Effective Properties of Multiphase Flow in Heterogeneous Porous Media

by

Bruce L. Jacobs

BSCE, Wayne State University (1985)
M.S., Massachusetts Institute of Technology (1987)

Submitted to the Civil and Environmental Engineering
in partial fulfillment of the requirements for the degree of
Doctor of Philosophy
Environmental Engineering

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

February 1999

© 1998 Massachusetts Institute of Technology, All rights reserved.

The author hereby grants to Massachusetts Institute of Technology permission to
reproduce and to distribute publicly paper and electronic copies
of this thesis document in whole or in part.

Signature of Author

Civil and Environmental Engineering
28 September 1998

Certified by

Lynn Gelhar
Professor, Civil and Environmental Engineering
Thesis Supervisor

Accepted by

Andrew Whittle
Chairperson, Departmental Committee on Graduate Students
Effective Properties of Multiphase Flow in Heterogeneous Porous Media

by

Bruce L. Jacobs

Submitted to the Civil and Environmental Engineering
on 28 September 1998, in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy
Environmental Engineering

Abstract

The impact of heterogeneity on multiphase flow is explored using a spectral perturbation technique employing a stationary, stochastic representation of the spatial variability of soil properties. A derivation of the system's effective properties - nonwetting phase moisture content, capillary pressure, normalized saturation and permeability - was developed which is not specific as to the form of the permeability dependence on saturation or capillary pressure. This lack of specificity enables evaluation and comparison of effective properties with differing characterization forms. Conventional characterization techniques are employed to parameterize the saturation, capillary pressure, relative permeability relationships and applied to the Cape Cod and Borden aquifers. An approximate solution for the characteristic width of a dense nonaqueous phase liquid (DNAPL) plume or air sparging contributing area is derived to evaluate the sensitivity of system behavior to properties of input processes.

Anisotropy is predicted for uniform, vertical flow in the Borden Aquifer consistent with both prior experimental observations and Monte Carlo simulations. Increases of the mean capillary pressure (increasing nonwetting phase saturation) is accompanied by reductions in nonwetting phase anisotropy. Similar levels of anisotropy are not found in the case of the Cape Cod aquifer; the difference is attributed largely to the mean value of the log of the characteristic pressure which is shown to control the rate of return to asymptotic permeability and hence system uniformity. A positive relation between anisotropy and interfacial tension was observed, consistent with prior numerical simulations. Positive dependence of lateral spreading on input flow rate is predicted for Cape Cod Aquifer with reverse response at Borden Aquifer due to capillary pressure dependent anisotropy of Borden Aquifer. The effective permeability for horizontal flow with core scale heterogeneity was found to be velocity dependent with features qualitatively similar to experimental observations and numerical experiments. Application of Leverett scaling as generally implemented in Monte Carlo simulations under represents aquifer heterogeneity and for the Borden Aquifer, van Genuchten characterization reduces system anisotropy by several orders of magnitude. Anisotropy of the effective properties proved to be less sensitive to Leverett scaling if the Brooks-Corey characterization was used due to insensitivity in this case to the variance of the slope parameter.

Thesis Supervisor: Lynn Gelhar
Title: Professor, Civil and Environmental Engineering
Acknowldgments

As is customary, I would like to use this space to express my gratitude to family and friends without whom I could not have carried my research to its somewhat prolonged conclusion.

I am profoundly moved by the emotional support and patience demonstrated by my family. As my "two year" program moved to three and finally four years, Cathy, Emma, Aaron, and Rose were all incredibly tolerant of their "senior citizen" student; of my frequent late nights, bad temper and too frequent absences from family activities.

Prof. Lynn Gelhar's support is also heartily acknowledged. Lynn was a tremendous mentor teaching both by example and direct instruction. He is a person of great integrity and patience with a sincere regard for the students placed under his supervision. The remainder of my committee also provided insight and grammar lessons without any direct benefit to themselves.

One of the most rewarding opportunities - spiritually, not financially - afforded to me while here at MIT has been the opportunity to teach Groundwater Hydrology and the M.Eng. project course. I am grateful to Lynn Gelhar, Dave Marks and the CEE department for making this possible and to the students who withstood my sometimes clumsy attempts to share my knowledge and experience.

Finally, the many friendships I have formed while here have sustained me through the many hours of hard work. Among many others, I am greatly beholden to the following individuals: Rosanna Tse, Enrique Lopez-Calva, Freddi Eisenburg, Sheila Frankel, and Cynthia Stewart.
# Contents

1 Introduction ........................................... 20

1.1 Motivation ........................................ 20

1.2 Related Work ...................................... 22

1.2.1 Numerical Investigations ....................... 23

1.2.2 Analytical Investigations ....................... 26

1.3 Objectives and Approach ......................... 29

1.4 Overview of Thesis Contents .................... 31

2 Evaluation of Effective Properties - General Case .............. 33

2.1 Introduction .................................... 33

2.2 Local Scale, Deterministic Representation of Multiphase Flow ...... 36

2.2.1 Conservation of Mass ............................. 36

2.2.2 Relative Permeability Characterization ............ 37

2.2.3 Leverett Scaling ................................ 40

2.3 Stochastic Properties of Independent Variables ............... 42

2.3.1 Definition of Independent Variables .............. 42

2.3.2 Fourier-Stieltjes Representation .................. 43

2.3.3 Spatial Correlation Model ....................... 44

2.4 Effective Properties .............................. 45

2.4.1 Effective Permeability .......................... 45

2.4.2 Normalized Wetting Phase Saturation ............... 49

2.4.3 Nonwetting Phase Volumetric Content ............. 50
2.5 Output Spectra .............................................. 54
2.6 Discussion .................................................. 59

3 Effective Properties - Vertical or Horizontal, Uniform Flow 61
3.1 Cross Products .............................................. 62
3.2 Evaluation of Effective Properties .......................... 67
  3.2.1 Dependence of Effective Properties on Horizontal Correlation Scale .... 68
  3.2.2 Analysis of Steady State Relative Permeability Measurements .......... 77
3.3 Summary ..................................................... 82

4 Effective Properties - Stratified Aquifer 84
4.1 Introduction .................................................. 84
4.2 Cross Products .............................................. 84
4.3 Uniform System with Static Wetting Phase ................. 90
4.4 Evaluation of Effective Properties at Borden Aquifer ............ 93
  4.4.1 Base Case ............................................... 93
  4.4.2 Brooks-Corey Characterization ................................ 105
  4.4.3 Leverett Scaling ....................................... 107
  4.4.4 Kueper-Frind Characterization ................................ 113
  4.4.5 Interfacial Tension ..................................... 119
  4.4.6 Summary ............................................... 122

5 Lateral Spreading of Nonwetting Phase through Static Wetting Phase 126
5.1 Integral Method ............................................. 127
5.2 Spreading in Planar Two Dimensional, Vertical Domain ........... 128
  5.2.1 Zero Moment ............................................ 130
  5.2.2 Second Moment ......................................... 130
  5.2.3 Rate of Plume Width Expansion ................................ 131
5.3 Analytical, Separable Solution in Planar Two Dimensional Domain .... 133
5.4 Spreading in Radially Symmetric Domain .......................... 134
  5.4.1 Zero Moment ............................................ 137
5.4.2 Second Moment ........................................... 137
5.4.3 Rate of Plume Width Expansion ......................... 138
5.5 Evaluation of Nonwetting Phase Solution ................. 139
  5.5.1 Analytical Solution ................................. 139
  5.5.2 Kueper and Frind Characterization .................. 140
  5.5.3 Base Case and Sensitivity Analysis .................. 142
5.6 Summary ................................................. 147

6 Cape Cod and Borden Aquifers: Effective Properties and Impact on Nonwetting Phase Plume Dimensions 159
  6.1 Introduction ........................................... 159
  6.2 Evidence of Field Scale Variability ...................... 160
    6.2.1 Borden Aquifer .................................. 160
    6.2.2 Cape Cod Aquifer ................................ 171
    6.2.3 Discussion ....................................... 181
  6.3 Effective Properties ................................... 183
  6.4 Lateral Spreading of Nonwetting Phase Plumes in the Cape Cod and Borden Aquifers ...................... 198
    6.4.1 DNAPL ............................................ 198
    6.4.2 Air Sparging ...................................... 198
  6.5 Summary ................................................. 199

7 Summary of Findings and Concluding Remarks 207
  7.1 Overview .............................................. 207
  7.2 Context of Prior Investigations .......................... 208
  7.3 Methodology .......................................... 209
  7.4 Findings .............................................. 210
    7.4.1 Capillary Pressure Sensitive Anisotropy .......... 210
    7.4.2 Effective Residual Wetting Phase Saturation .... 211
    7.4.3 Impact of p-s-k Characterization Form ............ 211
    7.4.4 Velocity Dependent Relative Permeability Effects 212
7.4.5 Implications for Lateral Spreading in Natural Aquifers .............. 213
7.5 Recommendations for Future Investigations .......................... 213
7.5.1 Local Scale Representation ........................................ 214
7.5.2 Direct Extensions of Current Work ............................... 215

A Notation 225

B Summary of Multiphase Monte Carlo Simulation References 227

C Evaluation of Integrals 236

C.1 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\pi^2 (1+u_1^2+u_2^2+u_3^2)^2} \frac{u_1^2 du_1 du_2 du_3}{(\rho^2 u_1^2+u_2^2+u_3^2)^2+u_1^2 \rho^2 \xi_1^2} .............................................. 236$

C.2 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{u_1^2}{\pi^2 (1+u_1^2+u_2^2+u_3^2)^2} \frac{u_1^2 du_1 du_2 du_3}{(\rho^2 u_1^2+u_2^2+u_3^2)^2+u_1^2 \rho^2 \xi_1^2 u_1^2} .............................. 239$

C.3 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{u_1^2}{\pi^2 (1+u_1^2+u_2^2+u_3^2)^2} \frac{u_1^2 du_1 du_2 du_3}{(\rho^2 u_1^2+u_2^2+u_3^2)^2+u_1^2 \rho^2 \xi_1^2 u_1^2} .............................. 242$

C.4 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(u_1^2+a_1) du_1}{\pi (u_1^2-r_2) (u_1^2-r_3)} .................................................. 243$

C.5 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(u_1^2+a_1) du_1}{\pi (u_1^2+u_2^2+u_3^2)} .................................................. 246$

C.6 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(u_1^2+a_1) du_1 du_2 du_3}{\pi^2 (u_1^2+a_1 u_1^2+a_2 u_1^2+a_3) (1+u_1^2+u_2^2+u_3^2)^2} .............. 247$

C.7 $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(u_1^2+a_1 u_1^2+a_2 u_1^2+a_3) du_1 du_2 du_3}{\pi^2 (u_1^2+a_1 u_1^2+a_2 u_1^2+a_3) (1+u_1^2+u_2^2+u_3^2)^2} .............. 249$

C.8 $\int_{-\infty}^{\infty} \frac{1}{\pi (1+u_1^2)} \frac{(u_1^2+A_1) du_1}{(u_1^2+A_2)} .................................................. 251$

D Borden Aquifer p-s-k Function Parameters 252
E  Cape Cod Moisture Retention Curve Parameters  257

F  Evaluation of Analytical Solution of Plume Half Width  259
   F.1  Find f Function with Separable Solution  259
   F.2  Develop Analytical Solution for W  262
   F.3  Evaluate $\int_{-\infty}^{\infty} u^2 f(u) \, du$  263
   F.4  Evaluate $\int_{-\infty}^{\infty} \int_{0}^{P_c(u)} \kappa_z(P_c) \, dP_c \, du$  264

G  Code for Evaluation of Integral Solution to Lateral Spreading of Nonwetting Phase Plume  265
List of Figures

3-1 First and second partial derivatives of $R_o$ with respect to $\tilde{P}_c$ ($= \alpha \tilde{P}_c$), $B$, $L$, and $F$ versus normalized capillary pressure $\tilde{P}_c$ for base case, Borden Aquifer, van Genuchten characterization. .................................................. 71

3-2 Mean capillary pressure-saturation curve for horizontal-vertical correlation scale ratio between 2 and $\infty$ and mean capillary pressure versus homogeneous saturation with mean input variable values, $S_e (\tilde{F})$, for the base case Borden Aquifer, van Genuchten characterization; where vertical correlation scale held constant at 18 cm. .......................................................... 72

3-3 Mean capillary pressure-saturation curve for horizontal-vertical correlation scale ratio between 2 and $\infty$ and mean capillary pressure versus homogeneous saturation at mean input values, $S_e (\tilde{F})$, for the base case Borden aquifer variable slope, van Genuchten characterization; where vertical correlation scale held constant at 18 cm. .......................................................... 73

3-4 Contributions, $S_{ij}$, to mean value of $S_e$ versus normalized mean capillary pressure for perfectly stratified condition with base case, Borden, van Genuchten characterization. .................................................................. 74

3-5 Normalized capillary pressure standard deviation versus normalized mean capillary pressure for horizontal-vertical correlation scales ranging between 2 and $\infty$, for base case, Borden aquifer, van Genuchten characterization; where vertical correlation scale held constant at 18 cm. .................................................. 75
3-6 Normalized effective permeability perpendicular to flow and \( \frac{k_0(f)}{\exp f} \) for uniform, vertical gravity flow (\( \delta_p = 0.6 \)) with horizontal-vertical correlation scales between 2 and \( \infty \), \( \xi_1 = 18 \) cm and base case, Borden Aquifer, van Genuchten characterization.

3-7 Effective permeability versus mean normalized saturation for uniform mean, horizontal flow with Capillary number, \( Ca = \frac{\theta \mu \xi_1}{\sigma \sqrt{k_h n}} \), ranging between 0.0016 and 16.0 with conditions similar to tested system of Dale et al and 50 to 1 vertical-horizontal correlation scale ratio.

3-8 Effective permeability versus mean normalized saturation for uniform horizontal flow subject to range of Capillary number, \( Ca = \frac{\theta \mu \xi_1}{\sigma \sqrt{k_h n}} \), between 0.00016 and 16, with van Genuchten, Leverett scaling, Borden aquifer conditions, and horizontal/vertical correlation scales of 0.2 cm and 20 cm.

4-1 Effective horizontal and vertical relative permeability, \( k_h \) and \( k_v \), and homogeneous relative permeability \( k_g = \exp (\bar{R} - \bar{F}) \) and \( k_m = \exp (R(\bar{F}) - \bar{F}) \) versus normalized mean capillary pressure, evaluated for base case, van Genuchten characterization of Borden aquifer with perfect stratification.

4-2 (a) Synthetic permeability curves based on base case, van Genuchten Borden Aquifer characterization and (b) envelope of permeability variability versus mean capillary pressure defined by \( \exp (\bar{R}_o \pm 2\sigma) \).

4-3 Nonwetting phase permeability response to abrupt transitions of intrinsic permeability.

4-4 Partial derivative \( \frac{\partial R_h}{\partial P_c} \) versus normalized mean capillary pressure for base case, Borden Aquifer, van Genuchten characterization and modified condition, whereby \( \bar{L} = 0 \).

4-5 Ratio of horizontal to vertical effective permeability versus normalized mean capillary pressure, evaluated for base case Borden aquifer conditions, and modified conditions whereby the correlation scale is increased to 60 cm and \( \bar{L} \) reduced to 0.102.
Contributions to horizontal - vertical permeability ratio, $A_{i,j}$, versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for base case van Genuchten characterization of Borden aquifer with perfect stratification.

Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o (\bar{S}_e)$ versus mean normalized saturation; evaluated for base case, Borden aquifer van Genuchten characterization with perfect stratification.

First and second partial derivatives of $R_o$ with respect to $\bar{P}_c (= \alpha_g P_c)$, $B$, $L$, and $F$ for variable slope, Brooks-Corey characterization of Borden aquifer versus normalized capillary pressure $\bar{P}_c$.

Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o (\bar{S}_e)$ versus mean normalized saturation; evaluated for Brooks-Corey, variable slope parameter characterization of Borden aquifer with perfect stratification.

Effective relative permeability versus normalized mean capillary pressure, evaluated for Brooks-Corey, variable slope, characterization of Borden aquifer with perfect stratification.

Effective permeability anisotropy ratio versus normalized mean capillary pressure, evaluated for both Brooks-Corey and van Genuchten, base case characterization of Borden aquifer with perfect stratification.

Contributions to horizontal - vertical permeability ratio versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for Brooks-Corey, variable slope, characterization of Borden aquifer with perfect stratification.

(a) Synthetic permeability curves based on Leverett scaling, constant slope, van Genuchten Borden Aquifer characterization. (b) Envelope of permeability variability as a function of capillary pressure defined by mean plus and minus two standard deviations for Leverett scaling, constant slope, van Genuchten Borden Aquifer characterization.
4-14 Effective relative permeability, $\kappa_u$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o \left( S_e \right)$ versus mean normalized saturation; for van Genuchten, constant slope parameter characterization with modified Leverett scaling of Borden aquifer with perfect stratification. .......................................................... 115

4-15 Effective relative permeability, $\kappa_u$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o \left( S_e \right)$ versus mean normalized saturation; for Borden aquifer parameters with perfect stratification and van Genuchten, constant slope parameter characterization without Leverett scaling. .......................................................... 116

4-16 Horizontal - vertical effective permeability ratio versus normalized mean capillary pressure, evaluated for van Genuchten, characterizations of Borden aquifer with perfect stratification and 1) base case conditions with variable slope parameter, 2) constant slope parameter with modified Leverett scaling ($\beta = 0.65$) and 3) constant slope parameter with no scaling and equivalent $\sigma_0^2$ to Leverett scaling condition. .......................................................... 117

4-17 Contributions, $A_{ij}$, to effective permeability anisotropy ratio for Leverett scaling, Borden Aquifer characterization, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for van Genuchten, Leverett scaling characterization of Borden aquifer with perfect stratification. 118

4-18 Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_u$, and homogeneous relative permeability $\kappa_y = \exp \left( \bar{R} - \bar{F} \right)$ and $\kappa_m = \exp \left( R \left( \bar{F} \right) - \bar{F} \right)$ versus normalized mean capillary pressure, evaluated for Kueper-Frind (1991) characterization of Borden Aquifer with Brooks-Corey p-s-k function, ln $k$ variability as measured by Sudicky, modified Leverett scaling. .................................................. 120

4-19 Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_u$, and homogeneous relative permeability $\kappa_y = \exp \left( \bar{R} - \bar{F} \right)$ and $\kappa_m = \exp \left( R \left( \bar{F} \right) - \bar{F} \right)$ versus normalized mean capillary pressure, evaluated for Borden Aquifer with Brooks-Corey p-s-k function and ln $k$ variability as measured by Sudicky, where parameter moments reflect independent measurements of p-s-k function parameters. 121
4-20 Effective permeability (a) and ratio of horizontal to vertical effective permeability (b) for low interfacial tension; Borden aquifer, base case, van Genuchten, variable slope characterization with $\tilde{B} = 7.8$. ............................................. 123

5-1 Power law permeability function exponents $\mu$ and $\nu$ for base case Borden Aquifer, van Genuchten characterization. ......................................................... 135

5-2 Spread function, $f$, versus lateral distance for function form of power law permeability function for exponents associated with normalized mean capillary pressure of 0.3, 0.6, 0.95 and 2.2. ......................................................... 136

5-3 Analytical and numerical solution of plume half width $w$ for power law permeability-capillary pressure function with $\mu = 13.4, \nu = 14.0$ ......................................................... 141

5-4 Kueper-Frind (1991b), Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: $w_o = 100$ cm, $\tilde{\kappa}_{z,0} = 0.11$. ......................................................... 143

5-5 Base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: $w_o = 100$ cm, $\tilde{\kappa}_{z,0} = 0.11$. ......................................................... 148

5-6 Gaussian shape function; base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: $w_o = 100$ cm, $\tilde{\kappa}_{z,0} = 0.11$. ......................................................... 149

5-7 Center line relative permeability for parabolic and Gaussian shape function for Borden, base case, van Genuchten characterization. ............................................. 150

5-8 Vertical relative permeability versus lateral distance from plume center line for both parabolic and Gaussian shape function at 500 cm below water table. .... 151

5-9 Mean nonwetting phase volumetric content versus lateral distance from plume center line for both parabolic and Gaussian shape function at 500 cm below water table. ............................................. 152
5-10 Second moment of nonwetting phase volumetric content versus elevation for parabolic and Gaussian shape functions. .......................................................... 153

5-11 Brooks-Corey, Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: \( w_o = 100 \text{ cm}, \bar{z}_{2,0} = 0.11 \). ........................................ 154

5-12 High flow, base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: \( w_o = 100 \text{ cm}, \bar{z}_{2,0} = 0.50 \). ......................... 155

5-13 Plume width profile for steady state gravity flow of nonwetting phase through static wetting phase with 1) base case, van Genuchten characterization and 2) wide source scenario \( (w_o = 1000 \text{ cm}) \). ......................................................... 156

5-14 Plume width profile for steady state gravity flow of nonwetting phase through static wetting phase with 1) base case, van Genuchten characterization, 2) low interfacial tension, 3) high flow and 4) modified Leverett scaling. .................. 157

6-1 Capillary pressure versus wetting phase saturation from seven Borden Aquifer soil samples from Kueper (1991a); measured under drainage conditions for perchloroethylene-water liquid pair. ......................................................... 163

6-2 Rescaled Borden aquifer capillary pressure-saturation curves using classic Leverett scaling (a) and modified Leverett scaling as in Kueper and Frind (1991b) with exponent \( \beta = 0.65 \) (b) and \( \beta = 1.0 \) (c). ................................. 165

6-3 Wetting and nonwetting phase permeability variability for Brooks-Corey characterization, with modified Leverett scaling for soils with permeability of \( F \pm 2\sigma_f \) \( (\sigma_f^2 = 0.29) \) and (a) and (b) Leverett exponent \( \beta = 0.65 \) and (c) and (d) \( \beta = 1.0 \). 168

6-4 Predicted relative permeability for seven soil samples from Borden Aquifer (based on data from Kueper and Frind, 1991b) for a) Brooks-Corey and b) van Genuchten p-s-k characterization functions. ................................. 170
6-5 Scatter plot of $L$, transformed van Genuchten slope parameter versus $\ln k$ (in cm$^2$) estimated for Borden aquifer soils in PCE-water system (based on data from Kueper and Frind, 1991b). ......................................................... 172

6-6 Scatter plot of $B$, transformed van Genuchten pressure normalization parameter versus $\ln k$ (in cm$^2$) estimated for Borden aquifer soils in PCE-water system (based on data from Kueper and Frind, 1991b). ......................................................... 173

6-7 (a) Synthetic permeability curves based on base case, van Genuchten Borden Aquifer characterization with variable slope parameter. (b) Envelope of permeability variability as a function of capillary pressure defined by mean plus and minus two standard deviations for base case van Genuchten Borden Aquifer characterization. ........................................................................................................... 174

6-8 Scatter plot of $B$, transformed van Genuchten characteristic pressure versus $\ln k$ (in cm$^2$) and estimated regression line for Cape Cod aquifer soils in air-water system (based on data from Mace, 1994). ................................................................. 178

6-9 Scatter plot of $L$, transformed van Genuchten slope parameter versus $\ln k$ (in cm$^2$) and estimated regression line for Cape Cod aquifer soils in air-water system (based on data from Mace, 1994). ................................................................. 179

6-10 (a) Synthetic permeability (cm$^2$) versus capillary pressure for estimated Cape Cod Aquifer van Genuchten p-s-k parameters based on data from Mace (1994) and (b) $\exp (R \pm 2\sigma_r)$ where $R$ and $\sigma_r$ are sample statistics of log permeability versus capillary pressure. ................................................................. 180

6-11 a) Mean normalized saturation versus mean capillary pressure for both perfectly stratified condition and measured correlation scale ratio and normalized saturation at mean parameters, $S_e (\tilde{\Gamma})$ and b) contributions to mean normalized saturation for base case, van Genuchten characterization of Cape Cod aquifer. ................................................................. 188

6-12 Mean and standard deviation of nonwetting phase volumetric content for base case, Cape Cod aquifer, van Genuchten characterization with zero porosity variance and zero residual saturation variance. ................................................................. 189
6-13 First and second partial derivatives of \( R_o \) with respect to \( \tilde{P}_c (= \alpha_g P_c) \), \( B \), \( L \), and \( F \) for variable slope parameter, van Genuchten characterization at Cape Cod aquifer versus normalized capillary pressure \( \tilde{P}_c \).

6-14 Effective horizontal and vertical relative permeability, \( \kappa_h \) and \( \kappa_v \), and homogeneous relative permeability, \( \kappa_g = \exp(\bar{R}) \) and \( \kappa_m = \exp(R(\bar{\Gamma})) \), versus normalized mean capillary pressure, evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.

6-15 Effective relative permeability, \( \kappa_v \) and \( \kappa_h \), and homogeneous permeability, \( \kappa_m = \exp R_o (\bar{S}_e) \) versus mean normalized saturation; evaluated for base case, van Genuchten Cape Cod aquifer characterization with perfect stratification.

6-16 Ratio of horizontal to vertical effective permeabilities versus mean normalized capillary pressure, evaluated for base case Cape Cod aquifer conditions.

6-17 Contributions to horizontal - vertical permeability ratio, \( A_{i,j} \), versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.

6-18 Contributions to horizontal - vertical permeability ratio, \( B_{i,j} = (|\epsilon| + 1) \ln A_{ij} \), versus normalized mean capillary pressure, where anisotropy is \( \exp \left( \frac{\Sigma E_i}{(|\epsilon| + 1)} \right) \), exponential of sum of individual contributions divided by \(|\epsilon| + 1\) at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.

6-19 Contributions to horizontal - vertical permeability ratio, \( B_{i,j} = (|\epsilon| + 1) \ln A_{ij} \), versus normalized mean capillary pressure, where anisotropy is \( \exp \left( \frac{\Sigma E_i}{(|\epsilon| + 1)} \right) \), exponential of sum of individual contributions divided by \(|\epsilon| + 1\) at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Borden aquifer with perfect stratification.

6-20 Ratio of horizontal to vertical effective permeability for Cape Cod base case characterization and selected modifications to mean parameters.
6-21 DNAPL release at Borden aquifer; system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Borden van Genuchten characterization, with variable slope parameter; boundary conditions: \( w_0 = 100 \text{ cm}, \kappa_{z,0} = 0.105 \) (same as Figure 5.2).

6-22 DNAPL release at Cape Cod aquifer; system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Cape Cod van Genuchten characterization, with variable slope parameter. Boundary conditions: \( w_0 = 100 \text{ cm}, \kappa_{z,0} = 0.105 \).

6-23 Air sparging at Borden aquifer; system profile for steady state simulation of air sparging, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Borden van Genuchten characterization, with variable slope parameter; boundary conditions: \( w_0 = 250 \text{ cm}, \kappa_{z,0} = 0.80 \).

6-24 Air sparging at Cape Cod Aquifer; system profile for steady state simulation of air sparging, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Cape Cod, van Genuchten characterization, with variable slope parameter. Boundary conditions: \( w_0 = 250 \text{ cm}, \kappa_{z,0} = 0.80 \).

6-25 Flow rate dependence of lateral spreading at Borden aquifer; nonwetting phase, lateral plume length scale for \( \tilde{r}_{r,0} = 0.2, 0.4, \) and \( 0.8 \) for base case characterization and \( w_0 = 250 \text{ cm} \).

6-26 Flow rate dependence of lateral spreading at Cape Cod aquifer; nonwetting phase, lateral plume length scale for \( \tilde{r}_{r,0} = 0.2, 0.4, \) and \( 0.8 \) for base case characterization and \( w_0 = 250 \text{ cm} \).
List of Tables

1.1 References containing descriptions of multiphase, Monte Carlo simulations. ........................................... 26

3.1 Base case, Borden Aquifer, van Genuchten parameters for independent estimation of parameters for each soil sample; based on data set of Kueper and Frind (1991b) ............................................................... 69

3.2 van Genuchten parameter moments for estimation of effective properties to approximate Dale et al (1997) system ................................................................. 79

4.1 Moments of transformed van Genuchten parameters for Borden Aquifer base case and alternative characterizations. ................................................................. 94

4.2 Parameters of variable slope, Brooks-Corey characterization for Borden Aquifer based on capillary pressure data set of Kueper and Frind (1991b) .................. 105

4.3 Moments of transformed van Genuchten parameters for Borden Aquifer with modified Leverett scaling and uncorrelated variability. ...................................... 113

4.4 Moments of transformed Brooks-Corey parameters for representation of Borden Aquifer characterization by Kueper and Frind (1991b). ...................................... 119

4.5 Reduced interfacial tension van Genuchten parameter moments (based on data from Kueper and Frind (1991b). ................................................................. 122

4.6 Summary of scenarios for estimation of effective properties under perfect stratification conditions. ................................................................. 125

5.1 Moments of transformed Brooks-Corey parameters for representation of Borden Aquifer characterization by Kueper and Frind (1991b). ...................................... 142
5.2 Moments of transformed van Genuchten parameters for Borden Aquifer base case and alternative characterizations. ........................................ 146

6.1 Moments and correlation scale of ln k estimates at the Borden Aquifer ....... 161
6.2 Keuper and Frind (1991) estimates of the Brooks-Corey parameters for the rescaled capillary pressure curve. ........................................ 166
6.3 Brooks-Corey parameter estimates for rescaled capillary pressure curves .... 166
6.4 Local displacement pressure (dynes/sq-cm) estimated based on modified Leverett scaling and local permeability spanning plus and minus two standard deviations from the mean ........................................ 167
6.5 Moisture Retention Parameters by Independent Evaluation of each Sample .... 169
6.6 Transformed Moisture Retention Parameters by Independent Evaluation of each Sample ......................................................... 171
6.7 Statistics of Hydraulic Conductivity at Cape Cod Aquifer ......................... 175
6.8 Statistics of estimated p-s-k parameters in Cape Cod aquifer (Mace, 1994) .... 176
6.9 Statistics of transformed p-s-k parameters in Cape Cod aquifer with original estimates as reported in Mace (1994). ................................. 176
6.10 Moments of transformed van Genuchten parameters for Cape Cod Aquifer base case and modified systems. ................................. 184
Chapter 1

Introduction

1.1 Motivation

The prevalence of subsurface contamination by slightly soluble, immiscible liquids is well documented (MacKay and Cherry, 1989; USEPA, 1993). These substances are primarily industrial chemicals or the byproducts of industrial processes which are introduced at the surface through improper handling or disposal practices or below the surface through leaks from storage or transmission facilities. They consist of a range of substances, but most are either petroleum based hydrocarbons or halogenated hydrocarbons. Their transport, above and below the water table, is controlled by a combination of gravitational, capillary and viscous forces, creating conditions whereby movement of the continuous nonaqueous phase liquid (NAPL) is difficult to predict and not necessarily consistent with that of the groundwater flow field.

The characterization of multiphase flow in porous media may be addressed at a number of scales. Pore scale analyses focus on the balance (or imbalance) of forces imposed at the interface. Pore radii, interfacial tension and fluid wetting characteristics are used to evaluate the capillary pressure and the pore scale trapping of residual nonwetting phase. Local scale characterizations are used to analyze mechanisms occurring at the scale of typical laboratory experiments (i.e., 10 - 50 cm). At this scale, the complexity of the physical domain prevents the development of exact analytical solutions. Progress at the local-scale has relied on both empirical evidence and physical and statistical arguments used to generalize pore-scale findings (Parker, 1989; Dullien, 1992). Advances in experimental technique have enabled the measurement of capillary
pressure and relative permeability, the development of analytical functions to represent the relation between saturation, capillary pressure and relative permeability and numerical codes to simulate multiphase systems. Progress in understanding of the local scale mechanisms has lent little to the understanding of field scale mechanisms (Parker, 1989; Wilson et al., 1989; Miller et al., 1998).

At present, there is only a vague understanding of the relation between spatial variability and field-scale flow. There appears to be agreement that alternating layers of fine and coarse grained soils\(^1\) increase lateral spreading and that spatial variability introduces large scale trapping mechanisms. There is however no agreement upon fundamental concepts such as the form of the mean scale equations, appropriate forms for derivation of effective parameters, the sensitivity of the plume depth and extent on the variability of hydraulic properties, or even which measurable hydraulic properties are of most importance for characterization of a site. The absence of a conceptual model for field-scale flow results in inadequate site characterization and inefficient data collection programs. If the field-scale flow mechanisms were better understood and methods were available for integration and analysis of data, then data collection could be more carefully planned and its impact enhanced.

The introduction of tetrachloroethylene (PCE) below the water table in a field experiment at the Borden aquifer (Kueper, et al., 1993) is particularly persuasive in emphasizing the role of heterogeneity in field scale flow. A 3 m by 3 m cell was constructed and PCE injected at constant head at a point below the water table. A total of 231 L of PCE were injected over a period of 29 hours and the results monitored using multilevel time domain reflectometry probes and multilevel piezometer bundles. Twenty seven days after injection, the upper 0.9 m of soil were excavated in 10 cm lifts and three continuous cores were driven an additional 2.5 m to the aquitard. PCE was found to have preferentially flowed along horizontal coarser grained sand units ranging in thickness from several mm to 5 cm. Interception of the sheet pile boundaries occurred at 10 cm below the injection point and nearly continuously thereafter to a depth of 2.0 m. Capillary forces, operating at the pore scale, prevent water from entering into the small

\(^1\)Soil is used to refer to all porous media irregardless of depth or organic content. This is consistent with the conventional use of the word in the hydrogeologic literature (see for example Bear, 1989; de Marsily, 1986 and Freeze and Cherry, 1989), notwithstanding narrower definitions applied by geochemists by which soil denotes only near surface deposits – usually with significant organic content.
pores of fine soils, but only by accounting for the spatial distribution of the local-scale properties could one account for the largely lateral PCE flow.

Even in the experimental emplacement of DNAPL's in soils which are by intent homogeneous (Schwille, 1988) fine horizontal structure inadvertently introduced into the soil column enhances the lateral spread of the nonwetting phase below the water table. On inspection of photos in this text, it is apparent that the red nonwetting phase liquid preferentially flows in the loosely packed soils between lifts which appear at regular intervals in the glass encased experimental trenches.

Until recently, little attention has been paid to analysis of field-scale phenomena. Field scale experimentation and numerical simulations with explicit depiction of small scale variability have demonstrated that spatial variability of hydraulic properties has a significant impact, but methods for describing the salient characteristics of that variation and predicting its impact are not available. Monte Carlo techniques have been applied to perform simulations of two-phase flow in media with explicit representation of local spatial variability, but these techniques have not yielded general analytical results for estimation of the dependence of flow on measurable characteristics. Not surprisingly, standard practices are generally inconsistent since there is not an understanding of what types of information are important, the number of measurements which should be taken or how to analyze the information so as to assist in characterization and remediation.

1.2 Related Work

Efforts to address the impact of heterogeneity on multiphase flow fall into two general categories:

- numerical investigations of flow in media with spatially variable hydraulic properties - in realizations of spatially correlated random fields or deterministic periodic media

- analytical evaluation of field scale properties using spectral models of random variability and a linearized continuity equation.

The following sections summarize some of the principal investigations in this area citing both the approach and important findings.
1.2.1 Numerical Investigations

Horizontal flow in spatially variable media represents a highly idealized domain, but the simplicity of the flow system and the availability of simple analytical solutions make it is attractive for exploration of the impact of variability. Yortsos and Chang (1990) presented an analysis of steady state, horizontal flow in periodic media. Starting with an analytical solution of the response to a rapid, ramped increase in permeability, they showed that the flow system on either side of the zone of increasing permeability eventually returns to an asymptotic saturation; where the value of the asymptotic saturation is a function of the rate of flow and the relative permeability characterization function. Further, they show that on the upgradient end of the change in permeability, the wetting phase saturation increases due to the downward shift in the capillary pressure-saturation function accompanying the change in permeability. The amplitude of this change in saturation is an inverse function of both the rate of flow and the rate of the change in permeability (the ramp slope) and conversely the saturation change amplitude increases with increases in the interfacial tension of the fluid pair. In the limit of high rates of flow and/or gradual changes in permeability, the amplitude of the change in saturation goes to zero. The saturation profile for a sequence of step changes in permeability appear as a near continuous line - at the asymptotic saturation - punctuated at each step change in permeability by a discontinuity on the downgradient end and a gradual return to the asymptotic saturation.

Dale et al. (1997) adopt the same model as Yortsos and Chang, in order to estimate the effective relative permeability as a function of the capillary number - an indicator of the ratio of viscous to capillary forces. They find that the rate of the approach to the asymptotic saturation is proportional to the flow velocity and inversely related to the capillary pressure curve slope magnitude. Consequently, they find that the effective relative permeability in one dimensional systems is dependent on the flow condition signified by the capillary number. For high capillary numbers (i.e., high velocity flows), the return to asymptotic saturation is immediate and the effective permeability is the harmonic mean of the relative permeability in each strata at this saturation. At low capillary numbers (low velocity flows), the capillary pressure throughout the system is constant and the saturation in each strata is at the constant value associated with this specified capillary pressure. These conditions are referred to as the viscous and capillary limits by the authors, who find an approach to the limiting conditions for inverse capillary
numbers ranging from 0.1 (viscous limit) to 100 (capillary limit). Qualitatively similar results were obtained by Ringrose et al. (1994).

Tests of the utility of the steady state estimates of effective permeability in transient systems were conducted (Dale et al., 1997) by numerical simulations of the displacement of oil by water in heterogeneous media and "equivalent" homogenous systems using the effective properties estimated for the steady state case. The authors find that the homogeneous systems provide reasonably good approximations of the mean behavior of the system and the time to breakthrough with, of course, the small scale perturbations characteristic of the heterogeneous system solutions.

The Monte Carlo technique employs deterministic numerical simulations in media whose properties are the realization of a spatially correlated random field. A single realization-flow simulation pair provides qualitative evidence of the impact of heterogeneity, while more general conclusions may be derived by systematic variation of properties and repetition of simulations in multiple realizations of the media. Special attention is required to the spatial discretization of simulations in spatially variable media and in particular for simulations of multiphase flow in spatially variable media. For the general problem of simulations in spatially variable media, the discretization must be adequate to resolve rapid changes in property values – the discretization therefore must be significantly smaller than the scale of variability.

Moreover for the case of multiphase flow in spatially variable media, a second discretization criteria was noted by Rathfelder and Abriola (1998). They note that the discretization must be small relative to the entry pressure (expressed as a water elevation) of the low permeability layers and that inadequate resolution reduces the simulated lateral spreading and vertical penetration in their transient simulations of a DNAPL release. For the van Genuchten type characterization, they note that vertical grid spacing on the order of 1/10 - 1/2 times the characteristic pressure normalized by the unit weight of water is adequate; while for the Brooks-Corey characterization, they were unable to reach solution convergence with increasing discretization, even with discretization on the order of 1/15 times the normalized entry pressure.

The resolution dependence of Monte Carlo investigations is demonstrated in a comparison of the simulations of multiphase flow below the water table at the Borden Aquifer by Kueper and Frind (1991b) and Brown et al. (1994). The resolution in the case of Brown et al. is
inadequate to resolve the fine scale lamination of the Borden Aquifer reducing the saturation variability and the lateral spread of the downward moving plumes. The increased resolution of Kueper and Frind (1991b) comes at a cost. Simulations of the 3.5 m deep by 9 m wide vertical, two-dimensional section required 25,200 finite difference cells and the simulation run time for a Cray X/MP (circa 1991) was on the order of 15 hours. Meaningful application of the Monte Carlo technique to a large scale, fully three dimensional plume would be near impossible with present day technology.

Table 1.1 contains a list of references documenting Monte Carlo simulations of multiphase flow – the titles are included in this list to provide some insight into the objectives and the simulated system. A more detailed list is included as Appendix B and includes information on the characterization form, simulation descriptions, grid dimensions and discretization. This Appendix is a working document and may not completely describe characterization schemes or simulated systems. The functions used to characterize the dependence of the relative permeability on the capillary pressure contain two parameters in all but one of the listed simulations. The value of these parameters are typically estimated for a particular soil by minimizing the deviance of measured capillary pressure values from the drainage phase of the capillary pressure curve. In general, one parameter is used to normalize the capillary pressure; this parameter is either in pressure or inverse pressure units. If in pressure units, it is generally thought to scale with a negative power of the local intrinsic permeability ($k$). The second parameter is generally thought of as a control on the slope of the capillary pressure curve and the relative permeability function. In every instance, in which the two parameter characterization was used, the slope parameter was specified at a constant value, perturbations from the mean of $\ln k$ varied independently and the value of the pressure normalization factor varied deterministically with $\ln k$ perturbations.

Only Dekker and Abriola (unpublished) and Kueper and Gerhard (1995) performed simulations in multiple realizations of the random field. In the other instances, single realizations were used to obtain a qualitative understanding of the dependence of multiphase flow on the mean and variance of the input parameters and the magnitude of the correlation scale. There is a general consensus that high mean entry pressure (or equivalently low interfacial tension), high variability and low correlation scales promote lateral plume spreading. Additional observations
<table>
<thead>
<tr>
<th>Reference</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dekker, T.J. and L.M. Abriola</td>
<td>The influence of field-scale heterogeneity on the infiltration and entrapment of dense nonaqueous phase liquids in saturated formations</td>
</tr>
<tr>
<td>(unpublished draft)</td>
<td></td>
</tr>
<tr>
<td>Essaid and Hess (1993)</td>
<td>Monte Carlo simulations of multiphase flow incorporating spatial variability of hydraulic properties</td>
</tr>
<tr>
<td>Essaid et al (1993)</td>
<td>Simulation of fluid distribution observed at a crude oil spill site incorporating hysteresis, oil entrapment, and spatial variability of hydraulic properties</td>
</tr>
<tr>
<td>Kueper, B.H. and E.O. Frind</td>
<td>Two phase flow in heterogeneous porous media</td>
</tr>
<tr>
<td>(1991a,b)</td>
<td></td>
</tr>
<tr>
<td>Kueper, B.H. and J.J. Gerhard</td>
<td>Variability of point source infiltration rates for two-phase flow in heterogeneous porous media</td>
</tr>
<tr>
<td>(1995)</td>
<td></td>
</tr>
<tr>
<td>Mayer, A.S. and C.T. Miller,</td>
<td>The influence of mass transfer characteristics and porous media heterogeneity on nonaqueous phase dissolution</td>
</tr>
<tr>
<td>(1996)</td>
<td></td>
</tr>
<tr>
<td>Rathfelder, K. and L.M. Abriola</td>
<td>The influence of capillarity in numerical modeling of organic liquid redistribution in two-phase systems</td>
</tr>
<tr>
<td>(1998)</td>
<td></td>
</tr>
<tr>
<td>Sleep, B.E. and J.F. Sykes</td>
<td>Compositional simulation of groundwater contamination by organic compounds: 1. Model development and verification</td>
</tr>
<tr>
<td>(1993a)</td>
<td></td>
</tr>
</tbody>
</table>

Table 1.1: References containing descriptions of multiphase, Monte Carlo simulations.

have been made regarding the simulation of hysteresis which are beyond the scope of this work. These results provide valuable insight into the qualitative system response to soil variability. They fail however to provide a means of quantitative estimation of effective properties for systems with other variability and in general provide only weak clues to the physical processes behind the system responses.

### 1.2.2 Analytical Investigations

The spectral-perturbation technique has been used in the analysis of saturated and unsaturated flow and transport. The technique relies on an assumption of separation of scales and low amplitude, spatially correlated random variability of property perturbations from the larger scale mean process. Yeh et al. (1985a, 1985b and 1985c) describe an investigation of effective properties in steady state, unsaturated flow where the relative permeability dependence on the
capillary pressure is assumed to be the negative exponential of a normalized capillary pressure. Both the log of the intrinsic permeability and the pressure normalizing factor are assumed to vary spatially in the most general case explored by the authors. Solutions for the variance of the capillary tension and the effective permeability are found for the case of uniform flow, perpendicular to the principal axes of the aquifer and for nonuniform flow in a perfectly stratified aquifer. Many of the effective property solutions of Yeh et al. are represented by analogous solutions in the present work. In fact, it may be easily shown that the present work encompasses the system described by Yeh, et al.. The principal finding is that of capillary pressure dependent anisotropy of the wetting phase, where the anisotropy of a horizontal, perfectly stratified system is proportional to the exponential of a measure of system variance and inversely proportional to the sum of one and the product of the correlation scale and the mean pressure normalizing factor. Mantoglou and Gelhar (1987a, 1987b, 1987c) extended this analysis to include dynamic effects in unsteady flow.

Polmann (1990) evaluated effective properties of the unsaturated flow system using the spectral-perturbation approach and a general, nonparametric description of capillary pressure and relative permeability. The impact of heterogeneity on a downward moving wetting phase plume was then evaluated using an integral analysis solution of the unsaturated flow problem.

Spectral perturbation solutions have been developed by Chang et al. (1995a) for field-scale, two phase flow under steady state conditions. A somewhat detailed description of the work of Chang et al. is presented here in order to understand the relevance of this work and important points of departure.

- The wetting phase relative permeability is the negative exponential of a normalized capillary pressure. The nonwetting phase relative permeability is one minus the wetting phase relative permeability, so that the relative permeability of the two phases sums to one for any capillary pressure. This model of relative permeability is inconsistent with the observation that the sum of the permeability of the two phases is less than one due to interference between flow paths of the two phases (Honarpour et al., 1986). It may be that this model is appropriate given the approximate nature of the subject, but this is not examined in any detail by Chang et al.
• The mean flow of both the wetting and nonwetting phase are assumed to be vertical, with zero capillary pressure gradients.

• Two spatial correlation models are evaluated. In the first, a hole type correlation model is adopted for the case of a one-dimensional domain. In the second case, a exponential correlation model is adopted for the ln $k$ field, where the system is assumed to be statistically isotropic. The heterogeneity of real soils is typically statistically anisotropic (Gelhar, 1993).

Their findings showed a positive dependence of the effective permeability on the mean ln $k$ for the three dimensional system and the reverse for the one dimensional domain, but for ln $k$ variance up to 1.0 in the isotropic three dimensional domain there is only minimal deviation of the effective permeability from the geometric mean, likely due to the isotropic media assumption allowing flow to bypass low permeability zones. The impact of anisotropy of the correlation scales is dismissed, despite field evidence which supports the notion that it is the stratified nature of heterogeneity which contributes to the lateral spreading of nonwetting phase plumes (Kueper and Frind, 1991). The authors miss the opportunity to examine the sensitivity to their mean parameter values or to associate these values with measured data. Further, implications of the use of relative permeability characterization which sum to one are not explored. The authors note that the difference in sign of the response of the effective wetting and nonwetting phase permeability to changes in the magnitude of the correlation scale is likely due to this feature of the characterization.

Abdin et al. (1995) compare the one dimensional, analytical stochastic results of Chang et al. (1995a) for the capillary pressure variance and effective permeability to analytical deterministic results in a domain with spatially variable permeability and characteristic pressure. Good comparisons are obtained for the effective permeability of both phases for the variance of the log permeability up to one and for the predicted relationship between mean capillary pressure and the variance of the wetting phase, nonwetting phase and capillary pressures.
1.3 Objectives and Approach

The overriding objective of this work is to enhance understanding of the role of aquifer heterogeneity in multiphase flow. The prior Monte Carlo and analytical investigations have initiated the process, but have not provided either a general understanding or specific techniques for predicting the impact of heterogeneity. Moreover, while these prior investigations may indicate that one or more properties is important, an important objective of our work is to supplement those observations with an explicit means of predicting the impact and describing the conditions under which these properties are significant.

The governing equations describing field scale behavior may be written in such a way that the equation parameters are effective properties, which in a physically justifiable way utilize information about local scale variability. The mathematical expressions by which one estimates the field scale properties are useful in that the form of the equation identifies the functional dependence of the effective properties on the input process variability (i.e., the local scale measurable properties of flow in porous media). Their utility is in suggesting physical models to improve the conceptual understanding of multiphase flow in heterogeneous aquifers, as engineering tools to anticipate the behavior of multiphase systems and to guide the rational collection of subsurface data for remedial investigations.

The focus will be on steady state systems of two fluid phases, with significant density differences such that gravitational forces are likely to be the primary factor in determination of the mean flow direction. In principle this may include fluids which are either lighter or denser than water. The former condition occurs in the case of air sparging where the natural buoyancy of air relative to water causes its upward movement toward the water table. Many common nonaqueous organic substances are however denser than water. Dense nonaqueous phase liquids (DNAPLs) for example may sink through a saturated zone and present particular issues which will be addressed as well. It is anticipated that problems of greater complexity, including transient systems will be addressed in future investigations, building on the findings summarized in this document.

Typically, in two phase systems in porous media one fluid preferentially wets the surfaces of the aquifer material. Generally, it is assumed for most surfaces that water is the wetting fluid relative to both air and organic compounds. For some media - organic compound pairs,
however, the media surface is preferentially wetted by the organic compound or is likely to do so after substantial contact periods. Still other media may have mixed wetting characteristics in which surfaces of varying composition have wetting characteristics which vary from point to point. The fluid of principal interest in this report is the nonwetting phase, while the impact of mixed wetting characteristics is not explored.

The proposed analysis of the field-scale process is based on the notion that spatial variation of media properties is responsible for the difference between field-scale conditions and conventional predictions of field-scale behavior in homogeneous media. Since a complete deterministic characterization of the spatially varying properties is not possible, soil properties are represented as a stationary, spatially correlated random field whose statistical properties are measurable from direct observation. The objectives of this type of analysis are to predict the large-scale mean response of the system derived from high frequency local-scale variation and the mean values of the independent properties.

In general, the approach will be to conceive of the observed variation of model parameters as a realization of a spatially correlated, random process and to employ perturbation techniques and spectral representation of the random fields so as to estimate the ensemble properties of the dependent variables. The spatial distribution of soil properties will be represented as the composite of two independent signals: a large-scale, slowly varying deterministic mean and high frequency random perturbation. Mean flow equations are developed from stochastic forms of the local flow equations, so as to provide a means of evaluating the field scale or effective properties. Linearized perturbation equations are derived from the local-scale equations to describe the dependence of saturation and capillary pressure on fluctuations in spatially variable random media properties. These are used in evaluation of cross-spectra to estimate the cross covariance of soil properties and system output parameters and thereby evaluate effective properties.

The approach utilizes a general formulation designed to be independent of the form of the functions describing the interdependence of capillary pressure, saturation and permeability (p-s-k functions). Evaluation of effective properties for any given characterization form was carried out by substitution of the functional representation of capillary pressure, saturation and permeability into a isolated set of routines. The symbolic computational capabilities of Maple V (1996) were employed to evaluate partial derivatives of the p-s-k functions and the
effective properties.

In support of the general objectives, effective properties are estimated for two aquifers, representing contrasting geological regimes. Further, an assessment of the sensitivity of these effective properties to factors identified in prior investigations is pursued, including: analytical form of relative permeability dependence on capillary pressure and saturation; scaling relationships suggested for capillary pressure and intrinsic permeability; and alternative interpretations of system variability. Finally an integral solution of the lateral spreading width of a nonwetting phase plume through static water is derived for use as a tool in describing the sensitivity of lateral spreading to the effective properties and ultimately the conditions for which the effective properties are estimated.

1.4 Overview of Thesis Contents

Chapter 2 provides a description of the conventional, local scale, deterministic mathematical representation of multiphase flow and a derivation of the effective properties under the most general conditions. Concepts addressed in this section include conservation of mass, relative permeability, capillary pressure-saturation-permeability (p-s-k) characterizations and Leverett scaling. This section serves as a reference to the conventional mathematical representation and introduces the notation including variables representing transformations of the p-s-k parameters to be used in the stochastic analysis.

In the second part of Chapter 2, the effective permeability and the first and second moments of normalized saturation, capillary pressure, and nonwetting phase volumetric content are derived for general flow and aquifer conditions. Solutions are presented as unresolved integrals of the output spectra found by the derivation and application of the stochastic differential equation based on the linearized continuity equation. Simplifying assumptions enable closed form evaluation of these integrals in subsequent chapters.

Following Yeh and Gelhar (1985c), two flow regimes are addressed which enable analytical evaluation of the effective property integrals. First, in Chapter 3, flow is assumed to be uniform and in the direction of one of the principal axes. Chapter 4 derives the effective property relationships for the perfectly stratified aquifer in nonuniform flow and addresses the case of
uniform flow and a static wetting phase in a perfectly stratified aquifer; this is a common condition of multiphase flow for which the effective property relationships are simple enough to permit a systematic analysis of the role of input moments. Effective properties are evaluated for conditions representing the Borden Aquifer. A description of the data set and its analysis are contained in Chapter 6. Chapter 3 contains a discussion exploring the relation of effective properties to horizontal correlation scales and the suitability of the perfect stratification assumption applied in Chapter 4 to natural systems. Further Chapter 3 contains an evaluation of the velocity dependence of relative permeability measurements in heterogeneous cores.

In Chapter 4, the effective property expressions are generated for the case of static wetting phase and vertical mean nonwetting phase flow in the perfectly stratified media. Efforts are made to develop a physical understanding of the form of the solution and the sensitivity of the effective properties to p-s-k function form, stochastic model, Leverett scaling and interfacial tension.

An approximate solution for the characteristic width of a dense or buoyant nonwetting phase plume is derived in Chapter 5. This solution serves as a means of evaluating the aquifer sensitivity to characterization form, soil properties, scaling techniques, correlation scales, and property cross-covariance. Estimates are made of plume half width in systems for which effective properties were estimated in Chapter 4.

Two case studies are described in Chapter 6 to broaden understanding of the nature of the effective property solutions. Stochastic descriptions of the Cape Cod and Borden Aquifers are developed, with the intent of demonstrating the impact of contrasting regimes. Effective properties are evaluated in the two systems and conclusions drawn as to the source of differing behavior predicted for the two aquifers. Integral solutions of lateral spreading of DNAPL and air sparging plumes are evaluated for both the Cape Cod and Borden aquifers, so as to further understanding of the significance of the effective property findings.

Finally, Chapter 7 contains a summary of findings and presents recommendations for future investigations.
2.1 Introduction

This chapter describes the derivation of effective properties for general flow and aquifer conditions. First, a deterministic, local scale representation of multiphase flow is presented consisting of a statement of conservation of mass and a modified Darcy equation. Closure of the system representation is achieved through functions defining the relation between capillary pressure, saturation and relative permeability (p-s-k functions). The objectives of this section are both to introduce notation and to serve as a point of reference for later sections where the local scale characterization is invoked.

Effective properties are defined and expressions for their value derived as functions of the moments of the input variables and the capillary pressure. Analytical expressions are presented for the output spectra and cross-spectra from which the moments will be derived for special conditions described in subsequent chapters.

The spectral perturbation technique relies on a highly idealized representation – ergodic, second-order stationary, random low amplitude deviations from a slowly varying mean. These assumptions, discussed elsewhere in great detail (Lumley and Panofsky, 1964, Gelhar, 1993) are in short:
• Separation of scales. Hydraulic properties are assumed to vary at two distinct scales represented by a slowly varying, large scale, mean and a stationary, local scale, random perturbation. It is assumed that the mean process is identifiable through conventional filtering techniques and that it varies slowly in space relative to the correlation scale of the random perturbation term. The presence of distinct scales should be reflected by a spectral gap, with low spectral density for some intermediate frequency range. This may not be strictly accurate at the front of a penetrating DNAPL where the mean saturation or mean capillary pressure may undergo rapid change, even relative to the small correlation scales of the perturbation terms. Nevertheless, it has been shown in other contexts such as the analysis of the movement of a wetting front in unsaturated media that this does not prevent the generation of reasonable results (Polmann, et al., 1991; Dale, et al., 1997; Aabdin et al., 1996).

• Low amplitude perturbation. Linearization of the governing equations is accomplished through the use of Taylor expansions in which terms exceeding second order are omitted. In cases of high variability, the accuracy of the approximations may be compromised. This is not a limitation of the stochastic methodology in general, but a consequence of the omission of higher order terms. In principal the problem of accuracy may be overcome by inclusion of higher order terms, however accurate estimation of higher order statistical moments will require more data than is normally available.

• Stationarity. The random input components are assumed to be second-order stationary.

• Ergodicity of the random perturbation. The proposed technique results in solutions for the ensemble moments of the dependent parameters. Since only a single realization of the input properties is available for direct measurement, it is assumed that the statistical properties of that realization are representative of the underlying process. The realization must be of sufficient length relative to the correlation scale of the input processes, so as to be statistically equivalent to a sequence of independent measurements. Ergodicity is essential but can not be proven through observation; supportive evidence is however possible through the generation of physically reasonable results and their validation in the field.
The proposed stochastic technique for estimation of the effective, field scale system properties relies on knowledge of both the independent variance of soil hydraulic properties, the joint covariances of these properties and a well defined spatial correlation model, defined by the shape of the correlation function and the magnitude of the correlation scales. Ideally, the application of the stochastic model ought to be based on multiple measurements of nonwetting phase relative permeability at a given site; however no publicly available source of information could be found which is adequate for this task. An alternative strategy was adopted to utilize measurements of capillary pressure and saturation performed in drainage experiments and to fit them to functions for which transformations have been devised which represent predictions of relative permeability. The same technique has been used in Monte Carlo simulations of nonwetting phase flow in heterogeneous aquifers, enabling direct comparisons with findings from this body of work.

The technique is attractive in that it allows for transformations between the predicted moments of capillary pressure, saturation and relative permeability, but is less than ideal due to the unreliability of predicted permeabilities. Tse (1997), through comparisons of measured unsaturated hydraulic conductivity, found that errors of several orders of magnitude are frequently encountered using the widely adopted van Genuchten relationship to predict wetting phase permeability. A similar assessment of nonwetting phase permeability predictions is not possible due to the lack of reliable data. It is considered likely however that the admittedly imperfect physical model underlying the transformation between capillary pressure and relative permeability does contain sufficient predictive capacity from which one may infer something of the variability of relative permeability with greater accuracy than the informed "guess". The goal at this point is to begin the process of understanding the impact of the spatial variability of multiphase flow properties and to provide motivation for the more frequent measurement of relative permeability in future studies. In the event that multiple, reliable measurements of relative permeability at a site were to made available, it would be worthwhile to reassess the findings of this document.
2.2 Local Scale, Deterministic Representation of Multiphase Flow

2.2.1 Conservation of Mass

In a locally isotropic, multiphase system the specific discharge, \( q_\beta \), of phase \( \beta \) is represented by the modified Darcy equation

\[
q_\beta = \frac{k \kappa_\beta}{\mu_\beta} \left( \nabla P_\beta + \rho_\beta g \right)
\]  

(2.1)

where

\[
\begin{align*}
k & = \text{intrinsic or saturated permeability} \ (L^2) \\
\kappa_\beta & = \text{relative permeability} \\
\mu_\beta & = \text{dynamic viscosity} \ (M/LT) \\
P_\beta & = \text{pressure of phase } \beta \ (M/T^2/L) \\
\rho_\beta & = \text{density of phase } \beta \ (M/L^3) \\
g & = \text{gravity vector} \ (L/T^2)
\end{align*}
\]  

(2.2)

The system to be addressed henceforth in this document consists of two fluid phases - a nonwetting phase and a wetting phase denoted, respectively, by \( \beta = o, w \). It is typically assumed that organic compounds and air are the nonwetting fluids relative to water. The relative permeability scalar, \( \kappa_\beta \), which varies between 0 and 1, is generally considered to be a nonlinear function of saturation with a number of characterizations proposed over the years to describe this relationship. A description of these functions is found in the subsequent section.

The steady state continuity equation for phase \( \beta \) in a locally isotropic system is

\[
\nabla \cdot q_\beta = \nabla \cdot \left[ \frac{k \kappa_\beta}{\mu_\beta} \left( \nabla P_\beta + \rho_\beta g \right) \right] = 0
\]

(2.4)

Alternatively, for a locally isotropic permeability field it may be written with respect to \( R = \ln(k \kappa_\beta) \) which will prove useful in later analysis.
\[ \nabla^2 P_\beta + \nabla R_\beta \cdot (\nabla P_\beta + \rho_\beta \mathbf{g}) = 0 \]  

(2.5)

At a pore scale the capillary pressure represents the pressure difference across an interface between the two liquid phases. Capillary pressure is also commonly used to refer to the local scale quantity representing the average pore scale capillary pressure over some representative elementary volume. Henceforth, references to capillary pressure will be used in that sense where the property is formally defined as

\[ P_c = P_o - P_w \]  

(2.6)

Increases in the nonwetting phase saturation are thought to be associated with the retreat of the fluid interfaces to the smaller radii pores and pore throats. The consequence is a reduction in the radius of curvature of the interface and an increase in the nonwetting phase permeability.

There are two common ways to complete the mathematical representation. The first is to assume that the relative permeability is a function of the capillary pressure as in Chang et al. (1995a). Alternatively, saturation based characterizations have been posited which describe the functional dependence of capillary pressure, normalized wetting phase saturation \((S_e)\) and relative permeability. In the latter case, the complete mathematical representation of two phase flow entails six equations to represent the system state with unknowns \(P_c, P_w, P_o, S_e, \kappa_w\) and \(\kappa_o\).

### 2.2.2 Relative Permeability Characterization

Functions characterizing the relation between permeability, saturation and capillary pressure are assumed to accurately represent the bulk, local system behavior, integrating the impact of processes occurring at the pore scale. The van Genuchten, Brooks-Corey and Gardner p-s-k models are described below, where the names refer to the principal originator of one or more components of the characterization. The relative permeability functions of two of the these characterizations, the van Genuchten and Brooks-Corey, propose the use of relative permeability functions which are transformations of empirical functions describing the capillary pressure-saturation curve. These are appealing in that relatively sparse or absent measurements
of the relative permeability may be supplemented or substituted for, by predictions based on inexpensive measurements of the capillary pressure-saturation curve. Predictions of wetting phase relative permeability based on capillary pressure-saturation curves are however, at best, uneven in their predictive capacity (Tse, 1997), a fact which is likely mirrored on the nonwetting phase side.

van Genuchten

van Genuchten (1980) proposed application of a capillary pressure-saturation curve of the form

\[
S_e = \left[1 + (\alpha P_c)^{1-m}\right]^{-m}
\]  

(2.7)

where

\[
S_e = \frac{\theta_w - \theta_r}{n - \theta_r}
\]

\[
\theta_w = \text{wetting phase volumetric content}
\]

\[
\theta_r = \text{residual wetting phase volumetric content}
\]

\[
n = \text{porosity}
\]

\[
m = \text{slope parameter; } 0 < m < 1
\]

\[
\alpha = \text{inverse characteristic pressure; } \alpha > 0
\]

The characteristic pressure is inversely related to the mean pore radius since the radius of curvature of the interface between the two fluids is smaller in the smaller pores. A simple balance of forces easily demonstrates the physical argument linking small radius of curvature - and hence smaller pore radii - and higher characteristic pressures.

Based on a statistical model of wetting phase relative permeability proposed by Mualem (1976) and later extended by Parker et al. (1987) for the nonwetting phase, the wetting and nonwetting phase relative permeabilities are related to (2.7) by

\[
\kappa_w = S_e^{1/2} \left[ \int_0^{S_e} \frac{dS_e}{P_c} \right]^2 
\]

(2.8)
\[ \kappa_o = (1 - S_e)^{1/2} \left[ \frac{\int_0^1 \frac{dS_e}{P_c}}{\int_0^1 \frac{dS_e}{P_c}} \right]^2 \]

The wetting and nonwetting phase relative permeability is stated as a function of \( S_e \) by introducing the capillary pressure-saturation function (2.7) into the statistical model of Mualem and evaluating the prior integrals

\[ \kappa_w = S_e^{1/2} \left[ 1 - \left( 1 - S_e^{1/m} \right)^m \right]^2 \]
\[ \kappa_o = (1 - S_e)^{1/2} \left( 1 - S_e^{1/m} \right)^{2m} \]

The variables \( B \) and \( L \), transformations of \( m \) and \( \alpha \), are defined as follows

\[ B = -\ln \alpha \] (2.10)
\[ L = -\ln \left( \frac{1}{m} - 1 \right) \]

Unlike \( \alpha \) and \( m \) whose values are constrained as described above, \( B \) and \( L \) may take on any real number. The intent of introducing these transformations is to avoid inadvertent, non-physical results in the stochastic analysis when the mean of \( \alpha \) or \( m \) approaches its physical limit expressed in (2.7).

**Brooks-Corey**

Brooks and Corey (1964) suggested a power law relationship between capillary pressure and saturation

\[ S_e = \left( \frac{P_c}{P_d} \right)^{-\lambda} \]

(2.11)

for \( P_c \geq P_d \). Physically reasonable results are obtained when the parameters, \( \lambda \) and \( P_d \) are constrained to be positive \((\lambda, P_d > 0)\). Employing Burdine's pore connectivity model,

\[ \kappa_w = S_e^2 \int_0^{S_e} \frac{dS_e}{P_c^2} \]
\[ \kappa_o = (1 - S_e)^2 \int_0^{1} \frac{dS_e}{P_c^2} \]

(2.12)
the wetting and nonwetting phase relative permeabilities are for the Brooks-Corey characterization:

\[
\kappa_w = S_e^{(2+3\lambda)/\lambda}
\]

\[
\kappa_o = (1 - S_e)^2 (1 - S_e^{(2+\lambda)/\lambda})
\]

As in the case of the van Genuchten characterization, the variables \( B \) and \( L \), transformations of \( \lambda \) and \( P_d \) are defined as follows:

\[
B = \ln P_d \tag{2.14}
\]

\[
L = \ln \lambda
\]

Gardner Characterization

Gardner proposed an exponential model for the wetting phase relative permeability

\[
\kappa_w = \exp(-\alpha P_c) \tag{2.15}
\]

which was extended by Chang et al. for application to the nonwetting phase

\[
\kappa_w = 1 - \exp(-\alpha P_c) \tag{2.16}
\]

This model does not include an explicit model of saturation and has the unrealistic property that the sum of the permeabilities of each phase equals the intrinsic permeability.

2.2.3 Leverett Scaling

Based on a pore scale balance of forces across the interface of two fluids, Leverett (1941) proposed a method by which the capillary pressure might be scaled by the square root of the local permeability
\[ P_c(S_e) = \sigma \cos \theta \frac{J(S_e)}{\sqrt{\frac{k}{n}}} \]  

(2.17)

where

\[ \sigma = \text{interfacial tension of fluid pair} \]
\[ n = \text{porosity} \]
\[ \theta = \text{contact angle} \]

and \( J \) is an undefined function representing a nondimensional form of the capillary pressure. The functional form of \( J(S_w) \) must be specified to complete the description of the relationship between saturation and capillary pressure. The conventional assertion is that \( J(S_w) \) is shared by all soils of a given type.

A modified form of Leverett scaling was proposed by Kueper and Frind (1991b) to improve the scaling effectiveness

\[ P_c(S_e) = \sigma J(S_e) \left( \frac{k}{n} \right)^{-\beta} \]  

(2.18)

This modified Leverett scaling neglects the contact angle, but introduces a new parameter \( \beta \), whose value is generally estimated using standard least squares techniques.

A common technique employed in numerical models of multiphase flow is to define the form of \( J(S_w) \) based on either the van Genuchten or Brooks-Corey characterizations. For example, given the Brooks-Corey capillary pressure function and the modified form of Leverett scaling, a dimensionless displacement pressure, \( P_d^* \) may be defined by the function

\[ P_d = P_d^* \sigma \cos \theta \left( \frac{k}{n} \right)^{-\beta} \]  

(2.19)

and the Brooks-Corey capillary pressure function utilized in its original form where the local value of \( P_d \) is expressed as a function of the local intrinsic permeability and the field scale constant \( P_d^* \).

Likewise, a nondimensional form of \( \alpha \) in the van Genuchten characterization may be defined
as

$$\alpha = \frac{\alpha^* \left( \frac{k}{\sigma} \right)^\beta}{\sigma} \quad (2.20)$$

Note that for $B$ defined as the log of the characteristic pressure (i.e., $B = \ln P_d$ or $B = -\ln \alpha$)

$$B = B^* + \ln \left( n^\beta \sigma \cos \theta \right) - \beta \ln k \quad (2.21)$$

where $B^*$ is a field scale log characteristic pressure, and the local value of the log characteristic pressure is a deterministic, linear function of the local value of $\ln k$. This expression provides a means of modifying the mean value of $B$ for different fluid pairs with differing interfacial tension or contact angle.

### 2.3 Stochastic Properties of Independent Variables

#### 2.3.1 Definition of Independent Variables

The value of the spatially variable, measurable soil properties controlling permeability are denoted by components of the vector $\Phi$. Each of the components of $\Phi$ may be decomposed into the sum of a slowly varying mean, $\Phi_i$, and a zero mean perturbation, $\phi'_i$, as in

$$\Phi_i = \Phi_i + \phi'_i \quad (2.22)$$

where

$$\Phi_i = E[\Phi_i] \quad (2.23)$$

$$E[\phi'_i] = 0$$

In the applications described in this document, the members of $\Phi_i$ are $F = \ln k$, $B$ and $L$, where $B$ and $L$ are transformations of either the Brooks-Corey or van Genuchten p-s-k function parameters as defined in (2.10) and (2.14). The derivation and resultant analytical expressions describing effective field scale properties in this Chapter and Chapters 3 and 4 are entirely general and may be used with alternative parameterizations of the relative permeability, where in that case $\phi_i$ take on alternative meanings.
The perturbation of each of the input variables is assumed to be correlated to the perturbation of \( F \) denoted by \( f' \), whereby

\[
\phi'_i = b_i f' + g'_i
\]  

(2.24)

and the zero mean, residual perturbation \( g'_i \) is an independent random variable such that

\[
E[g_i g_j] = \delta_{i,j} \sigma_{g_i}^2
\]  

(2.25)

where \( \delta_{i,j} \) is the Kronecker delta function equal to one for \( i = j \) and equal to zero otherwise. The covariance of two members of \( \Phi \) is therefore

\[
\text{cov}(\Phi_i, \Phi_j) = b_i b_j \sigma_f^2 + \delta_{i,j} \sigma_{g_i}^2
\]  

(2.26)

For convenience in the derivation and presentation of analytical results, a second parameter vector \( \Gamma \), is defined which includes the capillary pressure and the vector \( \Phi \) such that

\[
\Gamma = [\Phi, P_c]
\]  

(2.27)

The mean and perturbation of \( \Gamma \) denoted by \( \overline{\Gamma} \) and \( \gamma' \) are defined as

\[
\Gamma_i = \overline{\Gamma}_i + \gamma'_i
\]  

(2.28)

where

\[
\overline{\Gamma}_i = E[\Gamma_i]
\]

\[
E[\gamma'_i] = 0
\]

2.3.2 Fourier-Stieltjes Representation

Random fields and and the gradient of random fields which are stationary (statistically homogeneous) may also be represented in the wave number domain using the Fourier-Stieltjes integral
\[ \phi_i = \iiint_{-\infty}^{\infty} \exp (i\omega \cdot x) \, dZ_{\phi_i}(\omega) \]  
\[ \nabla \phi_i = \iiint_{-\infty}^{\infty} i\omega \exp (i\omega \cdot x) \, dZ_{\phi_i}(\omega) \]  

where \( dZ_{\phi_i}(\omega) \) is the spectral amplitude for the wave number \( \omega \).

### 2.3.3 Spatial Correlation Model

The findings of this chapter do not specify a correlation model. Subsequent chapters use the exponential correlation model, where the covariance between the value of the stationary random field at two points separated by the lag vector \( s \) is given by \( R(s) \) where

\[ R_{xy}(s) = \text{cov} \,(x, y) \exp \left( -\sqrt{\left( \frac{s_1}{\xi_1} \right)^2 + \left( \frac{s_2}{\xi_2} \right)^2 + \left( \frac{s_3}{\xi_3} \right)^2} \right) \]  

and \( \xi_1, \xi_2 \) and \( \xi_3 \) are the correlation scales in the direction of the three principal axes. All media properties are assumed to share this correlation model with identical correlation scales.

The covariance function and the spectrum of stationary random fields are related by Fourier transform pairs

\[ R_{xy}(s) = \int \int \int_{-\infty}^{\infty} e^{i\omega s} S_{xy}(\omega_1, \omega_2, \omega_3) \, d\omega_1 d\omega_2 d\omega_3 \]  
\[ S_{xy}(\omega) = \frac{1}{(2\pi)^3} \int \int \int_{-\infty}^{\infty} e^{-i\omega s} R_{xy}(s_1, s_2, s_3) \, ds_1 ds_2 ds_3 \]  

where the covariance is found by setting \( s = 0 \) in (2.33).

\[ \text{cov} \,(x, y) = \int \int \int_{-\infty}^{\infty} S_{xy}(\omega_1, \omega_2, \omega_3) \, d\omega_1 d\omega_2 d\omega_3 \]  

The spectrum associated with the exponential correlation model may be derived from (2.34) and (2.32) as:

\[ S_{xy}(\omega_1, \omega_2, \omega_3) = \frac{\text{cov} \,(x, y) \xi_1 \xi_2 \xi_3}{\pi^2 \left( 1 + (\xi_1 \omega_1)^2 + (\xi_2 \omega_2)^2 + (\xi_3 \omega_3)^2 \right)^2} \]  

It ought to be noted that the derivative of a random process with an exponential correlation
model is itself a random process with infinite variance. It is reasonable to question whether this is an appropriate correlation model to represent heterogeneous media properties. A related correlation model with the same analytical form, but where the spectrum of the high frequency components greater than some arbitrary value \( \omega_m \) are omitted, has a derivative with finite variance (Gelhar, 1993). Since the output signal is likely to be a filtered version of the input signal with the highest frequencies of little significance, the spectrum of the exponential covariance model may be safely used as an approximation of the cutoff model. The analytical simplicity of the exponential covariance model and documented successes in representing spatially variable aquifer properties with this model (Gelhar, 1993) are compelling reasons for its use in this instance.

2.4 Effective Properties

2.4.1 Effective Permeability

A field scale form of the multiphase Darcy equation (2.1) may be written to relate the mean specific discharge to the product of the effective permeability and the mean head gradient. The technique employed here to find the effective permeability is to

1. write the modified Darcy equation for multiphase flow, where the spatially variable properties and system variables are expressed as the sum of their mean and perturbation components,
2. linearize the expression by Taylor expansions of nonlinear terms about the mean of their parameters and
3. take the expected value of the resulting expression

In a locally isotropic system the specific discharge of the \( \beta \) phase is given by

\[
q_{\beta} = -\frac{k_{\beta}}{\mu_{\beta}} \left( \nabla P_o + \rho_o g \right)
\]

(2.37)

or

\[
q_{\beta} = \frac{\exp (R_{\beta}(\Gamma))}{\mu_{\beta}} j_{\beta}
\]

(2.38)
where

\[ R_\beta = \ln(k\kappa_\beta) \]  
\[ J_\beta = - (\nabla P_\beta + \rho_\beta g) \]

Assuming local isotropy, the specific discharge in the direction \( n \) is given by

\[ q_{\beta,n} = \frac{\exp(R_\beta(\Gamma))}{\mu_\beta} J_{\beta,n} \]

Now substituting the random terms by the sum of their mean and perturbation components and performing a Taylor expansion of \( \exp(R_\beta(\Gamma)) \) about \( \Gamma = \bar{\Gamma} \) the specific discharge in the direction \( n \) is

\[ q_{\beta,n} = \left( \frac{J_{\beta,n} + j'_{\beta,n}}{\mu_\beta} \right) \left( \exp(R_\beta(\bar{\Gamma})) + \gamma_i \frac{\partial \exp(R_\beta)}{\partial \Gamma_i} \bigg|_{\bar{\Gamma}} + \frac{\gamma_i \gamma_j}{2} \frac{\partial^2 \exp(R_\beta)}{\partial \Gamma_i \partial \Gamma_j} \bigg|_{\bar{\Gamma}} + \ldots \right) \]

where \( j'_{\beta} = -\nabla p'_{\beta} \) and the partial derivatives are evaluated at the value of the mean input properties, \( \Gamma = \bar{\Gamma} \). In the remainder of the text the value for which \( R_\beta \) and its derivatives are evaluated is omitted to simplify notation and it may be assumed that if not indicated that they are evaluated for the mean input parameter values. Expanding the derivatives of \( \exp(R_\beta(\bar{\Gamma})) \) the specific discharge becomes

\[ q_{\beta,n} = \frac{\exp(R_\beta) \left( J_{\beta,n} + j'_{\beta,n} \right)}{\mu_\beta} \left( 1 + \gamma_i \frac{\partial R_\beta}{\partial \Gamma_i} + \frac{\gamma_i \gamma_j}{2} \left( \frac{\partial R_\beta \partial R_\beta}{\partial \Gamma_i \partial \Gamma_j} + \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} \right) + \ldots \right) \]

The mean discharge is found by taking the expected value of the prior expression, neglecting terms greater than second order with respect to the perturbation terms and noting that the expected value of any perturbation is by definition zero
\[ E[q_{\beta,n}] = \frac{\exp(R_{\beta})}{\mu_{\beta}} \left\{ j_{\beta,n} \left[ 1 + \frac{E[\gamma_j \gamma_j']}{2} \left( \frac{\partial R_{\beta}}{\partial \Gamma_i} \frac{\partial R_{\beta}}{\partial \Gamma_j} + \frac{\partial^2 R_{\beta}}{\partial \Gamma_i \partial \Gamma_j} \right) \right] \right\} + E\left[ j'_{\beta,n} \gamma_i \right] \frac{\partial R_{\beta}}{\partial \Gamma_i} \right\} \] (2.44)

and the effective permeability defined as \( \hat{k}_{\beta,n} = \frac{E[q_{\beta,n}]\mu_{\beta}}{j_{\beta,n}} \) is given by

\[ \hat{k}_{\beta,n} = \exp(R_{\beta}) \left\{ 1 + \frac{E[\gamma_j \gamma_j']}{2} \left( \frac{\partial R_{\beta}}{\partial \Gamma_i} \frac{\partial R_{\beta}}{\partial \Gamma_j} + \frac{\partial^2 R_{\beta}}{\partial \Gamma_i \partial \Gamma_j} \right) \right\} + E\left[ j'_{\beta,n} \gamma_i \right] \frac{1}{j_{\beta,n}} \frac{\partial R_{\beta}}{\partial \Gamma_i} \right\} \] (2.45)

with no summation over \( n \) on the right hand side.

For a fully saturated system - wetting or nonwetting - all of the derivatives of \( R_{\beta} \) with respect to \( \Gamma \) evaluated for the Brooks-Corey and van Genuchten p-s-k functions go to zero except for \( \frac{\partial R_{\beta}}{\partial \Gamma} \). The saturated effective permeability, \( \hat{k}_{s,n} \), in a system with the principal coordinates aligned with the vertical and horizontal axes reduces to

\[ \hat{k}_{s,n} = \exp(\tilde{F}) \left( 1 + \frac{E[f^2]}{2} + \frac{E[j'_{n}f']}{J_n} \right) \] (2.46)

or as shown by Gelhar and Axness (1983) for a perfectly stratified aquifer

\[ \hat{k}_{s,n} = \exp(\tilde{F}) \left( 1 + \frac{E[f^2]}{2} \left( 1 - 2\delta_{1,n} \right) \right) \] (2.47)

where the direction 1 is perpendicular to stratification. As noted elsewhere, under conditions of large variability the prior result may yield physically unrealistic negative effective permeabilities in the direction perpendicular to stratification. Recognizing that the expression in parentheses represents the first two terms of a Taylor expansion of an exponential function, one might expect that under conditions of high variability where (2.47) becomes negative the exponential
function might be a reasonable approximation of the effective permeability.

\[ \hat{k}_{s,n} \approx \exp \left( \tilde{F} + \frac{E \left[ j^2 \right]}{2} (1 - 2\delta_{1,n}) \right) \]  

(2.48)

In fact, this expression is exact for a perfectly stratified medium with lognormal \( k \) (Gelhar and Axness, 1983). This modification is referred to in the remainder of this document as the exponential generalization of the effective permeability. The exponential generalization of \( \hat{k}_{s,n} \), \( \hat{k}^*_\beta,n \): is therefore

\[ \hat{k}^*_\beta,n = \exp (R_\beta (\bar{\Gamma})) \exp \left\{ \frac{E \left[ \gamma_i' \gamma_j' \right]}{2} \left( \frac{\partial R_\beta}{\partial \Gamma_i} \frac{\partial R_\beta}{\partial \Gamma_j} + \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} \right) \right\} + E \left[ j_{\beta,n}' \gamma_i' \right] \frac{1}{J_{\beta,n}} \frac{\partial R_\beta}{\partial \Gamma_i} \]  

(2.49)

An alternative means of arriving at the effective permeability is to perform the expansion about \( R_\beta \) as \( R_\beta = \bar{R}_\beta + \gamma' \), where

\[ r' = \gamma' \frac{\partial R_\beta}{\partial \Gamma_i} \]  

(2.50)

\[ \bar{R}_\beta = R_\beta (\bar{\Gamma}) + \frac{E \left[ \gamma_i' \gamma_j' \right]}{2} \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} \]  

(2.51)

The result is the same as found using the alternative scheme, however its simpler form is enlightening in that it provides a somewhat more intuitive understanding of the factors impacting the effective permeability. The exponential generalization using this notation is

\[ \hat{k}^*_\beta,n = e^{\bar{R}} \exp \left( \frac{\sigma^2}{2} + E \left[ j_{\beta,n}' r' \right] \right) \]  

(2.52)

The effective relative permeability is found by dividing each of the terms in the effective permeability tensor by the comparable term in the saturated permeability.

\[ \hat{\kappa}_{\beta,n} = \frac{\hat{k}_{\beta,n}}{\hat{k}_{s,n}} \]  

(2.53)
Using the exponential generalization for both the saturated and relative permeabilities, (2.48) and (2.49), the effective relative permeability is

\[
\tilde{\kappa}_{\beta,n} = \exp \left\{ R_{\beta} - F + \frac{E \left[ \gamma_i' \gamma_j' \right]}{2} \left( \frac{\partial R_{\beta}}{\partial \Gamma_i} \frac{\partial R_{\beta}}{\partial \Gamma_j} + \frac{\partial^2 R_{\beta}}{\partial \Gamma_i \partial \Gamma_j} \right) - \frac{E \left[ f^2 \right]}{2} \right\} + E \left[ j'_{\beta,n} \gamma_i' \right] \frac{1}{J_{\beta,n}} \frac{\partial R_{\beta}}{\partial \Gamma_i} - \frac{E \left[ j'_{\beta,n} f' \right]}{J_{\beta,n}} \right\}
\]

(2.54)

### 2.4.2 Normalized Wetting Phase Saturation

The mean, field scale saturation may be found by expanding the characterization of the saturation, and taking the expected value of the resulting stochastic expression.

\[
S_e = S_e(P_c, B, L)
\]

\[
\tilde{S}_e + s_e = S_e(\bar{\Gamma}) + \gamma_i' \frac{\partial S_e(\bar{\Gamma})}{\partial \Gamma_i} + \frac{\gamma_i' \gamma_j'}{2} \frac{\partial^2 S_e(\bar{\Gamma})}{\partial \Gamma_i \partial \Gamma_j} + ...
\]

Neglecting terms beyond second order, the mean saturation is therefore

\[
\tilde{S}_e = S_e(\bar{\Gamma}) + \frac{E \left[ \gamma_i' \gamma_j' \right]}{2} \frac{\partial^2 S_e(\bar{\Gamma})}{\partial \Gamma_i \partial \Gamma_j}
\]

(2.56)

The variance of the saturation, \( \sigma_{s_e}^2 \) is found by subtracting the mean expression (2.56) from the Taylor expansion (2.55)

\[
s_e' = \gamma_i' \frac{\partial S_e(\bar{\Gamma})}{\partial \Gamma_i}
\]

(2.57)

and taking the expected value of the square of the result

\[
\sigma_{s_e}^2 = E \left[ \gamma_i' \gamma_j' \right] \frac{\partial S_e(\bar{\Gamma})}{\partial \Gamma_i} \frac{\partial S_e(\bar{\Gamma})}{\partial \Gamma_j}
\]

(2.58)
2.4.3 Nonwetting Phase Volumetric Content

The nonwetting phase volumetric content, $\theta_o$, represents the volume of nonwetting phase compound per bulk volume. The moments may be found based on the definition of the normalized saturation.

\[
S_e = \frac{\theta_w - \theta_r}{n - \theta_r} \quad (2.59)
\]

- $\theta_o$ = nonwetting phase volumetric content
- $\theta_w$ = wetting phase volumetric content
- $n$ = porosity
- $\theta_r$ = irreducible wetting phase saturation

Now rewriting the definition with respect to $\theta_o$, $n$ and $\theta_r$.

\[
S_e = \frac{n - \theta_o - \theta_r}{n - \theta_r} = 1 - \frac{\theta_o}{n - \theta_r} \quad (2.60)
\]

So as to avoid problems in the estimation of the moments of $S_e$ for mean values near it natural limits, 0 and 1, a nonlinear transformation of $S_e$, $W$, is introduced which may take on any real value

\[
W = \ln \frac{S_e}{1 - S_e} \quad (2.61)
\]

The nonwetting phase volumetric content, $\theta_o$, may be found from (2.60) and (2.61) to be a function of $n$, $W$ and $\theta_r$

\[
\theta_o = \frac{n - \theta_r}{(e^W + 1)} \quad (2.62)
\]

Now introducing transformations of $n$ and $\theta_r$, such that the physically reasonable domain of the transformed variables $X$ and $Y$ is $[-\infty, \infty]$

\[
n = \frac{1}{e^{-X} + 1} \quad (2.63)
\]
\[ \theta_{wi} = \frac{1}{e^{-Y} + 1} \]  

\[ \theta_o = \frac{1}{(e^W + 1)} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \]  

The value of \( \theta_o \) as a function of \( W, X \) and \( Y \) is

\[ \Theta_o + \theta'_o = \frac{1}{(e^W + w + 1)} \left( \frac{1}{e^{-X} - z'_t + 1} - \frac{1}{e^{-Y} - y'_t + 1} \right) \]

and perform a Taylor expansion about mean of each variable

\[ \Theta_o + \theta'_o = \Theta_o(X, Y, W) + w' \frac{\partial \Theta_o}{\partial W} + x' \frac{\partial \Theta_o}{\partial X} + y' \frac{\partial \Theta_o}{\partial Y} + \frac{x'^2}{2} \frac{\partial^2 \Theta_o}{\partial X^2} + \frac{y'^2}{2} \frac{\partial^2 \Theta_o}{\partial Y^2} + w' x' \frac{\partial^2 \Theta_o}{\partial W \partial X} + w' y' \frac{\partial^2 \Theta_o}{\partial W \partial Y} \]

Evaluating each of the derivatives

\[ \Theta_o + \theta'_o = \frac{1}{(e^W + 1)} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \]

\[ + \frac{e^W}{(e^W + 1)} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \]

\[ - \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \]

\[ + \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \left( \frac{1}{2} + \frac{e^X}{e^{-X} + 1} \right) \]

\[ - \frac{e^Y}{(e^W + 1)^2} \left( \frac{1}{2} + \frac{e^Y}{e^{-Y} + 1} \right) \]

\[ + \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \left( \frac{1}{2} + \frac{e^W}{e^W + 1} \right) \]

\[ - \frac{e^W e^X}{(e^W + 1)^2 (e^{-X} + 1)^2} + \frac{e^W e^Y}{(e^W + 1)^2 (e^{-Y} + 1)^2} + \ldots \]

The mean is found by taking the expected value of the expansion result, where for the case
where terms greater than second order are neglected.

\[
\tilde{\theta}_o = \frac{1}{(e^W + 1)} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \\
+ \sigma_x^2 \frac{e^{-X}}{(e^W + 1)(e^{-X} + 1)^2} \left( -\frac{1}{2} + \frac{e^{-X}}{e^{-X} + 1} \right) \\
- \sigma_y^2 \frac{e^{-Y}}{(e^W + 1)(e^{-Y} + 1)^2} \left( -\frac{1}{2} + \frac{e^{-Y}}{e^{-Y} + 1} \right) \\
+ \sigma_w^2 \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \left( -\frac{1}{2} + \frac{e^W}{e^W + 1} \right) \\
- \text{cov}(W, X) \frac{e^W e^{-X}}{(e^W + 1)^2(e^{-X} + 1)^2} + \text{cov}(W, Y) \frac{e^W e^{-Y}}{(e^W + 1)^2(e^{-Y} + 1)^2}
\] (2.69)

The perturbation is found by subtracting the mean from the original expansion

\[
\theta'_o = x' \frac{e^{-X}}{(e^W + 1)(e^{-X} + 1)^2} - y' \frac{e^{-Y}}{(e^W + 1)(e^{-Y} + 1)^2} \\
- w' \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right)
\] (2.70)

The variance of \(\theta_o\) is the expected value of the square of the perturbation term.

\[
\sigma^2_{\theta_o} = \sigma_x^2 \left[ \frac{e^{-X}}{(e^{-X} + 1)^2(e^W + 1)} \right]^2 + \sigma_y^2 \left[ \frac{e^{-Y}}{(e^{-Y} + 1)^2(e^W + 1)} \right]^2 \\
+ \sigma_w^2 \left( \frac{e^W}{(e^W + 1)^2} \right)^2 \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right)^2 \\
- 2\text{cov}(X, Y) \frac{e^{-X} e^{-Y}}{(e^{-X} + 1)^2(e^W + 1)(e^{-Y} + 1)^2(e^W + 1)} \\
- 2\text{cov}(X, W) \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \frac{e^{-X}}{(e^{-X} + 1)^2(e^W + 1)} \\
+ 2\text{cov}(Y, W) \frac{e^W}{(e^W + 1)^2} \left( \frac{1}{e^{-X} + 1} - \frac{1}{e^{-Y} + 1} \right) \frac{e^{-Y}}{(e^{-Y} + 1)^2(e^W + 1)}
\] (2.71)
In order to evaluate the moments of \( \theta_e \) expressions must be derived for \( \sigma_w^2 \), \( \text{cov}(x,w) \) and \( \text{cov}(y,w) \). Assuming \( W \) to have a known functional dependence on the input properties vector, \( \Gamma \), the sum of its mean and perturbation may be written as the expansion.

\[
\bar{W} + w' = W(\bar{\Gamma}) + \gamma_i \frac{\partial W(\bar{\Gamma})}{\partial \Gamma_i} + \frac{\gamma_i \gamma_j}{2} \frac{\partial^2 W(\bar{\Gamma})}{\partial \Gamma_i \partial \Gamma_j} + ...
\]  

(2.72)

Therefore

\[
\bar{W} + w' = \ln \left( \frac{S_e}{1 - S_e} \right) + \gamma_i \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) + \frac{\gamma_i \gamma_j}{2} \left[ \frac{\partial^2 S_e}{\partial \Gamma_i \partial \Gamma_j} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) + \frac{\partial S_e}{\partial \Gamma_i} \frac{\partial S_e}{\partial \Gamma_j} \left( -\frac{1}{S_e^2} + \frac{1}{(1 - S_e)^2} \right) \right] + ...
\]  

(2.73)

where in this context \( S_e \) is the value of the normalized saturation evaluated for the mean input parameters, \( S_e(\bar{\Gamma}) \) and the partial derivatives with respect to \( S_e \) are evaluated at the mean input parameters. The mean value of \( W \) is found to be

\[
\bar{W} = \ln \left( \frac{S_e}{1 - S_e(\bar{\Gamma})} \right) + \text{cov}(\Gamma_i, \Gamma_j) \left[ \frac{\partial^2 S_e}{\partial \Gamma_i \partial \Gamma_j} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) + \frac{\partial S_e}{\partial \Gamma_i} \frac{\partial S_e}{\partial \Gamma_j} \left( -\frac{1}{S_e^2} + \frac{1}{(1 - S_e)^2} \right) \right]
\]  

(2.74)

The perturbation \( w' \) is therefore

\[
w' = \gamma_i \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right)
\]  

(2.75)

and the moments of \( W \) are

\[
\sigma_w^2 = \text{cov}(\Gamma_i, \Gamma_j) \frac{\partial S_e}{\partial \Gamma_i} \frac{\partial S_e}{\partial \Gamma_j} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right)^2
\]  

(2.76)

\[
\text{cov}(X,W) = \text{cov}(X, \Gamma_i) \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right)
\]  

(2.77)
\[ \text{cov}(Y, W) = \text{cov}(Y, \Gamma_i) \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) \]  

(2.78)

In the case where \(X\) and \(Y\) are correlated to \(F\) as in

\[ x' = b_x f' + g_x \]  

(2.79)

\[ y' = b_y f' + g_y \]

The covariance functions \(\text{cov}(X, W)\) and \(\text{cov}(Y, W)\) are given by

\[ \text{cov}(X, W) = \text{cov}(F, \Gamma_i) b_x \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) \]  

(2.80)

\[ \text{cov}(Y, W) = \text{cov}(F, \Gamma_i) b_y \frac{\partial S_e}{\partial \Gamma_i} \left( \frac{1}{S_e} + \frac{1}{1 - S_e} \right) \]

2.5 Output Spectra

As noted above, the mean normalized wetting phase saturation, \(\bar{S}_e\), and effective permeability, \(\bar{k}_{\beta}\), are functions of the mean, variance and covariance of the input variables \(\Phi\) and output variables \(j'\) and \(p'_e\). The mean, variance and covariance of the input variables are assumed to be known based on measurements or physical arguments related to the soil properties. Mean cross products of output and input variables are determined by the solution of the stochastic differential equation for multiphase flow. The continuity or flow equation for fluid phase \(\beta\) may be written in the following form

\[ \nabla^2 P_\beta - \nabla R_\beta \cdot J_\beta = 0 \]  

(2.81)

where \(R_\beta = \ln k_\beta\) and \(J_\beta = - (\nabla P_\beta + \rho_\beta \mathbf{g})\).

The linearized form of the stochastic differential equation is found by substituting the sum of the mean and perturbation for each of the random terms and performing a Taylor expansion of \(R_\beta (\bar{\Gamma})\) about \(\bar{\Gamma}\).

\[ 0 = \nabla^2 (\bar{P}_\beta + p'_\beta) - \nabla \left( R_\beta (\bar{\Gamma}) + \gamma_i \frac{\partial R_\beta}{\partial \Gamma_i} + \frac{\gamma_i' \gamma_j'}{2} \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} + \ldots \right) \cdot (\bar{J}_\beta + J'_\beta) \]  

(2.82)
where the partial derivatives are evaluated for the mean values of the input parameters.

The mean equation is found by taking the expected value of the previous term, while neglecting terms exceeding second order and noting that the mean of each of the perturbation terms is zero.

\[
0 = \nabla^2 \hat{P}_\beta - E \left[ \nabla \left( \gamma_i \frac{\partial R_\beta}{\partial \Gamma_i} \right) \cdot \hat{j}_\beta \right] - \nabla \left( R_\beta (\Gamma) + \frac{E \left[ \gamma_i \gamma_j \right]}{2} \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} \right) \cdot \hat{J}_\beta
\]  

(2.83)

The gradient of \( R_\beta \) may be written as

\[
\nabla R_\beta = \frac{\partial R_\beta}{\partial \hat{P}_c} \nabla \hat{P}_c + \frac{\partial R_\beta}{\partial \Phi_i} \nabla \Phi_i
\]  

(2.84)

but noting that the means of the input variables are assumed to be slowly varying, the second term on the right hand side may be neglected and the gradient of \( R \) related to the gradient of the capillary pressure

\[
\nabla R_\beta = \frac{\partial R_\beta}{\partial \hat{P}_c} \nabla \hat{P}_c
\]  

(2.85)

Similarly, the gradient of the partial derivative of \( R_\beta \) with respect to \( \Gamma_i \) may be approximated as

\[
\nabla \left( \frac{\partial R_\beta}{\partial \Gamma_i} \right) = \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \hat{P}_c} \nabla \hat{P}_c
\]  

(2.86)

Subtracting the mean equation from the linearized form of the continuity equation, while neglecting the difference \( \frac{E \left[ \gamma_i \gamma_j \right]}{2} \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} - \frac{\gamma_i \gamma_j}{2} \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \Gamma_j} \), results in a governing equation of the random, perturbation quantities

\[
0 = \nabla^2 \hat{P}_\beta - \frac{\partial R_\beta}{\partial \hat{P}_c} \nabla \hat{P}_c \cdot \hat{j}_\beta - \left( \gamma_i \frac{\partial^2 R_\beta}{\partial \Gamma_i \partial \hat{P}_c} \nabla \hat{P}_c + \frac{\partial R_\beta}{\partial \Gamma_i} \nabla \gamma_i \right) \cdot \hat{J}_\beta
\]  

(2.87)

This equation may also be expressed in the wave number domain, as in Lumley and Panofsky (1964), Gelhar and Axness (1983), and elsewhere using the Fourier-Stieljes integral representation of the random quantities described previously. Given \( dZ_{j' \beta} = -i\omega dZ_{p\beta} \) and recognizing the uniqueness of the spectral representation we find
\[ 0 = -\omega^2 dZ_{p_o} + i \frac{\partial R_o}{\partial P_c} \omega \cdot \nabla \bar{P}_c \, dZ_{p_o} \]

\[ - \left( \frac{\partial^2 R_o}{\partial \Gamma_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_o}{\partial \Gamma_i} \omega \right) \cdot \bar{J}_o \, d\gamma_i \]  

Thus, the solution for the spectral amplitude of the pressure perturbation is

\[ dZ_{p_o} = \left( \frac{\partial^2 R_o}{\partial \Gamma_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_o}{\partial \Gamma_i} \omega \right) \, \chi_o \, \bar{J}_o \]  

(2.89)

where

\[ \chi_o = \frac{1}{-\omega^2 + i \frac{\partial R_o}{\partial P_c} \omega \cdot \nabla P_c} \]

The spectral amplitude of the capillary pressure is given by the difference of the spectral amplitude of the nonwetting and wetting phase pressures.

\[ dZ_{p_c} = dZ_{p_c} - dZ_{p_w} \]

\[ = dZ_{\Gamma} \left[ \left( \frac{\partial^2 R_o}{\partial \Gamma_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_o}{\partial \Gamma_i} \omega \right) \chi_o \cdot \bar{J}_o \right. \]

\[ - \left. \left( \frac{\partial^2 R_w}{\partial \Gamma_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_w}{\partial \Gamma_i} \omega \right) \chi_w \cdot \bar{J}_w \right] \]

Since \( dZ_{\Gamma} \) includes \( dZ_{p_c} \), the solution for \( dZ_{p_c} \) is found by isolating \( dZ_{p_c} \) on the left hand side and writing the right hand side with respect to the parameter set \( \Phi \) which excludes \( P_c \) and \( p'_c \) respectively

\[ dZ_{p_c} = dZ_{\Phi} \]

\[ \frac{\left( \frac{\partial^2 R_o}{\partial \Phi_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_o}{\partial \Phi_i} \omega \right) \cdot \bar{J}_o \chi_o - \left( \frac{\partial^2 R_w}{\partial \Phi_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_w}{\partial \Phi_i} \omega \right) \cdot \bar{J}_w \chi_w}{1 - \left( \frac{\partial^2 R_o}{\partial P_c^2} \nabla \bar{P}_c + i \frac{\partial R_o}{\partial P_c} \omega \right) \cdot \bar{J}_o \chi_o + \left( \frac{\partial^2 R_w}{\partial P_c^2} \nabla \bar{P}_c + i \frac{\partial R_w}{\partial P_c} \omega \right) \cdot \bar{J}_w \chi_w} \]

To simplify the solution an additional variable, \( Y_m \), is introduced whereby for \( dZ_{\Phi} = dZ_{\phi} \) +
\[ dZ_{pc} = Y_m (dZ_{gm} + b_m dZ_f) \] (2.92)

where on expanding the right hand side of (2.91)

\[
Y_m = \left[ -\omega^2 \left( \frac{\partial^2 R_o}{\partial \Phi_m \partial P_c} - \frac{\partial^2 R_w}{\partial \Phi_m \partial P_c} \right) \cdot \nabla P_c - \left( \nabla P_c \cdot \omega \right) \left( \frac{\partial R_o}{\partial \Phi_m} \frac{\partial R_w}{\partial P_c} - \frac{\partial R_w}{\partial \Phi_m} \frac{\partial R_c}{\partial P_c} \right) \cdot \nabla P_c \right] \left[ \omega^4 + i\omega^2 \omega \cdot \left( -\frac{\partial R_w}{\partial P_c} \nabla P_c + \frac{\partial R_o}{\partial P_c} (\nabla P_c - \nabla \bar{P}_c) \right) \right. \\
\left. + \omega^2 \left( \frac{\partial^2 R_w}{\partial P_c^2} - \frac{\partial^2 R_o}{\partial P_c^2} \right) \cdot \nabla P_c + \left( \omega \cdot \left( J_o - J_w - \nabla \bar{P}_c \right) \left( \omega \cdot \nabla P_c \right) \frac{\partial R_w}{\partial P_c} \frac{\partial R_o}{\partial P_c} \frac{\partial R_w}{\partial \Phi_m} \frac{\partial R_c}{\partial P_c} \right) \cdot \nabla P_c \right]^{-1}
\] (2.93)

The remainder of this section documents derivation of cross-spectra expressions for \( S_{pc,\phi_i} \), \( S_{pc,pc} \), \( S_{j\phi,\phi_i} \), and \( S_{j\phi,pc} \) which will be utilized in Chapters 3 and 4 to evaluate the effective permeability for particular cases of uniform flow and flow in stratified systems.

The cross-spectra are found by taking the expected value of the cross product of the spectral amplitudes as in

\[
S_{pc,\phi_i} d\omega = \mathbb{E} \left[ dZ_{pc} dZ_{\phi_i}^* \right] = \mathbb{E} \left[ Y_m (b_m dZ_f + dZ_{gm}) (b_\epsilon dZ_f^* + dZ_{\phi_i}^*) \right] \] (2.94)

resulting in

\[
S_{pc,\phi_i} = Y_m (b_m b_\epsilon S_{f,f} + S_{gm,\phi_i}) \] (2.95)

Likewise
\[ S_{pc,pc} d\omega = E[dZ_p dZ_{pc}^*] \]
\[ = E \left[ Y_m (b_m dZ_f + dZ_{gm}) Y_i^* (b_i dZ_f^* + dZ_{gi}) \right] \]  

and

\[ S_{pc,pc} = Y_m (b_i b_m S_{f,f} + S_{gm,gi}) Y_i^* \]  
\[ = S_{pc,pc} Y_i^* \]  

By definition \( j'_\beta = -\nabla p'_\beta \) so the spectral amplitude of \( j'_\beta \) is given by

\[ dZ_{j_\beta} = -i\omega dZ_{p_\beta} \]  

From (2.89) the spectral amplitude of the pressure perturbation, \( dZ_{p_\beta} \), may be written with respect to \( dZ_{\phi_i} \) and \( dZ_{pc} \) as.

\[ dZ_{p_\beta} = x_\beta \bar{j}_\beta \left[ \left( \frac{\partial^2 R_{\beta}}{\partial P_c^2} \nabla \bar{P}_c + i \frac{\partial R_{\beta}}{\partial P_c} \omega \right) dZ_{pc} \right. \]
\[ + \left. \left( \frac{\partial^2 R_{\beta}}{\partial \Phi_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_{\beta}}{\partial \Phi_i} \omega \right) dZ_{\phi_i} \right] \]  

Introducing the variables \( X_{c,\beta} \) and \( X_{i,\beta} \) defined as

\[ X_{c,\beta} = x_\beta \bar{j}_\beta \left( \frac{\partial^2 R_{\beta}}{\partial P_c^2} \nabla \bar{P}_c + i \frac{\partial R_{\beta}}{\partial P_c} \omega \right) \]  
\[ X_{i,\beta} = x_\beta \bar{j}_\beta \left( \frac{\partial^2 R_{\beta}}{\partial \Phi_i \partial P_c} \nabla \bar{P}_c + i \frac{\partial R_{\beta}}{\partial \Phi_i} \omega \right) \]  

the pressure perturbation is

\[ dZ_{p_\beta} = X_{c,\beta} dZ_{pc} + X_{i,\beta} dZ_{\phi_i} \]  

58
and

\[ dZ_{j,s} = -i \omega \left( X_{c,\beta}dZ_{pc} + X_{i,\beta}dZ_{\phi_i} \right) \]
\[ = -i \omega \left( X_{c,\beta}dZ_{pc} + X_{i,\beta} \left( b_i dZ_f + dZ_{g_i} \right) \right) \]

Therefore equating \( S_{j,s,\phi_i}d\omega \) to the expected value of \( dZ_{j,s}dZ_{\phi_i}^* \)

\[ S_{j,s,\phi_i}d\omega = -i \omega E \left[ \left( X_{c,\beta}dZ_{pc} + X_{m,\beta} \left( b_m dZ_f + dZ_{g_m} \right) \right) \left( b_i dZ_f^* + dZ_{g_i}^* \right) \right] \]  \hspace{1cm} (2.103)

and

\[ S_{j,s,\phi_i} = -i \omega \left( X_{c,\beta}S_{pc,\phi_i} + X_{m,\beta} \left( b_m b_i S_{f,f} + S_{g_m,g_i} \right) \right) \]  \hspace{1cm} (2.104)

By the same reasoning, the spectra, \( S_{j,s,pc} \), is given by

\[ S_{j,s,pc}d\omega = E[dZ_{j,s}dZ_{pc}] \]
\[ = E \left[ i \omega \left( X_{c,\beta}^*dZ_{pc}^* + X_{i,\beta}^*dZ_{\phi_i}^* \right) dZ_{pc} \right] \]  \hspace{1cm} (2.105)

and

\[ S_{j,s,pc} = i \omega X_{c,\beta}^*S_{pc,pc} + i \omega X_{i,\beta}^*S_{\phi_i,pc} \]  \hspace{1cm} (2.106)

### 2.6 Discussion

This concludes the general derivation of the effective properties. In principal, this is sufficient for evaluation of effective properties for any condition by evaluation of integrals of the cross spectra. For instance, \( \sigma_{pc}^2 \), whose value is required for evaluation of the effective permeability is found by integration of \( S_{pc,pc} \) over the wave number space. Unfortunately, closed form solutions of these integrals were not found, so evaluation of effective permeabilities in this most general condition requires numerical integration. Alternatively, special conditions may be specified as in Yeh (1985a, b) which allow for analytical evaluation of the cross-product integrals. In Chapter
3, the condition of uniform flow perpendicular to the principal axes is examined and in Chapter 4 nonuniform flow in an arbitrary direction is addressed for the perfectly stratified aquifer.
Chapter 3

Effective Properties - Vertical or Horizontal, Uniform Flow

In this chapter, the general findings presented in Chapter 2 are applied for the particular case of uniform, mean flow aligned with a principal axis. The spectra functions presented in Chapter 2 are simplified by substitution of \( \nabla \hat{P}_c = 0 \) and \( \hat{J}_{\beta,2} = \hat{J}_{\beta,3} = 0 \). The simpler spectra expressions are then integrated analytically and the effective aquifer properties are evaluated for conditions representative of the Borden Aquifer under varying flow conditions.

The results of this chapter apply only to flow parallel to one of the principal axes. A more general solution allowing the estimation of effective permeability with flow not aligned to a principal axis is presented in Chapter 4, subject to the additional constraint that the aquifer is perfectly stratified.

A note on notation is included here to clarify differing uses of the directional index in this chapter and Chapter 4. In this chapter, \( J_{\beta,1} \) is used to indicate the head gradient in the direction of flow. The mean gradients in the other directions are taken to be zero, that is \( \hat{J}_{\beta,2} = \hat{J}_{\beta,3} = 0 \). In the next chapter, \( J_{\beta,1} \) is interpreted as the head gradient in the direction perpendicular to soil strata of infinite extent, while \( \hat{J}_{\beta,2} \) and \( \hat{J}_{\beta,3} \) are not restricted to be zero.
3.1 Cross Products

Moments of the cross products are derived below from general results developed in Chapter 2 for the special case of $\nabla \bar{P}_c = 0$ and $\bar{J}_{\beta,2} = \bar{J}_{\beta,3} = 0$. In uniform mean flow, the values of $\bar{J}_w$ and $\bar{J}_o$ are not independent. For horizontal flow,

$$\bar{J}_{w,1} = \bar{J}_{o,1}$$ (3.1)

For the case of vertical flow, on consideration of the condition $\frac{\partial \bar{P}_c}{\partial x_1} = \frac{\partial \bar{P}_c}{\partial x_1} - \frac{\partial \bar{P}_w}{\partial x_1} = 0$ and the definitions of $J_{w,1}$ and $J_{o,1}$ it is trivial to determine that

$$\bar{J}_{o,1} = \bar{J}_{w,1} - (\rho_o - \rho_w) g$$

$$= \bar{J}_{w,1} - \delta \rho g$$ (3.2)

In the remainder of this chapter, the deterministic interdependence of $\bar{J}_{w,1}$ and $\bar{J}_{o,1}$ is operative whether or not specifically stated.

Under these conditions $Y_m$ as defined in (2.93) reduces to

$$Y_m = \frac{-i \omega_1 \left( \frac{\partial R_o}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w}{\partial \Phi_m} \bar{J}_{w,1} \right)}{\omega^2 + i \omega_1 \left( \frac{\partial R_o}{\partial \bar{P}_c} \bar{J}_{o,1} - \frac{\partial R_w}{\partial \bar{P}_c} \bar{J}_{w,1} \right)}$$ (3.3)

or after eliminating the complex components from the denominator

$$Y_m = \frac{-i \omega_1 \left( \frac{\partial R_o}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w}{\partial \Phi_m} \bar{J}_{w,1} \right)}{\omega^4 + \omega_1^2 \left( \frac{\partial R_o}{\partial \bar{P}_c} \bar{J}_{o,1} - \frac{\partial R_w}{\partial \bar{P}_c} \bar{J}_{w,1} \right)^2}$$ (3.4)

and $X_{c,\beta}$ and $X_{i,\beta}$ from (2.100) reduce to

$$X_{c,\beta} = -\frac{i \bar{J}_{\beta,1} \omega_1 \frac{\partial R_\beta}{\partial \bar{P}_c}}{\omega^2}$$

$$X_{i,\beta} = -\frac{i \bar{J}_{\beta,1} \omega_1 \frac{\partial R_\beta}{\partial \Phi_i}}{\omega^2}$$ (3.5)
Given the spectra of the exponential correlation model (2.35) with a single correlation scale for all input variables and the output spectra (2.95), (2.97), (2.104), and (2.106), the moments of the output variables are found by evaluating the integral of the spectra functions. They are presented in the following section as unevauated integrals, however closed form solutions have been obtained and are presented along with their derivation in Appendix B.

From (2.35) and (2.95) the \( \text{cov}(P, \Phi_i) \) is equal to the integral

\[
\text{cov}(P, \Phi_i) = \int \int \int_{-\infty}^{\infty} Y_m (b_m b_i S_{f,f} + S_{g_m,g_i}) \, d\omega_1 d\omega_2 d\omega_3
\]

(3.6)

Substitute (3.4) for \( Y_m \) and the spectra function of the exponential correlation model (2.36) for \( S_{f,f} \) and \( S_{g_m,g_i} \). Then make the substitutions \( u_t = \omega_i \xi_i \) and \( \rho = \frac{\xi_2}{\xi_1} \), and omit the odd terms with respect to \( u_t \) which will integrate to zero

\[
\text{cov}(P, \Phi_i) = - \left( \frac{\partial R_o(\tilde{\Phi})}{\partial P_c} \tilde{J}_{o,1} - \frac{\partial R_w(\tilde{\Phi})}{\partial P_c} \tilde{J}_{w,1} \right)
\]

\[
\left( \frac{\partial R_o(\tilde{\Phi})}{\partial \Phi_m} \tilde{J}_{o,1} - \frac{\partial R_w(\tilde{\Phi})}{\partial \Phi_m} \tilde{J}_{w,1} \right) \left( b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_2^2 \right)
\]

\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} \rho^4 \xi_1^2 u_1^2
\]

\[
\left( \left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right)^2 + u_1^2 \rho^4 \xi_1^2 \left( \frac{\partial R_o(\tilde{\Phi})}{\partial P_c} \tilde{J}_{o,1} - \frac{\partial R_w(\tilde{\Phi})}{\partial P_c} \tilde{J}_{w,1} \right)^2 \right) \, du_1 du_2 du_3
\]

The closed form solution of this integral is derived in Appendix B.1.

\[
\text{cov}(P, \Phi_i) = - \left( \frac{\partial R_o(\tilde{\Phi})}{\partial P_c} \tilde{J}_{o,1} - \frac{\partial R_w(\tilde{\Phi})}{\partial P_c} \tilde{J}_{w,1} \right)
\]

\[
\left( \frac{\partial R_o(\tilde{\Phi})}{\partial \Phi_m} \tilde{J}_{o,1} - \frac{\partial R_w(\tilde{\Phi})}{\partial \Phi_m} \tilde{J}_{w,1} \right) \left( b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_2^2 \right) \rho^4 \xi_1^2 I_1(a, b)
\]

(3.8)
where

\[
I_1(a, b) = \begin{cases} 
- \frac{4 \tan^{-1}(\frac{2a+b}{\Delta})}{-\Delta \sqrt{\Delta}} + \frac{4 \tan^{-1}(\frac{b}{\sqrt{\Delta}})}{-\Delta \sqrt{\Delta}} + \frac{2+|b|}{-\Delta(a+|b|+1)}; & \Delta > 0 \\
- \frac{2}{2a+|b|} + \frac{2}{|b|}; & \Delta = 0 \\
- \frac{2+|b|}{\Delta(a+|b|+1)} + \frac{2}{(-\Delta)^{3/2}} \ln \left[ \frac{(2a+b+\sqrt{-\Delta})(|b|-\sqrt{-\Delta})}{(2a+b-\sqrt{-\Delta})(|b|+\sqrt{-\Delta})} \right]; & \Delta < 0 
\end{cases}
\]  

(3.9)

and

\[
a = \rho^2 - 1 \\
b = \rho^2 |\xi_1|
\]

(3.10)

By the same reasoning, from (2.95)

\[
\sigma_{pc}^2 = \iint_{-\infty}^{\infty} Y_m Y_n^* \left( b_m b_n S_{f,f} + S_{g_m,g_n} \right) d\omega_1 d\omega_2 d\omega_3
\]

(3.11)

and

\[
\sigma_{pc}^2 = \left( \frac{\partial R_0(\bar{\Phi})}{\partial \Phi_i} J_{o,1} - \frac{\partial R_w(\bar{\Phi})}{\partial \Phi_i} J_{w,1} \right) \\
\left( \frac{\partial R_0(\bar{\Phi})}{\partial \Phi_m} J_{o,1} - \frac{\partial R_w(\bar{\Phi})}{\partial \Phi_m} J_{w,1} \right) \left( b_i b_m \sigma^2_f + \delta_{i,m} \sigma^2_g \right) \\
\frac{1}{\pi^2 \left( 1 + u_1^2 + u_2^2 + u_3^2 \right)^2} \\
\frac{\rho^4 \xi^2_i u_1^2}{\left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right)^2 + u_1^2 \rho^4 \xi^2_1 \left( \frac{\partial R_0(\bar{\Phi})}{\partial \Phi_i} J_{o,1} - \frac{\partial R_w(\bar{\Phi})}{\partial \Phi_i} J_{w,1} \right)^2} du_1 du_2 du_3
\]

(3.12)

and

\[
\sigma_{pc}^2 = \left( \frac{\partial R_0(\bar{\Phi})}{\partial \Phi_i} J_{o,1} - \frac{\partial R_w(\bar{\Phi})}{\partial \Phi_i} J_{w,1} \right) \\
\left( \frac{\partial R_0(\bar{\Phi})}{\partial \Phi_m} J_{o,1} - \frac{\partial R_w(\bar{\Phi})}{\partial \Phi_m} J_{w,1} \right) \left( b_i b_m \sigma^2_f + \delta_{i,m} \sigma^2_g \right) \rho^4 \xi^2_1 I_1(a, b)
\]

(3.13)

From (2.104)

64
\[
\text{cov}(J_{\beta}, \Phi_i) = - \int \int \int_{-\infty}^{\infty} i\omega \left[ X_{c,\beta} S_{p_c,\phi_i} + X_{m,\beta} (b_m b_i S_{f,\phi} + S_{g_m,\phi_i}) \right] d\omega_1 d\omega_2 d\omega_3
\] (3.14)

and by the same process is found to be

\[
\text{cov}(J_{\beta,1}, \Phi_i) = (b_m b_i \sigma_f^2 + \delta_{i,m} \sigma_i^2) J_{\beta,1} \left[ \frac{\xi_1 \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} \rho^4 u_1^2}{(\rho^2 u_1^2 + u_2^2 + u_3^2)} + \frac{\xi_2 \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} \rho^6 u_1^4}{(\rho^2 u_1^2 + u_2^2 + u_3^2)} \right]
\]

\[
\left( \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} J_{\phi,1} - \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} J_{\phi,1} \right) \left( \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} J_{\phi,1} - \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} J_{\phi,1} \right)
\]

\[
\frac{1}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)} d\omega_1 d\omega_2 d\omega_3
\]

The closed forms of these integrals are derived in Appendices B.2 and B.3.

\[
\text{cov}(J_{\beta,1}, \Phi_i) = (b_m b_i \sigma_f^2 + \delta_{i,m} \sigma_i^2) J_{\beta,1} \xi_1^2 \rho^4 \left[ \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} \left( \sqrt{\rho^2 - 1} - \arctan \sqrt{\rho^2 - 1} \right) \right]
\]

\[
+ \left( \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} J_{\phi,1} - \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} J_{\phi,1} \right)
\]

\[
\left( \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} J_{\phi,1} - \frac{\partial R_0(\tilde{\Phi})}{\partial \Phi_m} J_{\phi,1} \right) \frac{\partial R_0(\tilde{\Phi})}{\partial P_c} \rho^2 I_2(a,b)
\]

\[
I_2 = \begin{cases} 
\frac{8
}{b^2 \Delta^{3/2}} \left( \tan^{-1} \left( \frac{2a+b}{\sqrt{\Delta}} \right) - \tan^{-1} \left( \frac{b}{\sqrt{\Delta}} \right) \right) - \frac{\tan^{-1}(\sqrt{\Delta})}{a^{3/2} b^2} - \frac{|b|+b^2-2a}{a \Delta b (1+a+b)} & \Delta \geq 0 \\
\frac{8 \Delta}{b^2 (-\Delta)^{3/2}} \left( \tanh^{-1} \left( \frac{b}{\sqrt{-\Delta}} \right) - \tanh^{-1} \left( \frac{2a+b}{\sqrt{-\Delta}} \right) \right) - \frac{\tan^{-1}(\sqrt{\Delta})}{a^{3/2} b^2} - \frac{b-2a+b^2}{a \Delta (1+a+b)} & \Delta < 0 
\end{cases}
\] (3.17)

From (2.106)

\[
\text{cov}(J_{\beta,1}, P_c) = \int \int \int_{-\infty}^{\infty} i\omega \left( X_{c,\beta}^* S_{p_c,\phi_i} + X_{i,\beta}^* S_{f,\phi_i, p_c} \right) d\omega_1 d\omega_2 d\omega_3
\] (3.18)
Separating the integral into the summation

$$\text{cov}(J_{\beta,1}, P_c) = A + B$$  \hspace{1cm} (3.19)

where

$$A = - (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_g^2) \left( \frac{\partial R_o (\bar{F})}{\partial \Phi_i} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial \Phi_i} \bar{J}_{w,1} \right) \left( \frac{\partial R_o (\bar{F})}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial \Phi_m} \bar{J}_{w,1} \right)$$  \hspace{1cm} (3.20)

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\xi_1^2 \rho^6 \frac{\partial R_o (\bar{F})}{\partial P_c} \bar{J}_{\beta,1}}{\pi^2 \left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right) \left( 1 + u_1^2 + u_2^2 + u_3^2 \right)^2} \, du_1 \, du_2 \, du_3$$

$$\frac{u_1^4}{\left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right)^2 + u_1^2 \rho^4 \xi_1^2 \left( \frac{\partial R_o (\bar{F})}{\partial P_c} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial P_c} \bar{J}_{w,1} \right)^2}$$

$$B = (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_g^2) \left( \frac{\partial R_o (\bar{F})}{\partial \Phi_i} \bar{J}_{\beta,1} \right) \left( \frac{\partial R_o (\bar{F})}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial \Phi_m} \bar{J}_{w,1} \right)$$  \hspace{1cm} (3.21)

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\xi_1^2 \rho^6 \left( \frac{\partial R_o (\bar{F})}{\partial P_c} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial P_c} \bar{J}_{w,1} \right)}{\pi^2 \left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right) \left( 1 + u_1^2 + u_2^2 + u_3^2 \right)^2} \, du_1 \, du_2 \, du_3$$

$$\frac{u_1^4}{\left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right)^2 + u_1^2 \rho^4 \xi_1^2 \left( \frac{\partial R_o (\bar{F})}{\partial P_c} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial P_c} \bar{J}_{w,1} \right)^2}$$

Substituting first $\beta = o$ and then $\beta = w$ in $A$ and $B$, one finds that $\text{cov}(J_{w,1}, P_c) = \text{cov}(J_{o,1}, P_c)$ and is identically zero when the gradient in either phase is zero.

$$\text{cov}(J_{\beta,1}, P_c) = \frac{\bar{J}_{o,1} \bar{J}_{w,1}}{\pi^2} (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_g^2) \left( \frac{\partial R_o (\bar{F})}{\partial P_c} \frac{\partial R_w (\bar{F})}{\partial \Phi_i} - \frac{\partial R_w (\bar{F})}{\partial P_c} \frac{\partial R_o (\bar{F})}{\partial \Phi_i} \right) \left( \frac{\partial R_o (\bar{F})}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w (\bar{F})}{\partial \Phi_m} \bar{J}_{w,1} \right)$$  \hspace{1cm} (3.22)

66
\[
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\xi_1^2 \rho^6}{u_1^4} \left( \rho^2 u_1^2 + u_2^2 + u_3^2 \right)^2 \left( \frac{\partial R_u(f)}{\partial \Phi_c} \bar{J}_{o,1} - \frac{\partial R_w(f)}{\partial \Phi_c} \bar{J}_{w,1} \right) \right)^2 du_1 du_2 du_3
\]

where the integral is evaluated in Section 2 of Appendix B.

\[
\text{cov}(J_{\beta,1}, P_c) = \frac{\bar{J}_{o,1}\bar{J}_{w,1}}{\pi^2} \left( b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_{\gamma_m}^2 \right) \left( \frac{\partial R_o(\bar{f})}{\partial P_c} \frac{\partial R_w(\bar{f})}{\partial \Phi_i} - \frac{\partial R_w(\bar{f})}{\partial P_c} \frac{\partial R_o(\bar{f})}{\partial \Phi_i} \right) \left( \frac{\partial R_o(\bar{f})}{\partial \Phi_m} \bar{J}_{o,1} - \frac{\partial R_w(\bar{f})}{\partial \Phi_m} \bar{J}_{w,1} \right)
\]

\( \xi_1^2 \rho^6 I_2(a, b) \)

and \( I_2 \) is presented in (3.17).

### 3.2 Evaluation of Effective Properties

The expressions for the moments are generic in that the form of the p-s-k functions and their derivatives are not specified. Effective properties were evaluated using the programming and symbolic algebra capabilities of Maple V Release 4 (1995), including routines for the automated evaluation of function derivatives. The bulk of the code was written as the derivation is presented here, in a manner such that it was independent of the selected p-s-k characterization. The specification of the characterization functions and the evaluation of the derivatives with respect to the random parameters were isolated to enable the characterizations to be easily modified to test the sensitivity to characterization form.

Two goals were identified for evaluation of effective properties under the conditions prescribed for this chapter.

1. Compare effective properties estimated for natural conditions to effective properties evaluated for the "perfectly" stratified case as presented in Chapter 4. The effective properties for the perfectly stratified aquifer reduce to simple expressions in which the role of individual parameters is readily understood. If as expected, based on results in unsaturated flow (Yeh, 1985b), the effective properties found for the perfectly stratified aquifer condition
can be shown to be a reasonable approximation of typical aquifer conditions, then there is a significant advantage to using the perfectly stratified condition. This will be addressed by evaluating the effective properties for a range of horizontal correlation scales, while keeping the vertical correlation scale constant.

2. Assess the velocity dependence of the effective permeability in horizontal, stratified heterogeneous systems through modification of the capillary number. It has been observed that steady state measurements of relative permeability are dependent on the flow velocity (Dullien, 1992; Demond and Roberts, 1993). Findings from analysis of one dimensional, multiphase flow with spatially variable properties (Dale et al., 1997) are consistent with those observations and suggest that heterogeneity may play a key role in the velocity dependence of relative permeability measurements.

3.2.1 Dependence of Effective Properties on Horizontal Correlation Scale

The effective permeability, the mean capillary pressure-saturation curve and the variance of the capillary pressure were evaluated for conditions representing the Borden aquifer subject to the following conditions:

- horizontal correlation scales ranging from 2 to 10000 times the vertical correlation scale
- uniform, vertical mean flow
- static wetting phase
- $\delta = 0.6 \text{ g/cm}^3$.

Table 3.1 summarizes the van Genuchten parameter moments used in estimating effective property. The values of the moments are based on measurements of capillary pressure during tetrachloroethylene (PCE)-water drainage experiments in seven soil samples from the Borden aquifer. A vertical correlation scale of 12 cm was used based on two studies of the permeability field at the Borden aquifer. The data sources and their analysis are explained in detail in Chapter 6. Consult Chapter 2 for the definition of $b_i$ and $\sigma_g$, and the assumptions of the underlying stochastic model.
Table 3.1: Base case, Borden Aquifer, van Genuchten parameters for independent estimation of parameters for each soil sample; based on data set of Kueper and Frind (1991b)

<table>
<thead>
<tr>
<th></th>
<th>mean</th>
<th>$b_i$</th>
<th>$\sigma_{b_i}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F$ (ln cm$^2$)</td>
<td>-16.4</td>
<td>-</td>
<td>0.35</td>
</tr>
<tr>
<td>$B$</td>
<td>10.4</td>
<td>-1.03</td>
<td>0.11</td>
</tr>
<tr>
<td>$L$</td>
<td>1.51</td>
<td>-0.83</td>
<td>0.17</td>
</tr>
</tbody>
</table>

The first and second derivatives of $R_o$ needed for estimation of the effective properties are plotted in Figure 3-1 versus a normalized mean capillary pressure, $\hat{P}_c = \frac{P}{\exp \bar{B}}$, where for $\alpha_g$, the geometric mean of a log normal $\alpha$ field, $\alpha_g = 1/\exp \bar{B}$ and $\hat{P}_c = \alpha_g \hat{P}_c$. The top row contains partial first derivatives of $R_o$ with respect to $\hat{P}_c (= \alpha_g \hat{P}_c)$, $B$, $L$, and $F$ respectively. The next three rows are plots of the second derivatives of the same quantities where the row and column heading indicate with respect to which variables the derivatives were evaluated. Second derivatives taken with respect to $F$ and any other input parameter are equal to zero and therefore are not shown.

Figure 3-2 shows the field scale capillary pressure-saturation retention curve for the partially stratified cases, the perfectly stratified case, and a homogeneous mean condition denoted $S_e (\bar{\Gamma})$; the labels in Figure 3-2 indicate the ratio, $\xi_2/\xi_1$ of horizontal correlation scale to vertical correlation scale. The perfectly stratified case is evaluated using the results of the Chapter 4 for the condition of static wetting phase. There is a minor increase in the magnitude of the capillary pressure-saturation curve slope for the heterogeneous cases, relative to that of the homogeneous case. The figure was replotted in log-log coordinates in Figure 3-3 to accentuate the differences between the field scale moisture retention at different horizontal scale values. The field scale normalized saturation is shifted to the right (greater wetting phase saturation for a given capillary pressure) relative to the homogeneous case, a trend that increases with increasing horizontal correlation scale. This issue is revisited in Chapter 6, where the mean capillary pressure-saturation curve is estimated for the Cape Cod Aquifer and its significant features identified and explained.

From Section 2.4.2 we note that a second order estimate of the mean saturation is

$$
\bar{S}_e = S_e (\bar{\Gamma}) + \frac{E \left[ \gamma_i' \gamma_j' \right]}{2} \frac{\partial^2 S_e}{\partial \Gamma_i \partial \Gamma_j} (3.24)
$$
Contributions to the deviation of the mean saturation from the homogeneous, mean parameter result are given by
\[ S_{i,j} = \frac{(2 - \xi_i\eta_j)}{2} \mathbb{E} \left[ \gamma_i^j \gamma_j^i \right] \frac{\partial^2 S_e}{\partial \Gamma_i \partial \Gamma_j} \]
where \( \tilde{S}_e = S_e (\tilde{\Gamma}) + \sum_{i=1}^{n} \sum_{j=1}^{n} S_{i,j} \). Figure 3-4 shows a plot of \( S_e (\tilde{\Gamma}) \) and \( S_{i,j} \), where the curves at any given capillary pressure sum to the mean normalized saturation. At low capillary pressures, all values of \( S_{i,j} \) are small relative to \( S_e (\tilde{\Gamma}) \). Around \( P_c \alpha_g = 1 \) there are significant contributions to \( \tilde{S}_e \) for all values of \( i, j \). At high capillary pressures, only the contribution from \( \sigma_{P_c}^2 \) persists, which is responsible for the high mean \( P_c \) shift seen in the log-log plot of the mean capillary pressure-saturation curve in Figure 3-3.

Figure 3-5 shows the normalized capillary pressure standard deviation versus the normalized mean capillary pressure for the same range of horizontal-vertical correlation scale ratios. Note that the capillary pressure standard deviation increases with increasing scale ratios (i.e., increasing stratification) for normalized capillary pressures exceeding one, and that the perfectly stratified case represents a limiting maximum standard deviation for all the curves. The same feature appears in the case of the wetting phase under these flow conditions (Yeh, 1985c) and may be thought of as the impact of low permeability layers of infinite lateral extent which permit greater variability in the capillary pressure, which would otherwise dissipate in a less than perfectly stratified system.

The effective relative permeability is plotted on both log and linear scales versus the normalized mean capillary pressure in Figure 3-6 for the same range of correlation scales encountered in Figures 3-2, 3-3 and 3-5. Figure 3-6 also shows the relative permeability value for the zero variance case, \( \exp \left( R (\tilde{\Gamma}) - \bar{R} \right) \), which exceeds the vertical relative permeability for all correlation scales and is approached by the nearly isotropic case of \( \xi_2 / \xi_1 = 2 \) for low capillary pressure (i.e., low nonwetting phase saturation). In aquifers which are less than perfectly stratified, flow may bypass low permeability units and the effective permeability becomes a complex function of the pattern of flow; however in a perfectly stratified aquifer flow must pass through units of extremely low permeability. Therefore the perfectly stratified aquifer represents a lower bound to the effective vertical permeability. By visual inspection, it may be concluded that the effective permeability estimated for the perfectly stratified aquifer provides a reasonably good approximation for aquifers with correlation scale ratios of approximately ten or more.
Figure 3-1: First and second partial derivatives of $R_o$ with respect to $\hat{P}_c = \alpha_g \hat{P}_c$, $B$, $L$, and $F$ versus normalized capillary pressure $\hat{P}_c$ for base case, Borden Aquifer, van Genuchten characterization.
Figure 3-2: Mean capillary pressure-saturation curve for horizontal-vertical correlation scale ratio between 2 and ∞ and mean capillary pressure versus homogeneous saturation with mean input variable values, $S_e\left(\bar{r}\right)$, for the base case Borden Aquifer, van Genuchten characterization; where vertical correlation scale held constant at 18 cm.
Figure 3-3: Mean capillary pressure-saturation curve for horizontal-vertical correlation scale ratio between 2 and $\infty$ and mean capillary pressure versus homogeneous saturation at mean input values, $S_e(\bar{\Gamma})$, for the base case Borden aquifer variable slope, van Genuchten characterization; where vertical correlation scale held constant at 18 cm.
Figure 3-4: Contributions, $S_{ij}$, to mean value of $S_r$ versus normalized mean capillary pressure for perfectly stratified condition with base case, Borden, van Genuchten characterization.
Figure 3-5: Normalized capillary pressure standard deviation versus normalized mean capillary pressure for horizontal-vertical correlation scales ranging between 2 and $\infty$, for base case, Borden aquifer, van Genuchten characterization; where vertical correlation scale held constant at 18 cm.
Figure 3-6: Normalized effective permeability perpendicular to flow and $\frac{k_{s}(f)}{\exp(F)}$ for uniform, vertical gravity flow ($\delta_{p} = 0.6$) with horizontal-vertical correlation scales between 2 and $\infty$, $\xi_{1} = 18$ cm and base case, Borden Aquifer, van Genuchten characterization.
3.2.2 Analysis of Steady State Relative Permeability Measurements

Velocity dependence of the effective relative permeability was found in numerical investigations by Dale et al. (1997) in simulations of one-dimensional, horizontal flow in spatially variable, periodic media. A negative correlation was observed between the capillary number and the nonwetting phase effective permeability for a given mean saturation where the total flow rate is held constant for any given value of $Ca$. The capillary number was defined as

$$Ca = \frac{q_t \mu d}{\sigma \sqrt{k_h n}}$$  \hspace{1cm} (3.25)

where

- $d$ = aquifer periodicity wave length ($L$)
- $\sigma$ = interfacial tension ($M/T^2$)
- $k_h$ = harmonic mean of the intrinsic permeability ($L^2$)
- $n$ = mean porosity
- $\mu$ = fluid viscosity ($M/L/T$, taken in simulations to be equivalent for both phases)
- $q_t$ = total specific discharge ($= q_w + q_o$), ($L/T$)

The effective permeability values were found to be bracketed by curves associated with extreme values of the capillary limit, whereby the maximum nonwetting phase permeabilities are found at the viscous limit ($Ca \gtrless 100$) and the minimum values found at the capillary limit ($Ca \lesssim 1$).

Several approaches were pursued herein to investigate the velocity dependence of effective properties as commonly encountered in relative permeability measurements. First effective properties were evaluated with soil properties selected to approximate the system simulated by Dale et al.. The $Ca$ was modified by changing the total discharge so as to observe the approach to the viscous and capillary limits with a correlation scale perpendicular to the flow 1000 times the correlation scale in the direction of flow.

Secondly, an evaluation was performed of velocity dependence in relative permeability measurements for an estimate of the core scale heterogeneity of Borden Aquifer soils. Demond and Roberts (1993) measured the relative permeability in organic compound-water systems where
the flow in the 7 cm long, 5.2 cm diameter permeameter device was maintained at 2.5 ml/min (specific discharge of 0.0020 cm/s). As is typical in measurements of this type, the samples are originally saturated with water and the flow of nonwetting phase increased gradually to increase the nonwetting phase volumetric content, while maintaining a constant total flow. This continues until measurable rates of water flow cease and the wetting phase saturation at this point is reported as the residual wetting phase saturation. The nonwetting phase permeability at the residual wetting phase saturation is sometimes referred to as the end point permeability. Typically end point permeabilities are on the order of 0.3 to 0.4 of the intrinsic permeability, as reported by Demond and Roberts (1993), Lin et al. (1982), Wilson et al. (1990). Demond and Roberts in one case increased the flow rate by a factor of three causing the end point permeability to increase from 0.38 to 0.70, while reducing the residual saturation from 0.086 to 0.021.

Estimation of the effective permeability for a given mean capillary pressure and total flow rate was found by a simple iterative procedure in which a first guess of the pressure gradient was used to solve for the effective permeability in the two phases. Then the pressure gradient was estimated for the computed effective permeability and specified flow and the process repeated until the difference in pressure gradient between sequential iterations falls below a specified tolerance.

**Approximation of Dale et al. Simulated System.** The p-s-k characterization used by Dale et al. is defined over a limited capillary pressure range, so a van Genuchten characterization was instead adopted. The Leverett scaling relationship was invoked using the standard technique, whereby the slope parameter variance is set to zero and the local log characteristic pressure is a deterministic linear function of the local natural log of the intrinsic permeability. The correlation scale in the direction of flow set to 10 cm and was used in place of the periodicity wavelength in estimation of $Ca$. The PCE-water interfacial tension of $\sigma = 45$ dynes/cm was adopted for use in the simulations.

Figure 3-7 shows the effective permeability versus mean normalized wetting phase saturation for $Ca$ between 0.0016 and 16 under the specified conditions. Note that there is a well defined limit to the effective permeability for high values of $Ca$ (i.e., at the viscous limit), but that the stochastic analysis does not produce a recognizable capillary limit at low $Ca$. Moreover
Table 3.2: van Genuchten parameter moments for estimation of effective properties to approximate Dale et al (1997) system

<table>
<thead>
<tr>
<th>Parameter</th>
<th>mean</th>
<th>b_i</th>
<th>σ_{g_i}</th>
</tr>
</thead>
<tbody>
<tr>
<td>F (ln σm^2)</td>
<td>-16.4</td>
<td>-</td>
<td>1.9</td>
</tr>
<tr>
<td>B</td>
<td>10.4</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>L</td>
<td>0.5</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

the nonwetting phase and wetting phase permeability values at the lowest tested capillary number, Ca = 0.0016, are nonmonotonic with respect to the mean normalized saturation. It is unlikely that this type of nonmonotonic behavior represents a physical behavior since it implies a reduction in permeability with increasing saturation. More likely it is the case that the nonmonotonic behavior is the result of the omission of higher order terms from the analysis. The effective permeability curves do demonstrate the principal features found in the effective permeability estimates of Dale et al. including:

1. downward shift of the nonwetting phase permeability for low capillary number flow

2. downward shift of the wetting phase effective permeability for low capillary number flow at low mean \( \bar{S}_e \)

3. upward shift of the wetting phase effective permeability for low capillary number flow at high mean \( \bar{S}_e \)

Extremely low nonwetting phase effective permeabilities are observed for low capillary number flow, \( Ca < 0.016 \), with normalized wetting phase saturation values short of one. The effective permeability for \( Ca = 0.016 \) for example is four orders of magnitude below the intrinsic permeability for a mean normalized wetting phase saturation of 0.8. The implication is that for flow near the capillary limit through a stratified system, the effective permeability falls to such low values that the wetting phase saturation might for all practical gradients and time frames be considered to be at a residual value. The same feature occurs for the wetting phase permeability where for example at \( Ca = 0.016 \) the wetting phase permeability is four orders of magnitude below the intrinsic permeability at a normalized wetting phase saturation greater than 0.3.

The reduction of the wetting phase effective permeability at high capillary pressure may
be responsible for the reported end-point permeabilities short of the intrinsic permeability. If one were to adopt the premise that the drainage phase of the relative permeability experiment would cease when the wetting phase permeability fell to a value one percent of the intrinsic permeability, then the measured end point nonwetting phase relative permeability and measured residual saturation would be the values corresponding to this wetting phase permeability. The lowermost of the horizontal dashed lines in Figure 3-7 indicates the permeability which is one percent of the intrinsic permeability. The intersection of this dashed line and the permeability curves identifies the mean normalized wetting phase saturation at which this postulated end point permeability is reached for a given capillary number. Finally, the nonwetting phase end point permeability may be found by noting the nonwetting phase permeability at this mean wetting phase saturation for the capillary number of concern.

The one percent wetting phase relative permeability is reached for the viscous limit case, \( Ca = 1.6 \), at approximately \( \bar{S}_e \approx 0.3 \), while for \( Ca = 0.016 \) it is reached at \( \bar{S}_e \approx 0.55 \). The approximate corresponding end-point nonwetting phase effective permeabilities are \( 1.5 \times 10^{-8} \text{cm}^2 \) for the viscous limit and \( 3 \times 10^{-9} \text{ cm}^2 \) for \( Ca = 0.016 \) – an increase in end point, nonwetting phase permeability of approximately 5 times.

**Borden Aquifer Relative Permeability Measurements.** Effective permeabilities were estimated for the base case, Borden aquifer, van Genuchten characterization with variable slope parameter (see Table 3.1), for correlation scales in the direction of flow of 0.2 cm. The small correlation scale was selected on the assumption that features at this scale are inadvertently introduced by the permeameter packing procedure. Figure 3-8 shows the effective wetting and nonwetting phase permeabilities plotted versus the mean saturation for \( Ca \) between 0.00016 and 16. At the original discharge rate of Demond and Roberts, the capillary number value is \( Ca = 0.00056 \). Increasing the rate of flow by a factor of three, as Demond and Roberts did in the experiment described, does not significantly change the "end point" saturation. The effective end point permeability does, however, nearly double between the flow regimes.

Whether or not the end-point saturation and permeability dependence on velocity may in this case be attributed to heterogeneity is inconclusive. The direction of both saturation and permeability dependence is consistent with that observed by Demond and Roberts, however the magnitude of the measured response is greater than predicted for the characterization as
Figure 3-7: Effective permeability versus mean normalized saturation for uniform mean, horizontal flow with Capillary number, \( C_a = \frac{q u x f}{\sigma \sqrt{k_0 n}} \), ranging between .0016 and 16.0 with conditions similar to tested system of Dale et al and 50 to 1 vertical-horizontal correlation scale ratio.
described. It may be that the heterogeneity has not been well characterized in this instance, that the impact of heterogeneity is not approximated well near the limiting conditions, or that heterogeneity is only one of several factors causing the velocity dependence; other factors might be caused by the dynamics of drainage which are not represented in the steady state analysis.

3.3 Summary

Analytical expressions are presented for effective properties in the case of uniform mean flow parallel to the principal aquifer axes. Using Borden Aquifer property moments as estimated in Chapter 6, the effective properties are evaluated for vertical mean uniform flow through static water, including the mean capillary pressure-saturation function, the standard deviation of the capillary pressure, and the effective permeability. These are contrasted with the homogeneous, mean parameter property values so as to understand the type of errors that occur when the p-s-k functions are evaluated at the mean parameter values and represented as field scale properties.

The mean saturation of the Borden Aquifer is greater than the homogeneous saturation at high capillary pressure, suggesting the presence of an effective wetting phase residual. The vertical effective permeability is found to converge to that of the perfectly stratified aquifer for correlation scale ratios exceeding 10, demonstrating that the vertical effective permeability may be approximated by the perfect stratification simplifications.

Effective permeabilities were estimated for horizontal, core scale systems of the type in which relative permeability measurements are generally performed. The results support the premise that the effective permeabilities are a function of the flow velocity as measured by the capillary number, an indicator of the ratio of viscous to capillary forces. Further, the end point permeability of the nonwetting phase and the end point saturation are also velocity-dependent in a manner which at least qualitatively matches experimental evidence.
Figure 3-8: Effective permeability versus mean normalized saturation for uniform horizontal flow subject to range of Capillary number, $Ca = \frac{\mu u L}{\alpha \sqrt{k_{s,n}}}$, between 0.00016 and 16, with van Genuchten, Leverett scaling, Borden aquifer conditions, and horizontal/vertical correlation scales of 0.2 cm and 20 cm.
Chapter 4

Effective Properties - Stratified Aquifer

4.1 Introduction

The results of Chapter 3 are based on the assumption of uniform flow in the direction of one of the principal axes. This enabled analytical evaluation of the cross-spectra and the evaluation of the effective property functions. In this chapter, the aquifer is assumed to be perfectly stratified. That is bedding is of infinite horizontal extent aligned with the horizontal axes. The conditions of uniformity and flow in the direction of the principal axes are however relaxed. The first section presents the derivation of cross products for the general, perfectly stratified aquifer condition. The next section presents the same with the additional condition of a static wetting phase and uniform mean condition. Effective properties are then evaluated for the Borden aquifer and selective modifications of this restricted case.

4.2 Cross Products

The effective properties found for the general condition as presented in Chapter 2 are in this case adapted by assigning an infinite correlation scale length in two directions ($\xi_2$ and $\xi_3$). Making the substitution for the wave number $\omega_i = \frac{2\pi}{\xi_i}$ one finds that dot products with $\omega$ are reduced to only the components aligned with the direction perpendicular to the plane for which
the correlation scales are infinite. The moment expressions are reduced to forms for which analytical evaluation of the integrals is possible.

The quantities \( Y_m, X_{c,\beta}, \) and \( X_{t,\beta}, \) defined in (2.93) and (2.100), under these conditions may be written as:

\[
Y_m = \left[ -u_1^2 \xi_1 \left( J_o \frac{\partial^2 R_o(\tilde{\Gamma})}{\partial \Phi_m \partial P_c} - J_w \frac{\partial^2 R_w(\tilde{\Gamma})}{\partial \Phi_m \partial P_c} \right) \cdot \nabla \tilde{P}_c \right] - \frac{\partial \tilde{P}_c}{\partial x_1} u_1^2 \xi_1^2 \left( J_o \frac{\partial R_o(\tilde{\Gamma})}{\partial \Phi_m} \frac{\partial R_w(\tilde{\Gamma})}{\partial P_c} - J_w \frac{\partial R_w(\tilde{\Gamma})}{\partial \Phi_m} \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} \right) + i \left( -u_1^2 \xi_1 \left( \frac{\partial R_o(\tilde{\Gamma})}{\partial \Phi_m} \frac{\partial R_w(\tilde{\Gamma})}{\partial P_c} - J_w \frac{\partial R_w(\tilde{\Gamma})}{\partial \Phi_m} \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} \right) \cdot \nabla \tilde{P}_c \right] \left( u_1^3 + iu_1^2 \xi_1 \left( -\frac{\partial R_w(\tilde{\Gamma})}{\partial x_1} + J_w \right) - \frac{\partial R_o(\tilde{\Gamma})}{\partial x_1} \left( \frac{\partial \tilde{P}_c}{\partial P_c} - J_o \right) \right) + u_1^2 \xi_1 \left( J_o \frac{\partial^2 R_o(\tilde{\Gamma})}{\partial P_c^2} - J_w \frac{\partial^2 R_w(\tilde{\Gamma})}{\partial P_c^2} \right) \cdot \nabla \tilde{P}_c + u_1^2 \xi_1 \left( J_o - J_w \right) \frac{\partial \tilde{P}_c}{\partial x_1} \frac{\partial R_o(\tilde{\Gamma})}{\partial x_1} \frac{\partial R_w(\tilde{\Gamma})}{\partial P_c} + i \frac{\partial \tilde{P}_c}{\partial x_1} \xi_1 \left( J_w \frac{\partial^2 R_w(\tilde{\Gamma})}{\partial P_c^2} - J_o \frac{\partial^2 R_o(\tilde{\Gamma})}{\partial P_c^2} \right) \cdot \nabla \tilde{P}_c \right]^{-1}.
\]

\[
X_{c,\beta} = \frac{-\xi_1^2 \frac{\partial^2 R_o(\tilde{\Gamma})}{\partial P_c^2} J_o \cdot \nabla \tilde{P}_c - iu_1 \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} \xi_1}{u_1^2 - i \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} - u_1 \xi_1 \frac{\partial \tilde{P}_c}{\partial x_1}}.
\]

\[
X_{t,\beta} = \frac{-\xi_1^2 \frac{\partial^2 R_o(\tilde{\Gamma})}{\partial P_c^2} J_o \cdot \nabla \tilde{P}_c - iu_1 \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} \xi_1}{u_1^2 - i \frac{\partial R_o(\tilde{\Gamma})}{\partial P_c} - u_1 \xi_1 \frac{\partial \tilde{P}_c}{\partial x_1}}.
\]

Define \( C_1, C_2, \ldots, C_{11} \) based on (4.1) and (4.2)

\[
Y_m = \frac{iu_1^2 C_{1,m} + u_1 C_{2,m} + iC_{3,m}}{u_1^3 + iu_1^2 C_4 + u_1 C_5 + iC_6}.
\]
\[ X_{c,\beta} = \frac{(C_7 + iu_1 C_8)}{u_1^2 + iu_1 C_9} \]  \hspace{1cm} (4.4)

\[ X_{i,\beta} = \frac{C_{10,i} + iu_1 C_{11,i}}{u_1^2 + iu_1 C_9} \]

The spectral functions are found by substituting \( Y_m, X_{c,\beta}, X_{i,\beta} \) and the spectral function of the independent variables \( g_i^j \) into equations (2.95), (2.97), (2.104) and (2.106). For an exponential correlation function

\[ S_{g_i,g_i} = \frac{\sigma_{g_i}^2 \xi_1 \xi_2 \xi_3}{\pi^2 \left( 1 + (\xi_1 \omega_1)^2 + (\xi_2 \omega_2)^2 + (\xi_3 \omega_3)^2 \right)} \]  \hspace{1cm} (4.5)

Then the mean cross products are evaluated by the integration of the cross-spectra as in (2.35)

Noting that (see Appendix B.5)

\[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{du_2 du_3}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} = \frac{1}{\pi (1 + u_1^2)} \]  \hspace{1cm} (4.6)

the \( \text{cov}(P_c, \Phi_i) \) and \( \sigma_{p_c}^2 \) are

\[ \text{cov}(P_c, \Phi_i) = \int_{-\infty}^{\infty} \left( b_i b_m \sigma_{f_i}^2 + \delta_{i,m} \sigma_{g_i}^2 \right) \frac{1}{\pi (1 + u_1^2)} \frac{u_1^4 (C_4 C_{1,m} + C_{2,m}) + u_1^2 (C_6 C_{1,m} + C_4 C_{3,m} + C_5 C_{2,m}) + C_6 C_{3,m}}{(u_1^6 + u_1^4 (C_4^2 + 2C_5) + u_1^2 (C_5^2 + 2C_4 C_6) + C_6^2)} du_1 \]  \hspace{1cm} (4.7)

\[ \sigma_{p_c}^2 = \left( b_i b_m \sigma_{f_i}^2 + \delta_{i,m} \sigma_{g_i}^2 \right) \int_{-\infty}^{\infty} \frac{u_1^4 C_{1,m} C_{1,i} + u_1^2 (C_{2,m} C_{2,i} + C_{1,m} C_{3,i} + C_{1,i} C_{3,m}) + C_{3,m} C_{3,i}}{\pi (1 + u_1^2) (u_1^6 + u_1^4 (C_4^2 + 2C_5) + u_1^2 (C_5^2 + 2C_4 C_6) + C_6^2)} du_1 \]  \hspace{1cm} (4.8)

where the closed form solution of integrals of this form is given in Appendix B.6.

In order to evaluate \( \text{cov}(J_{\beta}, \Phi_i) \)

\[ \text{cov}(J_{\beta}, \Phi_i) = -\int \int \int \frac{i\omega \left( b_i b_m \sigma_{f_i}^2 + \delta_{i,m} \sigma_{g_{2m}}^2 \right)}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} \left( X_{c,\beta} Y_m + X_m \right) du_1 du_2 du_3 \]  \hspace{1cm} (4.9)
Consider first the expression

\[ i\omega (X_{c,\beta} Y_m + X_m) = \frac{i\omega u_1^2 C_{1,m} + u_1 C_{2,m} + i C_{3,m} (C_7 + i u_1 C_8)}{u_1^2 + i u_1^2 C_4 + u_1 C_5 + i C_6} \left( \frac{1}{u_1^2 + i u_1 C_9} \right) \]

(4.10)

+ \frac{i\omega C_{10,m} + i u_1 C_{11,m}}{u_1^2 + i u_1 C_9}

Eliminate all complex components from the denominator by multiplying the numerator and denominator by the complex conjugate of the denominator

\[ i\omega (X_{c,\beta} Y_m + X_m) = \frac{i\omega}{u_1 (u_1^2 + C_9^2)} \]

\[ \left[ u_1^4 (C_4 C_{1,m} + C_{2,m}) + i u_1^3 (C_1,m C_5 - C_{2,m} C_4 + C_{3,m}) \right. \]

\[ + u_1^2 (C_6 C_{1,m} + C_4 C_{3,m} + C_5 C_{2,m}) \]

\[ + i (C_5 C_{3,m} - C_6 C_{2,m}) + C_6 C_{3,m} \]

\[ \left. \frac{C_7 + i u_1 C_8}{(u_1^2 + C_9^2 + 2 C_5) + u_1^2 (C_8^2 + 2 C_4 C_6) + C_6^2} \right] \]

\[ + i\omega \left( \frac{C_{10,m} + i u_1 C_{11,m}}{u_1 (u_1^2 + C_9^2)} \right) \]

(4.11)

Substitute \( \frac{\omega}{\xi_1} \) for \( \omega \) and eliminate all odd components which will integrate to zero; the latter is equivalent to maintaining only the real components so that

\[ \text{Re} \left[ i \frac{u_1}{\xi_1} (X_{c,\beta} Y_m + X_m) \right] = \left[ (u_1^2 C_8 - C_7 C_9) u_1^4 (C_4 C_{1,m} + C_{2,m}) \right. \]

\[ + u_1^2 (C_6 C_{1,m} + C_4 C_{3,m} + C_5 C_{2,m}) + C_6 C_{3,m}) \]

\[ - (C_7 + C_8 C_9) u_1^4 (C_{1,m} C_5 - C_{2,m} C_4 + C_{3,m}) \]

\[ + u_1^2 (C_5 C_{3,m} - C_6 C_{2,m})) \right] \]

\[ \frac{1}{(u_1^2 + C_9^2) (u_1^2 + u_1^4 (C_2^2 + 2 C_5) + u_1^2 (C_9^2 + 2 C_4 C_6) + C_6^2)} \frac{1}{\xi_1} \]

\[ \frac{1}{\xi_1} \left( \frac{C_{11,m} - C_9 C_{10,m}}{u_1^2 + C_9^2} \right) \]

(4.12)
while
\[
\text{Re} \left[ \frac{u_2}{\xi_2} (X_{c,\beta} Y_m + X_m) \right] = \text{Re} \left[ \frac{u_3}{\xi_3} (X_{c,\beta} Y_m + X_m) \right] = 0 \tag{4.13}
\]

Now substitute the result back into (4.9) and carry out the trivial integrals with respect to \(u_2\) and \(u_3\). Therefore
\[
\text{cov}(J_{\beta,1}, \Phi_1) = -(b_m b_1 \sigma_f^2 + \delta_{i,m} \sigma_g^2) \int_{-\infty}^{\infty} \frac{1}{\pi (1 + u_1^2)} \frac{1}{(u_1^2 C_8 - C_7 C_9)} \left[ (u_1^2 C_8 - C_7 C_9) \right. \\
\left. + (u_1^4 (C_4 C_{1,m} + C_{2,m}) + u_1^2 ((C_6 C_{1,m} + C_4 C_{3,m} + C_5 C_{2,m}) + C_6 C_{3,m}) \\
- (u_1^4 (C_{1,m} C_5 - C_{2,m} C_4 + C_{3,m}) + u_1^2 (C_6 C_{3,m} - C_6 C_{2,m}) \right) (C_7 + C_8 C_9) \\
\frac{1}{(u_1^2 C_4^2 + 2 C_8) + u_1^2 (C_4^2 + 2 C_4 C_6 + C_6^2)} du_1 \\
+ (b_m b_1 \sigma_f^2 + \delta_{i,m} \sigma_g^2) \int_{-\infty}^{\infty} \frac{1}{\pi (1 + u_1^2)} \frac{(u_1^2 C_{11,m} - C_9 C_{10,m})}{\xi_1 (u_1^2 + C_8)} du_1
\]

and
\[
\text{cov}(J_{\beta,2}, \Phi_1) = \text{cov}(J_{\beta,3}, \Phi_1) = 0 \tag{4.15}
\]

where the closed form solutions of integrals of this form are given in Appendices B.7 and B.8.

Finally, consider evaluation of \(\text{cov}(J_{\beta}, P_c)\) by substitution of (2.106) into (2.35)
\[
\text{cov}(J_{\beta}, P_c) = -\int \int \int \frac{i \omega (b_m b_1 \sigma_f^2 + \delta_{i,m} \sigma_g^2)}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} (X_{c,\beta} Y_m Y_i^* + X_{m,\beta} Y_i^*) du_1 du_2 du_3 \tag{4.16}
\]

Substitute (4.3) and (4.4) into (4.16), simplify and eliminate the odd components of
\(-i \omega (X_{c,\beta} Y_m Y_i^* + X_{m,\beta} Y_i^*)\) and then evaluate the resulting integral. Consider first \(-i \omega X_{c,\beta} Y_m Y_i^*\).

\[
-i \omega X_{c,\beta} Y_m Y_i^* = -i \omega \left( \frac{i u_1^2 C_{1,m} + u_1 C_{2,m} + i C_{3,m}}{u_1^3 + i u_1^2 C_4 + u_1 C_5 + i C_6} \right) \frac{(C_7 + i u_1 C_8)}{u_1^2 + i u_1 C_9} \left( \frac{u_1^3 - i u_1^2 C_4 + u_1 C_5 - i C_6}{u_1^3 + i u_1^2 C_4 + u_1 C_5 + i C_6} \right) \tag{4.17}
\]

Substitute \(u_n = \omega_n \xi_n\), simplify and eliminate the odd components so that
\[
\text{Re} [-i\omega_1 X_{c,\beta} Y_m Y_i^*] = \frac{1}{\xi_1} \left[ \left( u_1^2 C_8 - C_7 C_9 \right) \left( u_1^2 C_{1,1} + C_{3,1} \right) \left( u_1^2 C_{1,m} + C_{3,m} \right) + u_1^2 C_{2,m} C_{2,i} \right] + u_1^2 \left( \left( u_1^2 C_{1,1} + C_{3,1} \right) C_{2,i} + \left( u_1^2 C_{1,m} + C_{3,m} \right) C_{2,m} \right) \left( C_{7} + C_{8} C_{9} \right) \left( \frac{1}{u_1^2 + C_9^2} \right) \left( \frac{u_1^8 + u_1^4 \left( C_4^2 + 2C_5 \right) + u_1^2 \left( C_5^2 + 2C_4 C_6 \right) + C_6^2}{u_1^4 + C_9^2} \right)
\]

and

\[
\text{Re} [-i\omega_2 X_{c,\beta} Y_m Y_i^*] = \text{Re} [-i\omega_3 X_{c,\beta} Y_m Y_i^*] = 0
\]

Simplify the expression \(-i\omega X_{m,\beta} Y_i^*\) from (4.16) where

\[
-i\omega X_{m,\beta} Y_i^* = -i\omega \left( \frac{-iu_1^2 C_{1,1} + u_1 C_{2,1} - iC_{3,1}}{u_1^3 - iu_1^2 C_4 + u_1 C_5 - iC_6} \right) \left( \frac{C_{10,m} + iu_1 C_{11,m}}{u_1^2 + iu_1 C_9} \right)
\]

Substitute \(u_n = \omega_n \xi_n\) simplify and eliminate the odd components so that

\[
\text{Re} [-i\omega_1 X_{m,\beta} Y_i^*] = -\frac{1}{\xi_1} \left[ \left( u_1^3 + u_1 C_5 \right) u_1 + \left( u_1^2 C_4 + C_6 \right) C_9 \right] \left( u_1^2 C_{1,1} + C_{3,1} \right) C_{10,m} - u_1^2 C_{2,m} C_{11,m} \right] \left( \frac{1}{u_1^2 + C_9^2} \right) \left( \frac{u_1^8 + u_1^4 \left( C_4^2 + 2C_5 \right) + u_1^2 \left( C_5^2 + 2C_4 C_6 \right) + C_6^2}{u_1^4 + C_9^2} \right)
\]

\[
\text{Re} [-i\omega_2 X_{m,\beta} Y_i^*] = \text{Re} [-i\omega_3 X_{m,\beta} Y_i^*] = 0
\]

To evaluate \(\text{cov}(J_{\beta,1}, P_c)\), substitute (4.18) and (4.20) into (4.16) and rearrange into the following form where the closed form solution of this integral is given in Appendix B.

\[
\text{cov}(J_{\beta,1}, P_c) = \int \int \int \frac{\left( a_7 u_1^6 + a_8 u_1^4 + a_9 u_1^2 + a_{10} \right) du_1 du_2 du_3}{\pi^2 \left( a_1 u_1^6 + a_2 u_1^4 + a_3 u_1^2 + a_4 \right) \left( a_5 u_1^2 + a_6^2 \right) \left( 1 + u_1^2 + u_2^2 + u_3^2 \right)^2}
\]

and

\[
\text{cov}(J_{\beta,2}, P_c) = \text{cov}(J_{\beta,3}, P_c) = 0
\]
4.3 Uniform System with Static Wetting Phase

The cross-products and the effective permeability are evaluated in this section for the case of a perfectly stratified aquifer, uniform mean flow ($\nabla P_c = 0$), static wetting phase ($J_w = 0$), and vertical mean nonwetting phase flow ($\bar{J}_{o,2} = \bar{J}_{o,3} = 0$). Under these conditions, which combine the restrictive conditions of both Chapter 3 (flow aligned with principal axes) and Chapter 4 (perfect stratification), the cross-products reduce to relatively simple forms in which the dependencies on input parameters may be easily determined.

To find the $\text{cov}(P_c, \Phi_i)$ under these more restrictive conditions, take the limit of $\text{cov}(P_c, \Phi_i)$ in (3.7) as $\rho \to \infty$, set $\bar{J}_w = 0$. Alternatively, one might set $\bar{J}_{o,2} = \bar{J}_{o,3} = 0$ and $\nabla \bar{P}_c = 0$ in (4.7). Recognizing the solution of integrals from Appendix B

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{du_2 du_3}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} = \frac{1}{\pi (1 + u_1^2)}$$

and

$$\int_{-\infty}^{\infty} \frac{1}{\pi (1 + u_1^2) (u_1^2 + A^2)} du_1 = \frac{1}{(1 + |A|)|A|}$$

the covariance is given by

$$\text{cov}(P_c, \Phi_i) = (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_{g_i}^2) \frac{-\xi_2^2 J_{o,1} \frac{\partial R_a}{\partial \Phi_i} \frac{\partial R_a}{\partial \Phi_m}}{|\varepsilon| (|\varepsilon| + 1)}$$

(4.23)

$$= - (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_{g_i}^2) \frac{\partial R_a}{\partial \Phi_i} \frac{\partial R_a}{\partial \Phi_m} (|\varepsilon| + 1)$$

(4.24)

where $\varepsilon = \xi_1 \bar{J}_{o,1} \frac{\partial R_a}{\partial P_c}$ and $\bar{J}_{o,1} = -\delta \rho g$. By the same reasoning, the limit of the expression (3.9) becomes

$$\sigma_{P_c}^2 = (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_{g_i}^2) \frac{|\varepsilon| \frac{\partial R_a}{\partial \Phi_i} \frac{\partial R_a}{\partial \Phi_m}}{(|\varepsilon| + 1) \left(\frac{\partial R_a}{\partial P_c}\right)^2}$$

(4.25)

The $\text{cov}(J_{o,n}, \Phi_i) = 0$ for $n \neq 1$ while otherwise

$$\text{cov}(J_{o,1}, \Phi_i) = - (b_i b_m \sigma_f^2 + \delta_{i,m} \sigma_{g_i}^2) \int_{-\infty}^{\infty} \frac{1}{\pi (1 + u_1^2)}$$

(4.26)
\[
\begin{align*}
&\left[ J_{o,1} \frac{\partial R_o}{\partial \Phi_m} - \frac{\xi^2 J^3}{(u_1^2 + \left( \xi_1 J_{o,1} \frac{\partial R_o}{\partial \Phi_c} \right)^2)} \right] du_1 \\
&= - (b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2) \int_{-\infty}^{\infty} \frac{1}{\pi (1 + u_1^2)} \frac{u_1^2 J_{o,1} \frac{\partial R_o}{\partial \Phi_m}}{u_1^2 + \left( \xi_1 J_{o,1} \frac{\partial R_o}{\partial \Phi_c} \right)^2} du_1 \\
&= - \left( b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2 \right) \frac{\xi_1 \frac{\partial R_o}{\partial \Phi_m}}{\xi_1 \frac{\partial R_o}{\partial \Phi_c} (|\varepsilon| + 1)} \\
&\quad \quad \quad (4.27)
\end{align*}
\]

From Chapter 3 we know that the \( \text{cov}(J_{o,1}, P_c) = 0 \) for uniform flow along one of the principal axes when the gradient in either phase is zero.

The effective permeability is found by substituting the prior expressions into the general form for the effective permeability (2.49) represented here in its most general form

\[
\hat{k}_n^* = \exp \left\{ R \left( \bar{\Gamma} \right) + \frac{E \left[ \gamma_i \gamma'_j \right]}{2} \left( \frac{\partial R \left( \bar{\Gamma} \right)}{\partial \Gamma_i} \frac{\partial R \left( \bar{\Gamma} \right)}{\partial \Gamma_j} + \frac{\partial^2 R \left( \bar{\Gamma} \right)}{\partial \Gamma_i \partial \Gamma_j} \right) + E \left[ \bar{\gamma}_i \gamma'_j \right] \frac{1}{J_n} \frac{\partial R \left( \bar{\Gamma} \right)}{\partial \Gamma_i} \right\} \\
(4.28)
\]

On substituting (4.25), (4.24) and (4.27) the effective permeability is given by

\[
\hat{k}_n^* = \exp \left\{ R_o \left( \bar{\Gamma} \right) + \frac{(b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2)}{2} \left( \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} + \frac{\partial^2 R_o}{\partial \Phi_i \partial \Phi_j} \right) - \frac{(b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2)}{\xi_1 \frac{\partial R_o}{\partial \Phi_m} (|\varepsilon| + 1)} \left( \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} + \frac{\partial^2 R_o}{\partial \Phi_i \partial \Phi_j} \right) \\
+ \frac{(b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2)}{2 \left( \xi_1 \frac{\partial R_o}{\partial \Phi_c} \right)^2 (|\varepsilon| + 1)} \left( \frac{\partial R_o}{\partial \Phi_c} \frac{\partial R_o}{\partial \Phi_c} + \frac{\partial^2 R_o}{\partial \Phi_c \partial \Phi_c} \right) \\
- \frac{\delta_{i,n} (b_m b_i \sigma_j \sigma_i + \delta_{i,m} \sigma_{g_i}^2)}{J_n} \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_m} \right\} \\
(4.29)
\]
Finally, on simplification the effective permeability reduces to

$$
\hat{k}_n^* = \exp \left\{ R_o (\tilde{\Gamma}) + \left( b_i b_j \sigma_{ij}^2 + \delta_{i,j} \sigma_{g_j}^2 \right) \left[ \frac{1}{2} \frac{\partial^2 R_o}{\partial \Phi_i \partial \Phi_j} + \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} \frac{1 - 2 \delta_{i,n}}{2 (|\varepsilon| + 1)} \right] \right\} - \frac{|\varepsilon|}{2 (|\varepsilon| + 1)} \left( \frac{\partial R_o}{\partial P_c} \right)^2 \left[ \frac{\partial^2 R_o}{\partial \Phi_i \partial \Phi_j} \frac{\partial^2 R_o}{\partial \Phi_i \partial P_c} \frac{\partial^2 R_o}{\partial \Phi_j \partial P_c} - \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} \frac{\partial^2 R_o}{\partial P_c^2} \right] \right\}
$$

(4.30)

The ratio of horizontal-vertical effective permeability \( \frac{k_x}{k_y} \) is given by

$$
A = \exp \left[ \frac{\left( b_i b_j \sigma_{ij}^2 + \delta_{i,j} \sigma_{g_j}^2 \right) \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j}}{(|\varepsilon| + 1)} \right]
$$

(4.31)

where anisotropy is introduced because of the inequality of the covariance of the input variables with the pressure gradient in the directions parallel and perpendicular to stratification. Specifically, \( \text{cov}(J_{i,2}, \Phi_i) = \text{cov}(J_{i,3}, \Phi_i) = 0 \) and \( \text{cov}(J_{i,1}, \Phi_i) \neq 0 \). Since the perturbation of the nonwetting phase permeability at a given capillary pressure (i.e., \( p'_c = 0 \)) is given by \( \tau' = \phi'_t \frac{\partial R_o}{\partial \Phi_t} \), the term in the numerator of the exponential argument, \( \left( b_i b_j \sigma_{ij}^2 + \delta_{i,j} \sigma_{g_j}^2 \right) \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} \) of (4.31), is the variance of the log permeability for a fixed capillary pressure. That is, this term represents the variance of the log permeability sampled over the set of soil samples at a given capillary pressure. The variance is scaled by \( (|\varepsilon| + 1) \) whose physical significance is discussed in the following section.

Similarly, the mean value of \( S_e \) may be found from

$$
\bar{S}_e = S_e (\tilde{\Gamma}) + \frac{1}{2} \frac{\partial^2 S_e}{\partial \tilde{\Gamma}_i \partial \tilde{\Gamma}_j} \mathbb{E} [\gamma'_i \gamma'_j]
$$

(4.32)

or on substitution of the cross products

$$
\bar{S}_e = S_e (\tilde{\Gamma}) \left( \frac{b_i b_j \sigma_{ij}^2 + \delta_{i,j} \sigma_{g_j}^2}{2} \right) \left[ \frac{\partial^2 S_e}{\partial \Phi_i \partial \Phi_j} \right] - \frac{\partial^2 S_e}{\partial \Phi_i \partial P_c} \frac{|\varepsilon|}{\partial \Phi_m} \left( \frac{\partial R_o}{\partial \Phi_m} \right) \frac{\partial^2 S_e}{\partial P_c^2} \left( \frac{|\varepsilon|}{\partial \Phi_c} \right)^2 \left( \frac{|\varepsilon|}{\partial \Phi_c} \right)^2
$$

(4.33)

92
4.4 Evaluation of Effective Properties at Borden Aquifer

Effective properties were evaluated for conditions representing the Borden Aquifer for the perfectly stratified aquifer assumption and

- vertical mean flow
- static wetting phase
- $\delta_p = 0.6 \text{ g/cm}^3$

A detailed description of the data source and its analysis is presented in Chapter 6. The effective properties are estimated for a characterization referred to as the base case characterization of the Borden aquifer, van Genuchten p-s-k function with parameters independently estimated for each of seven soil samples. Then the analogous Brooks-Corey characterization is examined, followed by an evaluation of effective properties where the system is governed by a modified form of Leverett scaling as in Kueper and Frind (1991b). Next, effective properties are estimated for a characterization reflecting the analysis of Kueper and Frind (1991b), with Brooks-Corey p-s-k functions, modified Leverett scaling and an elevated $\ln k$ variance as estimated in former studies of the Borden aquifer permeability field. Lastly, effective properties are evaluated and discussed for a low interfacial tension fluid pair using the otherwise base case stochastic characterization.

4.4.1 Base Case

The effective vertical and horizontal relative permeabilities, $\kappa_v$ and $\kappa_h$, are plotted versus the mean normalized capillary pressure in Figures 4-1a and 4-1b for the Borden Aquifer base case (see Table 4.1) where, as defined in Chapter 2, the relative permeabilities are normalized by dividing by the the saturated, anisotropic effective permeabilities. The capillary pressure is, in this case, normalized by the geometric mean of the inverse characteristic pressure ($\alpha_g = \ln B$) as previously defined in Chapter 2. Also plotted are indicators of the relative permeability of homogeneous media, $\kappa_m$ and $\kappa_g$, defined as
\[
\kappa_m = \exp \left( R \left( \bar{F} \right) - \bar{F} \right)
\]
\[
\kappa_g = \exp \left( \bar{R} - \bar{F} \right)
\]
(4.34)

For all values of \( \bar{F} \), the horizontal relative permeability exceeds the vertical relative permeability. As expected, the effective nonwetting phase permeabilities reduce to the saturated effective permeability solution of Gelhar and Axness (1983) for high capillary pressure values. Additional variability, over and above that of the intrinsic permeability occurs due to the variance of the input properties and the value of the partial derivatives in the form of \( \frac{\partial R_0}{\partial \Phi_i} \frac{\partial R_0}{\partial \Phi_j} \text{cov}(\Phi_i, \Phi_j) \). Sensitivity of the anisotropy on the mean value of the input variables and the mean capillary pressure is induced through their effect on the value of these partial derivatives.

Table 4.1: Moments of transformed van Genuchten parameters for Borden Aquifer base case and alternative characterizations.

<table>
<thead>
<tr>
<th></th>
<th>( F ) (ln cm (^2))</th>
<th>( \sigma_f )</th>
<th>( B ) (ln dynes/cm (^2))</th>
<th>( \sigma_{gb} )</th>
<th>( b_b )</th>
<th>( L )</th>
<th>( \sigma_{gl} )</th>
<th>( b_l )</th>
<th>( \xi_1 ) (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
<td>12</td>
</tr>
<tr>
<td>Increased ( \xi_1 )</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
<td>60</td>
</tr>
<tr>
<td>Increased ( \frac{\partial R_0}{\partial F} )</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>0.00</td>
<td>0.174</td>
<td>-0.83</td>
<td>12</td>
</tr>
</tbody>
</table>

Since a set of relative permeability measurements are not available for the Borden Aquifer soils, the predicted relative permeability curves based on the p-s-k function properties serve in lieu of real relative permeability observations. In order to visualize the variability of the relative permeability between samples, 100 independent random replicates are drawn for the base case van Genuchten, Borden Aquifer p-s-k parameter moments, where the independent random variables \( f' \), \( g'_i \) are assumed to be normally distributed. The properties of a given soil sample, are represented by \( F = \bar{F} + f' \), \( B = B + b_b f' + g'_b \), and \( L = L + b_l f' + g'_l \). The permeability, \( k_o \), at a given capillary pressure is estimated by evaluation of (2.7), (2.9) and (2.10). Figure 4-2a shows the permeability of each of the 100 "samples" as a function of the capillary pressure. Sample statistics, \( \bar{R}_o \) and \( \bar{R}_o \pm 2\sigma_r \) were estimated as a function of capillary pressure for the 100 "samples" and \( \exp \bar{R}_o \), \( \exp (\bar{R}_o \pm 2\sigma_r) \) plotted versus capillary pressure in Figure 4-2b. Approaching a nonwetting phase saturated media, (i.e., high capillary pressures),
Figure 4-1: Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_v$, and homogeneous relative permeability $\kappa_g = \exp (R - \bar{F})$ and $\kappa_m = \exp (R (\bar{\Gamma} - \bar{F})$ versus normalized mean capillary pressure, evaluated for base case, van Genuchten characterization of Borden aquifer with perfect stratification.
the variability is due only to the variability of the intrinsic permeability field, but significantly
greater, pressure dependent variability occurs at lower capillary pressures.

For a normally distributed $R_o$ the quantity $\exp (\bar{R}_o \pm 2\sigma_r)$ would bound 95 percent of the
parent population. That the upper bound exceeds the saturated permeability by approximately
two orders of magnitude for $P_c \approx 25$ cm demonstrates that $R_o$ is not normally distributed and
that the distribution is skewed towards lower permeabilities. The mean value $\exp \bar{R}_o$ does seem
to be a reliable indicator of centrality in the distribution of $R_o$. However, the perturbation
technique which assumes symmetry of the random perturbations, will therefore in the case of
large amplitude variability over estimate the arithmetic mean of the relative permeability.

In order to understand the dependence of anisotropy on the correlation scale and $\frac{\partial R}{\partial \xi}$,
consider vertical one-dimensional flow through a system of homogeneous layers of thickness
equivalent to the vertical correlation scale. Now consider the system behavior at a transition
between layers of contrasting permeability as in Figure 4-3, where a layer of low intrinsic
permeability is sandwiched between layers of greater intrinsic permeability. Moving upward
from the middle unit into the overlying high permeability unit, the permeability is abruptly
increased, while maintaining continuity of the capillary pressure. This corresponds to a jump
from the permeability-capillary pressure curve of the low permeability unit to that of the high
permeability unit as in the transition from state 0 to state 1 shown in Figure 4-3. Continuing to
move upward, within the homogeneous high permeability unit, the capillary pressure and the
nonwetting phase permeability will continue to increase, as the system returns to a uniform,
gravity flow condition (state 1 to state 2) where

$$\frac{\partial P_z}{\partial z} = 0$$

(4.35)

and

$$q_o = -\frac{k_o \delta \rho g}{\mu_o}$$

(4.36)

The asymptotic nonwetting phase permeability, $k_o$, is common to all units regardless of its
intrinsic permeability. Its value depends on only the fluid viscosity, the rate of flow and the
density difference of the two fluids.

The return to gravity flow conditions also occurs in unsaturated flow, where in that case the
Figure 4-2: (a) Synthetic permeability curves based on base case, van Genuchten Borden Aquifer characterization and (b) envelope of permeability variability versus mean capillary pressure defined by \( \exp \left( \bar{K}_c \pm 2\sigma_r \right) \).
Figure 4-3: Nonwetting phase permeability response to abrupt transitions of intrinsic permeability.
system approaches a unit gradient. In the case of multiphase flow with a static wetting phase of not inconsequential density the capillary pressure gradient is given by

\[
\frac{\partial P_c}{\partial z} = -\frac{\mu_o g_o}{k_o} - \delta \rho g
\]  

(4.37)

where for downward flow the first term on the right hand side, \(-\frac{\mu_o g_o}{k_o}\), is positive and the second term, \(-\delta \rho g\), negative. When the first term is greater in magnitude \(\left| \frac{\mu_o g_o}{k_o} \right| > |\delta \rho g|\) then \(\frac{\partial P_c}{\partial z} > 0\), and the nonwetting phase permeability will increase in the upward direction until the two terms equilibrate and the capillary pressure gradient approaches zero. Conversely, when the second term is greater \(\left| \frac{\mu_o g_o}{k_o} \right| < |\delta \rho g|\) the capillary pressure gradient is negative and the nonwetting phase permeability will continue to decrease moving upward in the aquifer, increasing the magnitude of the positive term and returning the capillary pressure gradient to zero.

If we consider the effective permeability to be the harmonic mean of the local permeability over the vertical, it follows that greater uniformity will increase the value of the harmonic mean relative to the effective horizontal permeability, approximated by the arithmetic mean of the local permeability. Increasing the rate at which the system returns to the asymptotic permeability and/or increasing the unit thickness will therefore have the effect of increasing system uniformity and reducing the anisotropy of the effective permeability. The rate at which the permeability approaches its asymptotic value may be found by substituting \(\frac{\partial k_o}{\partial z} \frac{dP_c}{dk_o}\) for \(\frac{\partial P_c}{\partial z}\) in the Darcy equation and solving for \(\frac{\partial k_o}{\partial z}\)

\[
\frac{\partial k_o}{\partial z} = -(q \mu_o + k_o \delta \rho g) \frac{d \ln k_o}{dP_c}
\]  

(4.38)

It is apparent that the return of the permeability to its asymptotic value is proportional to \(\frac{d \ln k_o}{dP_c} = \frac{dR_k}{dP_c}\), so greater values of \(\frac{dR_k}{dP_c}\) will increase system uniformity and reduce anisotropy – consistent with its role in the expression (4.31) for the effective permeability anisotropy ratio. Similar arguments have been made in descriptions of one-dimensional, horizontal flow (Yortsos and Chang, 1990) and vertical flow (Chang et al., 1995a).

In order to illustrate the impact of correlation scale and \(\frac{dR_k}{dP_c}\), effective permeabilities were evaluated for two modifications from the base case condition; in one case the correlation scale
was increased five-fold and in the second case the value of $\frac{\partial R_a}{\partial P_c}$ was increased (for $\alpha_q P_c < 1$) by setting $\bar{L} = 0$ (see Figure 4-4). The parameter statistics for these two cases are presented in Table 4.1. The value of $L$ may be thought of as an indicator of soil uniformity, where by comparison, the mean value for the Hanford site in Washington is −0.52, the mean value of the Maddock sandy loam from Oakes, North Dakota is 0.56 (based on Tse, 1997) and the mean value for soils from the Cape Cod aquifer is 0.53 (based on Mace, 1994). Based on the analysis of the preceding paragraph, each of the modifications should have the effect of reducing the system anisotropy. The ratio, $\frac{k_A}{k_e}$, was plotted versus the mean capillary pressure in Figure 4-5 for the base case condition and for the two modified cases. Note the extreme anisotropic conditions reached by the base case for low capillary pressure (i.e., low nonwetting phase content), while the anisotropy of the modified systems were, as expected, less.

Contributions to anisotropy, $A_{i,j}$, were plotted versus mean capillary pressure for the base case condition in Figure 4-6 where

$$A_{i,j} = \exp \left[ \left( 2 - \delta_{i,j} \right) \frac{\left( b_i b_j \sigma_i^2 + \delta_{i,i} \sigma_j^2 \right)}{(|\epsilon| + 1)} \frac{\partial R_o \partial R_o}{\partial \Phi_i \partial \Phi_j} \right]$$

(4.39)

and the anisotropy ratio of the effective permeabilities, $A = \frac{k_A}{k_e}$, is the product $\prod_{i=1}^{n} \prod_{j=i}^{n} A_{i,j}$, where $n$ in this context is the number of input variables. The principal contributor to the anisotropy for $\bar{P}_c \approx 1/\alpha_q$ is due to the variability of $B$. At lower mean capillary pressure values – for which the anisotropy is at its peak value – the covariance of $B$ and $L$ are the principal factors, while the variance of $L$ and the variance of $B$ are still significant.

The effective relative permeabilities and the homogeneous relative permeability, $\kappa_m = \exp \left( R_o (\bar{S}_e, \bar{\Phi}) - \bar{F} \right)$ for the base case condition are plotted versus the mean saturation in Figure 4-7. The difference between either of the effective permeabilities and $\kappa_m$ in Figure 4-7 represents the error in the relative permeability estimate which occurs when the field scale conditions are assumed to be represented by the local scale p-s-k function evaluated at the mean input values.
Figure 4-4: Partial derivative $\frac{\partial R_c}{\partial P_c}$ versus normalized mean capillary pressure for base case, Borden Aquifer, van Genuchten characterization and modified condition, whereby $\bar{L} = 0$. 
Figure 4-5: Ratio of horizontal to vertical effective permeability versus normalized mean capillary pressure, evaluated for base case Borden aquifer conditions, and modified conditions whereby the correlation scale is increased to 60 cm and $L$ reduced to 0.
Figure 4-6: Contributions to horizontal - vertical permeability ratio, $A_{ij}$, versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for base case van Genuchten characterization of Borden aquifer with perfect stratification.
Figure 4-7: Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o (\bar{S}_e)$ versus mean normalized saturation; evaluated for base case, Borden aquifer van Genuchten characterization with perfect stratification.
4.4.2 Brooks-Corey Characterization

Stochastic analysis of the Brooks-Corey characterization is problematic in the vicinity of mean capillary pressures near the mean threshold pressure due to the discontinuity of derivatives of \( R_o \) at this point. The partial derivatives with respect to \( R_o \) are plotted in Figure 4-8 for the Brooks-Corey p-s-k function mean parameter values tabulated Table 4.2. The moments were estimated for the same Borden aquifer capillary pressure data set (Kueper and Frind, 1991b) used in the base case, van Genuchten characterization. The partial derivatives \( \frac{\partial R_o}{\partial T_c} \) and \( \frac{\partial^2 R_o}{\partial P_c^2} \) approach infinity while the derivatives \( \frac{\partial R_o}{\partial B} \) and \( \frac{\partial^2 R_o}{\partial B^2} \) approach negative infinity for capillary pressures approaching the threshold pressure. Another way to comprehend the analytical problems confronted for capillary pressures in this region is to think of sampling the relative permeability of soils, where the capillary pressure in all soils is near the mean threshold pressure. Soils with threshold pressures greater than the mean will retain water at this capillary pressure and thus have finite nonwetting phase permeability, while soils with threshold pressures less than the mean will have zero permeability at this capillary pressure. In a stratified media, the vertical effective permeability approximated by the harmonic mean will approach zero and the ratio of horizontal to effective permeabilities will approach infinity.

Table 4.2: Parameters of variable slope, Brooks-Corey characterization for Borden Aquifer based on capillary pressure data set of Kueper and Frind (1991b)

<table>
<thead>
<tr>
<th></th>
<th>( F )</th>
<th>( \sigma_f )</th>
<th>( B )</th>
<th>( \sigma_{gb} )</th>
<th>( b_0 )</th>
<th>( L )</th>
<th>( \sigma_{g_h} )</th>
<th>( b_1 )</th>
<th>( \xi_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brooks-Corey</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.16</td>
<td>0.096</td>
<td>-1.04</td>
<td>1.02</td>
<td>0.078</td>
<td>-0.53</td>
<td>12</td>
</tr>
</tbody>
</table>

The effective relative permeabilities and the homogeneous relative permeability, \( \kappa_m = \exp \left( R_o \left( \bar{S}_e, \bar{\Phi} \right) - \bar{F} \right) \), are plotted versus the mean normalized saturation in Figure 4-9. Figure 4-10 shows the effective relative permeability versus the mean capillary pressure, normalized by the geometric mean of the characteristic pressure \( \bar{P}_c/P_{d,g} = \bar{P}_c/\exp \bar{B} \). This figure shows clearly the large disparity between the vertical and horizontal relative permeability for \( \bar{P}_c \) approaching \( P_{d,g} \). Figure 4-11 shows the anisotropy ratio of the effective permeability, \( \frac{k_h}{k_v} \), for the Brooks-Corey and van Genuchten cases versus the mean normalized capillary pressure. The anisotropy of the two characterizations differs little over the high capillary pressure range, but deviate from each other in the capillary pressure range which are problematic for the estimation.
Figure 4-8: First and second partial derivatives of $R_g$ with respect to $\dot{P}_c (= \alpha_g P_c)$, $B$, $L$, and $F$ for variable slope, Brooks-Corey characterization of Borden aquifer versus normalized capillary pressure $\dot{P}_c$. 
of effective properties with the Brooks-Corey characterization. Figure 4-12 shows the contributions to anisotropy, \(A_{ij}\), plotted versus the normalized mean \(P_c\). It is of interest to note two significant differences between the values of \(A_{ij}\) for the Brooks-Corey and van Genuchten characterizations. The contribution due to the variance of \(L\), \(A_{L,L}\), is not significant for the Brooks-Corey characterization as it was for the van Genuchten characterization due to the low magnitude of the partial derivative of \(R_o\) with respect to \(L\); not surprising since the permeability at low capillary pressures in the Brooks-Corey characterization is governed principally by the value of \(B\). Secondly, the direction of the \(A_{B,L}\) contribution tends to reduce anisotropy, while significant \(A_{B,L}\) contributions were encountered in the van Genuchten characterization which tended to enhance anisotropy.

### 4.4.3 Leverett Scaling

It is common practice in Monte Carlo simulations of multiphase flow in heterogeneous media to employ Leverett scaling, whereby the characteristic pressure parameter of the p-s-k function is a deterministic function of the local permeability. The generation of random media therefore consists of 1) selection of field scale slope and characteristic pressure parameters, 2) the generation of a spatially correlated \(\ln k\) field and 3) the deterministic computation of the local characteristic pressure at each computational node. For the Brooks-Corey characterization and modified Leverett scaling as in Kueper and Frind (1991b) this would be in the form

\[
P_d = P^*_d \sigma \left( \frac{k_s}{n} \right)^{-\beta}
\]  

(4.40)

where \(P^*_d\) is the field scale displacement pressure, \(n\) is the aquifer porosity, \(\sigma\) is the interfacial tension of the fluid pair, and \(k_s\) is the local saturated permeability. The practice and its application for the Borden aquifer capillary pressure measurements is discussed in somewhat more detail in Chapter 6. It is interesting to note that the Leverett scaling relationship is consistent with a deterministic linear relationship between \(\ln k_s\) and \(B (= \ln P_d)\) where from (2.21)

\[
B = \bar{B} - \beta \ln k_s
\]

(4.41)
Figure 4-9: Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o (\bar{S}_e)$ versus mean normalized saturation; evaluated for Brooks-Corey, variable slope parameter characterization of Borden aquifer with perfect stratification.
Figure 4-10: Effective relative permeability versus normalized mean capillary pressure, evaluated for Brooks-Corey, variable slope, characterization of Borden aquifer with perfect stratification.
Figure 4-11: Effective permeability anisotropy ratio versus normalized mean capillary pressure, evaluated for both Brooks-Corey and van Genuchten, base case characterization of Borden aquifer with perfect stratification.
Figure 4-12: Contributions to horizontal - vertical permeability ratio versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for Brooks-Corey, variable slope, characterization of Borden aquifer with perfect stratification.
enabling simulation of the Leverett scaling relationship within the correlation model outlined in Chapter 2 by setting the residual variance of $B$ to zero \( \sigma_{b_0} = 0 \) and $b_b = -\beta$.

Figure 4-13a shows synthetic permeability curves for a modified base case condition, with constant slope parameter ($\sigma_l = 0$) and modified Leverett scaling (parameter moments in Table 4.3); the envelope of permeability values defined by two standard deviations above and below the mean is presented in Figure 4-13b. Note the regularity of the permeability curves and the sharp reduction in the width of the envelope of permeability values, relative to that depicted for the base case in Figure 4.2. Figure 4.14 shows the effective vertical and horizontal nonwetting phase permeabilities versus mean normalized wetting phase saturation for these conditions. Figure 4.15 shows the effective permeabilities for a constant slope factor ($\sigma_l = 0$) as before, but without the Leverett scaling relationship between $B$ and $F$ (see No Leverett Scaling entry in Table 4.3). In the latter case where the variability in $B$ is not correlated with $F$ (i.e., $\beta = 0$), the variance, $\sigma_b$, is specified to be of the same magnitude as in the Leverett scaling formulation (i.e., $\sigma_b = |\beta| \sigma_f$). Figure 4-16 shows the ratio of the vertical to horizontal effective permeabilities as a function of the mean capillary pressure for three cases:

1. base case characterization
2. Leverett scaling characterization
3. non-Leverett scaling characterization with constant slope parameter and variance of the log characteristic pressure equal to the Leverett scaling characterization

The highest anisotropy is reached for the base case, with significantly diminished values of anisotropy with a constant slope factor, with or without Leverett scaling. It is apparent that the form of the variability of $B$, whether correlated in $k$ or not, is not important under these conditions. It is however, of significant importance to represent the correct magnitude of the variability of $B$ and under these conditions the correct magnitude of the variability of the transformed slope factor, $L$. It is apparent that Monte Carlo simulations which employ the van Genuchten characterization and Leverett scaling, underrepresent the variability in a way which dramatically changes the system response. The contribution of individual terms to the anisotropy ratio versus the normalized mean capillary pressure is presented for the Leverett
scaling case in Figure 4-17, where the contributing terms related to the variability of \( L \) are of course zero. By comparison, in the same plot constructed for the base case conditions, Figure 4-6, there are significant contributions related to variability of \( L \).

Table 4.3: Moments of transformed van Genuchten parameters for Borden Aquifer with modified Leverett scaling and uncorrelated variability.

<table>
<thead>
<tr>
<th></th>
<th>( F )</th>
<th>( \sigma_f )</th>
<th>( B )</th>
<th>( \sigma_{gb} )</th>
<th>( b_b )</th>
<th>( L )</th>
<th>( \sigma_{gi} )</th>
<th>( b_l )</th>
<th>( \xi_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leverett Scaling</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.0</td>
<td>-0.65</td>
<td>1.50</td>
<td>0.0</td>
<td>0.0</td>
<td>12</td>
</tr>
<tr>
<td>No Leverett Scaling</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.225</td>
<td>0.0</td>
<td>1.50</td>
<td>0.0</td>
<td>0.0</td>
<td>12</td>
</tr>
</tbody>
</table>

4.4.4 Kueper-Frind Characterization

Kueper and Frind (1991b) employed a Brooks-Corey p-s-k function and modified Leverett scaling to represent variability at the Borden aquifer; with \( \sigma_f^2 = 0.29 \) as estimated for the Borden aquifer by Sudicky (1986). The effective relative permeabilities with input parameter moments as listed in Table 4.4 are plotted for this case versus the mean capillary pressure in Figure 4-18. These effective permeabilities will be used in estimation of plume width for a qualitative comparison with the Monte Carlo simulations described by Kueper and Frind (1991b).

The effective properties of the variable \( L \), Brooks-Corey characterization, without Leverett scaling – as in section 4.4.2, but with \( \sigma_f^2 = 0.29 \) – were estimated and plotted in Figure 4-19. Parameter moments for this case are in the second row of Table 4.4. The estimated effective relative permeability takes on the physically unreasonable values greater than one. Analogous physically unrealistic estimates of effective relative permeability with a van Genuchten characterization also result in relative permeabilities greater than one over some range of mean capillary pressures. This is due to the process of linearization of the governing equations and a violation of the assumption of low amplitude variability. These are obviously unreasonable results, but more troubling is that the impact of these nonlinearities most likely effects even those effective permeability estimates which appear to be physically reasonable. The reader should bear in mind that all effective property estimates in this document are correct to second order and that there may occur situations where errors occur due to significant, but unrepresented, higher order nonlinearities. Further, the exponential generalization has been applied

113
Figure 4-13: (a) Synthetic permeability curves based on Leverett scaling, constant slope, van Genuchten Borden Aquifer characterization. (b) Envelope of permeability variability as a function of capillary pressure defined by mean plus and minus two standard deviations for Leverett scaling, constant slope, van Genuchten Borden Aquifer characterization.
Figure 4-14: Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_v (\bar{S}_e)$ versus mean normalized saturation; for van Genuchten, constant slope parameter characterization with modified Leverett scaling of Borden aquifer with perfect stratification.
Figure 4-15: Effective relative permeability, $\kappa_v$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_0 (\bar{S}_e)$ versus mean normalized saturation; for Borden aquifer parameters with perfect stratification and van Genuchten, constant slope parameter characterization without Leverett scaling.
Figure 4-16: Horizontal - vertical effective permeability ratio versus normalized mean capillary pressure, evaluated for van Genuchten, characterizations of Borden aquifer with perfect stratification and 1) base case conditions with variable slope parameter, 2) constant slope parameter with modified Leverett scaling ($\beta = 0.65$) and 3) constant slope parameter with no scaling and equivalent $\sigma^2_0$ to Leverett scaling condition.
Figure 4-17: Contributions, $A_{ij}$, to effective permeability anisotropy ratio for Leverett scaling, Borden Aquifer characterization, where anisotropy is product of individual contributions at given mean capillary pressure; evaluated for van Genuchten, Leverett scaling characterization of Borden aquifer with perfect stratification.
to alleviate problems which occur with high variability. This generalization is a first guess of system behavior for "large" variability, which may itself inadvertently introduce errors due to inconsistency of this guess with real high variability system behavior.

Table 4.4: Moments of transformed Brooks-Corey parameters for representation of Borden Aquifer characterization by Kueper and Frind (1991b).

<table>
<thead>
<tr>
<th></th>
<th>$F$ (ln cm$^2$)</th>
<th>$\sigma_f$ (ln dynes/cm$^2$)</th>
<th>$B$</th>
<th>$\sigma_{b_0}$</th>
<th>$b_b$</th>
<th>$L$</th>
<th>$\sigma_{b_l}$</th>
<th>$b_l$</th>
<th>$\xi_1$ (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>based on Kueper / Frind (1991b)</td>
<td>-16.01</td>
<td>0.538</td>
<td>10.16</td>
<td>0.0</td>
<td>-0.65</td>
<td>0.96</td>
<td>0.0</td>
<td>0.0</td>
<td>12</td>
</tr>
<tr>
<td>non-Leverett</td>
<td>-16.01</td>
<td>0.538</td>
<td>10.16</td>
<td>0.096</td>
<td>-1.04</td>
<td>1.02</td>
<td>0.078</td>
<td>-0.53</td>
<td>12</td>
</tr>
</tbody>
</table>

### 4.4.5 Interfacial Tension

The lateral spread of simulated nonwetting phase plumes in heterogeneous media has been shown in numerical simulations to be strongly dependent on the interfacial tension of the fluid pair (Kueper and Frind, 1991b; Rathfelder and Abriola, 1998). Typically, the impact of interfacial tension is adjusted by application of Leverett scaling relationships, whereby the local characteristic pressure of the p-s-k function is proportional to the interfacial tension. Reductions in the interfacial tension, therefore reduces both the mean and variance of the characteristic pressure. The effect may be represented by rewriting the Leverett relationship as

$$B = -\ln \alpha = -\ln \alpha^* + \ln \sigma - \alpha \ln n + \alpha \ln k$$

(4.42)

and recognizing that the mean value of $B$ may be written as

$$\bar{B} = -\ln \alpha^* + \ln \sigma - \alpha \ln n + E[\alpha \ln k]$$

(4.43)

Therefore the mean value of $B$ changes with the log of the interfacial tension. The effective permeabilities were recomputed for the base case Borden aquifer, van Genuchten characterization with $\bar{B} = 7.8$, representing a thirteen-fold reduction in the interfacial tension – since from (4.43), $S_T = \exp(10.4 - 7.8) = 13$. Figure 4-20 (a) and (b) show the effective permeabilities and the ratio of horizontal-vertical effective permeabilities for this low interfacial tension case. The pressure dependent anisotropy is nearly eliminated in the reduced interfacial tension case due
Figure 4-18: Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_v$, and homogeneous relative permeability $\kappa_g = \exp \left( \bar{R} - \bar{F} \right)$ and $\kappa_m = \exp \left( R \left( \bar{\Gamma} \right) - \bar{F} \right)$ versus normalized mean capillary pressure, evaluated for Kueper-Frind (1991) characterization of Borden Aquifer with Brooks-Corey p-s-k function, ln $k$ variability as measured by Sudicky, modified Leverett scaling.
Figure 4-19: Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_v$, and homogeneous relative permeability $\kappa_g = \exp(R - F)$ and $\kappa_m = \exp(RF - F)$ versus normalized mean capillary pressure, evaluated for Borden Aquifer with Brooks-Corey p-s-k function and ln k variability as measured by Sudicky, where parameter moments reflect independent measurements of p-s-k function parameters.
to an order of magnitude increase in $\frac{\partial R_e}{\partial P_c}$ and consequently $\varepsilon$. The system is far less anisotropic than the base case from which it differs only in the mean value of $B$.

Table 4.5: Reduced interfacial tension van Genuchten parameter moments (based on data from Kueper and Frind (1991b)).

<table>
<thead>
<tr>
<th>$F$ (ln cm$^2$)</th>
<th>$\sigma_f$</th>
<th>$B$ (ln dynes/cm$^2$)</th>
<th>$\sigma_{gb}$</th>
<th>$b_b$</th>
<th>$L$</th>
<th>$\sigma_{gb}$</th>
<th>$b_l$</th>
<th>$\xi_1$ (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low interfacial tension</td>
<td>-16.01</td>
<td>0.346</td>
<td>7.80</td>
<td>0.113</td>
<td>-1.03</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
</tr>
</tbody>
</table>

4.4.6 Summary

The effective properties were estimated in this Chapter for vertical, uniform mean flow in a perfectly stratified aquifer for a number of scenarios as summarized in Table 4.6. Initially, the base case, van Genuchten, Borden Aquifer conditions were represented whereby the parameter moments are based on individual estimates of the p-s-k parameter values. The solution replicates the saturated, effective permeability solution, and predicts large anisotropy for low mean capillary pressure values. From the moments of the random input variables, the principal contributors to the pressure dependent anisotropy for the van Genuchten characterization were found to be the variance of the characteristic pressure, $\sigma_h^2$, the variance of the slope parameter, $\sigma_l^2$, and the covariance of the two p-s-k parameters, $\text{cov}(L,B)$. A simplified model of one-dimensional, vertical flow was used to explain the inverse dependence of anisotropy on the vertical correlation scale and the partial derivative, $\frac{\partial R_e}{\partial P_c}$.

Effective permeabilities were estimated using the Brooks-Corey p-s-k functions for the same conditions as in the base case. The solution is less than perfectly reliable under these conditions for mean capillary pressure values near the mean threshold pressure; however, large anisotropy values indicated for mean capillary pressures in this range are not unexpected. There is less effect of the variability of $\sigma_h^2$ on the anisotropy of the Brooks-Corey system than for the base case.

Far less anisotropy was predicted for Leverett scaling conditions than the base case conditions – that is for the case of a field scale slope parameter and for deterministic dependence of the log characteristic pressure, $B$ on the value of $\ln k$. A similar characterization based on Kueper and Frind (1991b) was implemented where in this case, the Brooks-Corey p-s-k func-
Figure 4-20: Effective permeability (a) and ratio of horizontal to vertical effective permeability (b) for low interfacial tension; Borden aquifer, base case, van Genuchten, variable slope characterization with $\bar{B} = 7.8$. 

123
tions were used and the variability of ln $k$ was set at the field scale value measured by Sudicky (1986) – slightly more than twice the ln $k$ variance of the soils for which the p-s-k parameters were estimated.

Lastly, the effective permeability was estimated for the case of reduced interfacial tensions, introduced by reducing the mean value of $B$. As anticipated the pressure dependent anisotropy is nearly eliminated due to increases in $\frac{\partial R_a}{\partial P_e}$. 
Table 4.6: Summary of scenarios for estimation of effective properties under perfect stratification conditions

<table>
<thead>
<tr>
<th>no.</th>
<th>description</th>
<th>p-s-k form</th>
<th>anisotropy ratio of effective permeabilities</th>
<th>$\bar{F}$ (in cm$^2$)</th>
<th>$\sigma_I$</th>
<th>$\sigma_L$</th>
<th>$\sigma_B$</th>
<th>$\bar{B}$</th>
<th>$\sigma_B$</th>
<th>$b_b$</th>
<th>$\xi_1$ (cm)</th>
<th>$\xi_2$ (cm)</th>
<th>$\rho_o$ (g/cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>base case, Borden</td>
<td>VG</td>
<td>high pressure dependent anisotropy, peak value approx. 4000</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>2</td>
<td>Borden base case, increased $\xi_i$</td>
<td>VG</td>
<td>peak value &lt;10</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>60</td>
<td>1.6</td>
</tr>
<tr>
<td>3</td>
<td>Borden base case, increased dRo/dPc</td>
<td>VG</td>
<td>peak value &lt;10</td>
<td>-16.40</td>
<td>0.346</td>
<td>0.00</td>
<td>0.174</td>
<td>-0.83</td>
<td>10.4</td>
<td>0.113</td>
<td>-1.03</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>4</td>
<td>analogous to Borden Base case with BC p-s-k</td>
<td>BC</td>
<td>extreme values on approach of mean capillary pressure to mean displacement pressure</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.02</td>
<td>0.079</td>
<td>-0.53</td>
<td>10.16</td>
<td>0.096</td>
<td>-1.04</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>5</td>
<td>Borden, Leverett scaling</td>
<td>VG</td>
<td>peak value &lt;10</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.50</td>
<td>0.000</td>
<td>0</td>
<td>10.4</td>
<td>0.000</td>
<td>-0.65</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>6</td>
<td>Borden, no Leverett, $c_0$ same as Lev. (5)</td>
<td>VG</td>
<td>similar in form and magnitude to Leverett scaling (5)</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.50</td>
<td>0.000</td>
<td>0</td>
<td>10.4</td>
<td>0.225</td>
<td>0.00</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>7</td>
<td>Borden, Kueper-Frind characterization</td>
<td>BC</td>
<td>extreme values on approach of mean capillary pressure to mean displacement pressure</td>
<td>-16.01</td>
<td>0.538</td>
<td>0.96</td>
<td>0.000</td>
<td>0</td>
<td>10.16</td>
<td>0.000</td>
<td>-0.65</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>8</td>
<td>Borden, no Leverett scaling, elevated $c_0$ as in (7)</td>
<td>BC</td>
<td>unrealistic result - horizontal effective permeability exceeds saturated horizontal permeability for mean capillary pressure approaching mean displacement pressure</td>
<td>-16.01</td>
<td>0.538</td>
<td>0.96</td>
<td>0.078</td>
<td>-0.53</td>
<td>10.16</td>
<td>0.096</td>
<td>-1.04</td>
<td>12</td>
<td>1.6</td>
</tr>
<tr>
<td>9</td>
<td>Borden base case, low interfacial tension</td>
<td>VG</td>
<td>minimal, &lt;2</td>
<td>-16.40</td>
<td>0.346</td>
<td>1.50</td>
<td>0.174</td>
<td>-0.83</td>
<td>7.8</td>
<td>0.113</td>
<td>-1.03</td>
<td>12</td>
<td>1.6</td>
</tr>
</tbody>
</table>
Chapter 5

Lateral Spreading of Nonwetting Phase through Static Wetting Phase

Consider the case of a nonwetting phase liquid or gas introduced into an aquifer in which density instabilities cause the flow of the nonwetting liquid. Based on observations of continuous air sparging sources, the nonwetting phase flow will initially cause the displacement of the wetting phase at a front defined by a zone of rapidly changing saturation. The lateral extent of the nonwetting phase will gradually diminish as the vertical wetting phase flow is arrested and the plume reaches a steady state configuration (McKay and Acomb, 1996; Schima et al., 1996). This chapter describes an approximate steady state solution to vertical nonwetting phase flow through static water. The solution is derived using the effective properties, homogeneous within the solution domain, to predict field scale behavior in response to local heterogeneities. The objective is to test aquifer sensitivity to characterization form and properties of input processes. This builds on the findings of Chapter 4, providing a means of testing the implications of the predicted effective properties for common multiphase flow scenarios.

The integral method is introduced briefly. For more information the reader is referred to Crank (1979) or Goodman (1964), or to Polmann (1990) where the same procedure was employed for estimation of the lateral spreading of the wetting phase in unsaturated flow. Then the technique is applied to derive a nonlinear, first order ordinary differential equation whose solution is the lateral plume half-width as a function of elevation. The equation is derived
for both the planar, X-Z and cylindrical R-Z domains. The planar X-Z solution represents the system response to a horizontal planar source extending infinitely in the direction perpendicular to the solution plane. The solution is the mean lateral extent (in the X direction) of the nonwetting phase averaged over the horizontal in the direction perpendicular to the solution plane.

In general, the integral approach presumes both the existence of a separable solution and the solution's functional form. A solution of this type is described for the case where the effective permeability is a power law function of the mean capillary pressure. Both the functional form of the vertical effective permeability lateral dependence and an analytical solution for the plume half-width are presented. This provides support for the application of the technique to more general cases and enabled a formal check of the numerical code used to estimate the plume width. Finally, the code for the numerical solution of the plume half width is described and used in evaluation of plume width in systems for which effective properties were estimated in Chapter 4.

5.1 Integral Method

The integral method has been useful in the development of approximate solutions for the nonlinear diffusion equation, where the diffusivity is a function of the potential. The technique converts nonlinear, partial differential equations to ordinary differential equations by assuming the analytical form of the equation's solution and introducing a width parameter as the independent variable. Consider for instance a nonlinear diffusion equation

\[
\frac{\partial}{\partial x} \left( \alpha_z(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial z} \left( \alpha_z(T) \frac{\partial T}{\partial z} \right) = 0 \tag{5.1}
\]

The first step is to assume an approximate solution \( \tau(x, z) \) and define the spatially variable error, \( \varepsilon \), of the flow divergence as

\[
\frac{\partial}{\partial x} \left( \alpha_z(\tau) \frac{\partial \tau}{\partial x} \right) + \frac{\partial}{\partial z} \left( \alpha_z(\tau) \frac{\partial \tau}{\partial z} \right) = \varepsilon \tag{5.2}
\]
If the solution is assumed to have a separable form (i.e., \( \tau(x, z) = \tau_o(z) \cdot f(x/L) \) with known or assumed \( f \)), then the problem is reduced from one of solving for \( T \) at every \( x, z \) point to finding a solution for \( \tau_o \) and \( L \) as a function of the vertical distance, \( z \). One desirable property of \( \tau \) would be if the value of \( \varepsilon \) were on average equal to zero over the solution domain:

\[
\int \left( \frac{\partial}{\partial x} \left( \alpha_x(\tau) \frac{\partial \tau}{\partial x} \right) + \frac{\partial}{\partial z} \left( \alpha_z(\tau) \frac{\partial \tau}{\partial z} \right) \right) dx = \int \varepsilon dx = 0 \tag{5.3}
\]

or further that the moments of \( \varepsilon \) over the solution domain are also equated to zero

\[
\int x^j \varepsilon dx = 0 \tag{5.4}
\]

Further it may be shown that the function \( \tau(x, z) \) which satisfies

\[
\int_a^b x^j L(\tau(x, z)) dx = 0, \quad j = 0, 1, 2, \ldots n \tag{5.5}
\]

will make \( L(\tau(x, z)) = 0 \) at least \( n \) times in the interval \( a \leq x \leq b \) (Goodman, 1964). Therefore, each additional moment, equated on average to zero, improves the accuracy of the result at the expense of additional analytical complexity. In the solution presented in the next section, the zero and second moment are utilized. The first moment is omitted since the first moment is identically zero for any symmetrical trial solution.

### 5.2 Spreading in Planar Two Dimensional, Vertical Domain

The horizontal functional form of the vertical relative permeability is assumed to be known whereby

\[
\kappa_z = \tilde{\kappa}_z(z) f \left( \frac{x}{w(z)} \right) \tag{5.6}
\]

\( \tilde{\kappa}_z(z) \) is the center point vertical relative permeability and \( f \) is a physically reasonable function whose argument is the horizontal distance relative to the plume center-line normalized by a characteristic plume half-width, \( w(z) \). The integral technique converts the partial differential equation to a nonlinear, ordinary differential equation with respect to \( w \) and a secondary constraint with respect to \( \tilde{\kappa}_z \); with boundary conditions \( w = w_o \) and \( \tilde{\kappa}_z = \tilde{\kappa}_{z,0} \) specified for \( z = 0 \).
Two forms of $f$ were considered:

\[
f(u) = \begin{cases} 
1 - u^2, & |u| \leq 1 \\
0, & |u| > 1 
\end{cases} \quad (5.7)
\]

\[
f(u) = \exp(-u^2) \quad (5.8)
\]

In both cases, there is no lateral flow at the center line, \(\frac{\partial f}{\partial u}\big|_{u=0} = 0\), and the peak value of $f$ occurs at the center line, $x = 0$.

In the presence of a static wetting phase and homogeneous effective intrinsic permeability, the steady state continuity equation is

\[
k_x \frac{\partial}{\partial x} \left( \kappa_x \frac{\partial P_c}{\partial x} \right) + k_z \frac{\partial}{\partial z} \left( \kappa_z \left( \frac{\partial P_c}{\partial z} + \delta \rho g \right) \right) = 0 \quad (5.9)
\]

For the case of gravity flow, \(\left| \frac{\partial P_c}{\partial z} \right| < \delta \rho g\), the flow equation may be written as

\[
k_x \frac{\partial}{\partial x} \left( \kappa_x \frac{\partial P_c}{\partial x} \right) + \delta \rho g k_z \frac{\partial \kappa_z}{\partial z} = 0 \quad (5.10)
\]

By reducing the equation to first order with respect to $z$, the boundary condition of the problem need be stated only at the source elevation. This reduces the complexity of the solution, but imposes a lower bound on the source width for which the solution is applicable for a given rate of flow. This assumption is technically equivalent to the assumption of zero longitudinal dispersion in the advection-dispersion equation. Checks for violations of the gravity flow assumption were carried out by estimation of the capillary pressure gradient along the center line following numerical solution under the gravity flow assumption. In some cases, the capillary pressure gradient is of the same order of magnitude as the gravity term, but this condition occurs over a narrow vertical range near the source point. See for example Figure 5-4b which is a plot of the estimated mean capillary pressure gradient, along the plume center line, versus elevation. Note that the capillary pressure gradient in this case in fact exceeds the gravity flow term of 580 dynes/cm$^3$, but only in the first 10 cm below the water table. Below this point, the gradient is far less than the gravity term indicating that the assumption of gravity flow below this point is appropriate.
The problem may be written with respect to the Kirchoff transform \( s(P_c) = \int_0^{P_c} \kappa_x(P'_c) dP'_c \) as

\[
k_x \frac{\partial^2 s(P_c)}{\partial x^2} + \delta \rho g k_z \frac{\partial \kappa_z}{\partial z} = 0 \quad (5.11)
\]

### 5.2.1 Zero Moment

The horizontal, zero moment of the governing equation where the trial solution \( \tilde{\kappa}_z f \) has been substituted for \( \kappa_z \), is

\[
k_x \int_{-\infty}^{\infty} \frac{\partial^2 s(P_c)}{\partial x^2} dx + \delta \rho g k_z \int_{-\infty}^{\infty} \frac{\partial \tilde{\kappa}_z f}{\partial z} dx = 0 \quad (5.12)
\]

The first integral evaluates to zero, therefore, the zero moment reduces to

\[
\delta \rho g k_z \int_{-\infty}^{\infty} \frac{\partial \tilde{\kappa}_z f}{\partial z} dx = 0 \quad (5.13)
\]

On reversing the order of integration and differentiation and making the change of variable \( u = \frac{z}{w} \)

\[
\frac{\partial (w \tilde{\kappa}_z)}{\partial z} \int_{-\infty}^{\infty} f du = 0 \quad (5.14)
\]

The obvious solution is

\[
\tilde{\kappa}_z w = C
\]

which for the specified boundary conditions, \( w(0) = w_0, \tilde{\kappa}_z(0) = \tilde{\kappa}_{z,0} \) the zero moment reduces to

\[
w_0 \tilde{\kappa}_z = w_0 \tilde{\kappa}_{z,0} \quad (5.15)
\]

This is simply a statement that the downward flow through any horizontal section does not change with elevation.

### 5.2.2 Second Moment

The second moment of the continuity equation is equated to zero

\[
k_x \int_{-\infty}^{\infty} x^2 \frac{\partial^2 s}{\partial x^2} dx + \delta \rho g k_z \int_{-\infty}^{\infty} x^2 \frac{\partial \tilde{\kappa}_z f}{\partial z} dx = 0 \quad (5.16)
\]
Reversing the order of integration and differentiation in the second integral and making the substitution \( u = \frac{z}{w} \)

\[
w k_x \int_{-\infty}^{\infty} u^2 \frac{\partial^2 s}{\partial u^2} du + \delta \rho g k_x \frac{\partial}{\partial z} \left( w^3 \tilde{\kappa}_z \int_{-\infty}^{\infty} u^2 f(\tilde{u}) du \right) = 0
\]  

(5.17)

The first integral is evaluated by twice applying integration by parts and recognizing that \( \lim_{u \to -\infty} \frac{\partial s}{\partial u} = \lim_{u \to -\infty} \frac{\partial s}{\partial u} = 0 \) and \( \lim_{u \to -\infty} s = \lim_{u \to \infty} s = 0 \).

\[
\int_{-\infty}^{\infty} u^2 \frac{\partial^2 s}{\partial u^2} du = u^2 \frac{\partial s}{\partial u} \bigg|_{-\infty}^{\infty} - 2 \int_{-\infty}^{\infty} usdu = u^2 \frac{\partial s}{\partial u} \bigg|_{-\infty}^{\infty} - 2 \left[ us \bigg|_{u=-\infty}^{\infty} - \int_{-\infty}^{\infty} sdu \right] = 2 \int_{-\infty}^{\infty} sdu
\]

(5.18)

The simplified second moment expression is therefore

\[
2w k_x \int_{-\infty}^{\infty} sdu + \delta \rho g k_x \frac{\partial}{\partial z} \left( w^3 \tilde{\kappa}_z \right) \int_{-\infty}^{\infty} u^2 f(\tilde{u}) du = 0
\]

(5.19)

where the integral \( \int_{-\infty}^{\infty} u^2 f(\tilde{u}) du \) can be resolved analytically or numerically depending on the form of \( f(u) \).

### 5.2.3 Rate of Plume Width Expansion

Substituting the zero moment result (5.16) into the second moment expression (5.20)

\[
2w k_x \int_{-\infty}^{\infty} sdu + \delta \rho g k_x \frac{\partial}{\partial z} \left( w^3 \tilde{\kappa}_z \frac{w_0 u_0}{w} \right) \int_{-\infty}^{\infty} u^2 f(\tilde{u}) du = 0
\]

(5.20)

and the rate of plume growth \( \frac{\partial w}{\partial z} \) is given by

\[
\frac{\partial w}{\partial z} = -\frac{k_x \int_{-\infty}^{\infty} sdu}{k_x \tilde{\kappa}_z,0 w_0 \rho g \int_{-\infty}^{\infty} u^2 f(u) du}
\]

(5.21)

Recognizing that the total vertical flow per unit width \( Q_1 \) is \( -\frac{k_x \tilde{\kappa}_z,0 w_0 \rho g}{\mu_0} \int_{-1}^{1} f(u) du \) the
rate of plume expansion may be written as

\[
\frac{\partial w}{\partial z} = \frac{\int_{-\infty}^{\infty} s \, du \int_{-\infty}^{\infty} f(u) \, du}{Q_t \mu_o \int_{-\infty}^{\infty} u^2 f(u) \, du}
\]  

(5.22)

For the parabolic \( f(u) = 1 - u^2 \) this reduces to

\[
\frac{\partial w}{\partial z} = \frac{5 \int_{-1}^{1} s \, du}{Q_t \mu_o}
\]  

(5.23)

while for \( f(u) = \exp(-u^2) \)

\[
\frac{\partial w}{\partial z} = \frac{2 \int_{-\infty}^{\infty} s \, du}{Q_t \mu_o}
\]  

(5.24)

It would be incorrect to conclude from this result that the rate of \( w \) expansion is inversely proportional to \( Q_t \) since the numerator is also a function of flow in an unspecified manner.

Evaluation of the double integral \( \int_{-\infty}^{\infty} s \, du = \int_{-\infty}^{\infty} \int_{0}^{P_c(u)} \kappa_x \, dP_c \, du \) is accomplished by numerical evaluation of the equivalent single integral found by inverting the order in which the integrals are evaluated

\[
\int_{-\infty}^{\infty} \int_{0}^{P_c(u)} \kappa_x \, dP_c \, du = \int_{0}^{P_c(\kappa_x)} \left( \int_{-u(P_c)}^{u(P_c)} \kappa_x \, dP_c \right) \kappa_x \, dP_c
\]  

(5.25)

\[
= 2 \int_{0}^{P_c(\kappa_x)} u(P_c) \kappa_x \, dP_c
\]

where \( u(P_c) \) is evaluated by inverting the \( f \) function, \( u(P_c) = f^{-1} \left( \frac{\kappa_x(P_c)}{\kappa_x} \right) \) and the integral’s upper bound \( P_c(\kappa_x) \) is found by interpolation of the tabulated effective property functions.

The value of \( w \) may be used to numerically estimate the second moment of the nonwetting phase plume as a function of \( z \) based on the tabulated functional relationship \( \bar{\theta}_o(\kappa_x) \)

\[
M_2 = \left( \frac{\int x^2 \bar{\theta}_o(x) \, dx}{\int \bar{\theta}_o(x) \, dx} \right)^{1/2}
\]  

(5.26)

\[
= \left( \frac{w^2 \int \kappa_x(\kappa_x(u)) \, du}{\int \kappa_x(\kappa_x(u)) \, du} \right)^{1/2}
\]
5.3 Analytical, Separable Solution in Planar Two Dimensional Domain

The integral method presumes the solution is the product of two functions: the first, $\bar{\kappa}_z (z)$, describing the center line vertical relative permeability versus elevation and the second, $f \left( \frac{x}{u(z)} \right)$, describing the relative permeability’s lateral dependence. It is not necessarily the case that separable solutions are available for shape functions of arbitrary form. Assuming that the horizontal and vertical effective, relative permeabilities are described by power functions of the capillary pressure

$$\kappa_x = aP_c^\nu$$
$$\kappa_z = bP_c^\mu$$

then the problem does have a separable solution (Gelhar, personal communication, 1998) with a shape function of form

$$f (u) = \left( 1 - \frac{\nu - \mu + 1}{2\mu} u^2 \right)^{\mu/(\nu - \mu + 1)}$$

(5.28)

where $u = \frac{x}{u(z)}$. The derivation of $f$ and the analytical solution for $w$ with this spreading function is described in Appendix F. The function $f$ ranges from a strictly parabolic form in the case of $\mu = \nu = 1$, to other more Gaussian-like forms.

It is also informative in providing insight into the appropriate form of the lateral spreading function, $f (u)$ for the non-power law effective permeability function. In these cases, one interpretation might be to consider the permeability function to be locally approximated by a power law function. Figure 5-1 shows the local exponent values versus the mean capillary pressure, where the exponents are computed as $\nu = \frac{\partial \ln \kappa_x}{\partial \ln P_c}$ and $\mu = \frac{\partial \ln \kappa_z}{\partial \ln P_c}$ for the base case Borden Aquifer conditions using the tabulated effective permeability function. For low capillary pressures, the exponents are constant over nearly an order of magnitude change in mean capillary pressure. In this region, the effective permeability is well approximated by the power law permeability function, however these capillary pressure values are associated with nonwetting phase permeability values too low to be of any practical value. Four exponent pair values were selected for
normalized mean capillary pressure values: $P_{G} \alpha_{g} = 0.3, 0.6, 0.95, \text{ and } 2.2$. The $f$ function for these four mean capillary pressures as well as for the case of $\mu = \nu = 1$ are plotted in Figure 5-2. For the latter set of exponents, $\mu = \nu = 1$, the $f$ function of the analytical solution reduces to a parabolic function. The value of $w$ is selected for each curve so that the area under the curves is equivalent. The most abrupt reduction in $f$ with increasing $u$ is found for the case of the highest capillary pressure. Curiously, the next lowest capillary pressure has the largest tail, with reductions in this tailing effect found for further reductions in the mean capillary pressure. This implies that the lateral front of the nonwetting phase plume is sharpest at the highest elevation where the mean capillary pressure is greatest. Beyond some lesser critical capillary pressure, moving away from the source into the body of the plume, the front will broaden and become less sharp.

The solution for the plume half width as a function of elevation is in this case

$$w = \left( w_0^{(\nu+1+\mu)/\mu} - \frac{\left( \mu + \nu + 1 \right) k_a a (\kappa_w w_0)^{(\nu-\mu+1)/\mu} \delta_p g b (\nu+1)/\mu g^2}{z} \right)^{\mu/(\nu+1+\mu)}$$

(5.29)

This finding is valuable in that it shows that exact separable solutions exist at least for the case of a simple power law, permeability function. Further, this result supports the presumption that a physically reasonable, separable solution exists for the more general case, whose shape function is likely to be reasonably approximated by a quadratic function.

### 5.4 Spreading in Radially Symmetric Domain

To obtain the equation describing lateral spreading in a radial domain, the same technique is applied as for the vertical two-dimensional plane. The vertical effective relative permeability is assumed to be described by $\kappa_z = \hat{k}_z f \left( \frac{r}{R} \right)$. For a static wetting phase, the nonwetting phase continuity equation may be written as

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r k_z \kappa_z \frac{\partial P_c}{\partial r} \right) + \frac{\partial}{\partial z} \left( k_z \kappa_z \left( \frac{\partial P_c}{\partial z} + \delta_p g \right) \right) = 0$$

(5.30)
Figure 5-1: Power law permeability function exponents $\mu$ and $\nu$ for base case Borden Aquifer, van Genuchten characterization.
Figure 5-2: Spread function, $f$, versus lateral distance for function form of power law permeability function for exponents associated with normalized mean capillary pressure of 0.3, 0.6, 0.95 and 2.2.
while assuming as before that $|\frac{\partial P_c}{\partial z}| \ll \delta_p g$ and that the effective saturated permeabilities, $k_x$ and $k_z$ are homogeneous

$$\frac{k_x}{k_z} \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa_z \frac{\partial P_c}{\partial x} \right) + \frac{\delta_p g \kappa_z}{\partial z} = 0 \quad (5.31)$$

### 5.4.1 Zero Moment

By substitution of $\kappa_z = \tilde{k}_z f$, the zero moment of the continuity equation is

$$\frac{k_x}{k_z} \int_0^{2\pi} \int_0^\infty \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa_z \frac{\partial P_c}{\partial r} \right) r \, dr \, d\theta + \int_0^{2\pi} \int_0^\infty \delta_p g \frac{\partial \tilde{k}_z f}{\partial z} r \, dr \, d\theta = 0 \quad (5.32)$$

Integration with respect to $\theta$ is trivial due to radial symmetry

$$\frac{2\pi k_x}{k_z} \int_0^\infty \frac{\partial}{\partial r} \left( r \kappa_z \frac{\partial P_c}{\partial r} \right) dr + 2\pi \delta_p g \int_0^\infty \frac{\partial \tilde{k}_z f}{\partial z} r \, dr = 0 \quad (5.33)$$

Recognizing that $\kappa_z r \frac{\partial P_c}{\partial r} \bigg|_0^\infty = 0$, the zero moment reduces to

$$\int_0^\infty \frac{\partial \tilde{k}_z f}{\partial z} r \, dr = 0 \quad (5.34)$$

Applying the same reasoning as in the planar domain, leads to the zero moment result

$$\tilde{k}_z = \frac{\tilde{k}_{z,0} R_0}{R^2} \quad (5.35)$$

### 5.4.2 Second Moment

Equating the second moment of the continuity equation to zero

$$\frac{k_x}{k_z} \int_0^{2\pi} \int_0^\infty r^2 \frac{1}{r} \frac{\partial}{\partial r} \left( r \kappa_z \frac{\partial P_c}{\partial r} \right) r \, dr \, d\theta + \int_0^{2\pi} \int_0^\infty r^2 \delta_p g \frac{\partial \tilde{k}_z f}{\partial z} r \, dr \, d\theta = 0 \quad (5.36)$$

Employing integration by parts on the first integral and reversing the order of integration and differentiation in the second integral

$$\frac{k_x}{k_z \delta_p g} \left[ r^2 r \kappa_z \frac{\partial P_c}{\partial r} \bigg|_0^\infty - \int_0^\infty 2rr \kappa_z \frac{\partial P_c}{\partial r} \, dr \right] + \frac{\partial}{\partial z} \int_0^\infty r^3 \tilde{k}_z f \, dr = 0 \quad (5.37)$$

137
Recognizing that $r^2 \kappa_x \frac{\partial P_c}{\partial r} \bigg|_0^\infty = 0$ and applying integration by parts again

$$- \frac{k_x}{k_z \delta \rho g} \left[ r^2 \int_0^{P_c(r)} \kappa_x dP_c \bigg|_0^\infty - \int_0^\infty 4r \int_0^{P_c(r)} \kappa_x dP_c dr \right] + \frac{\partial}{\partial z} \int_0^\infty r^3 \tilde{\kappa}_z f dr = 0 \quad (5.38)$$

and

$$\frac{4k_x}{k_z \delta \rho g} \int_0^\infty r \int_0^{P_c(r)} \kappa_x dP_c dr + \frac{\partial}{\partial z} \int_0^\infty r^3 \tilde{\kappa}_z f dr = 0 \quad (5.39)$$

Now, on substitution of $u = \frac{r}{R}$

$$\frac{4k_x}{k_z \delta \rho g} R^2 \int_0^\infty \int_0^{P_c(r)} \kappa_x udP_c du + \frac{\partial}{\partial z} \int_0^\infty R^4 \tilde{\kappa}_z \int_0^\infty u^3 f du = 0 \quad (5.40)$$

### 5.4.3 Rate of Plume Width Expansion

Substituting the zero moment result $\tilde{\kappa}_z = \frac{\kappa_z \rho R^2}{R^2}$ in the second moment expression

$$\frac{4k_x}{k_z \delta \rho g} R^2 \int_0^\infty \int_0^{P_c(r)} \kappa_x udP_c du + \frac{\partial}{\partial z} \int_0^\infty \frac{R^4 \tilde{\kappa}_z}{\delta \rho g} \int_0^\infty u^3 f du = 0 \quad (5.41)$$

resulting in an expression for the rate of plume width expansion

$$\frac{\partial R}{\partial z} = -\frac{2k_x R}{\kappa_z \rho \delta \rho g \frac{R^2}{\mu_o}} \int_0^\infty \frac{P_c(u)}{u^3 f(u)} du \quad (5.42)$$

Recognizing that the total flow $Q_t = \frac{k_x \rho \delta \rho g 2\pi R^2}{\mu_o} \int_0^\infty u f(u) du$

$$\frac{\partial R}{\partial z} = \frac{4\pi R k_x}{Q_t \mu_o} \int_0^\infty \frac{P_c(u)}{u^3 f(u)} du \quad (5.43)$$

For the case of $f = 1 - u^2$

$$\frac{\partial R}{\partial z} = \frac{12\pi R k_x}{Q_t \mu_o} \int_0^\infty \frac{P_c(u)}{u^3 f(u)} du \quad (5.44)$$

while for $f = \exp(-u^2)$

$$\frac{\partial R}{\partial z} = \frac{4\pi R k_x}{Q_t \mu_o} \int_0^\infty \frac{P_c(u)}{u^3 f(u)} du \quad (5.45)$$
Evaluation of the double integral \( \int_0^\infty \int_0^{P_c(u)} \kappa_x u \, dP_c \, du \) is accomplished by numerical evaluation of the equivalent single integral found by inverting the order in which the integrals are evaluated

\[
\int_0^\infty \int_0^{P_c(u)} \kappa_x u \, dP_c \, du = \int_0^{P_c(\bar{\kappa}_z)} \left( \int_0^{u(P_c)} u \, du \right) \kappa_x dP_c = \frac{1}{2} \int_0^{P_c(\bar{\kappa}_z)} u \left( \frac{\kappa_x(P_c)}{\bar{\kappa}_z} \right)^2 \kappa_x dP_c \tag{5.46}
\]

and as in the planar domain \( u(P_c) \) is evaluated as \( f^{-1} \left( \frac{\kappa_x(P_c)}{\bar{\kappa}_z} \right) \).

The value of \( w \) may be used to numerically estimate the second moment of the nonwetting phase plume as a function of \( z \) based on the tabulated functional relationship \( \bar{\theta}_o(\kappa_z) \)

\[
M_2 = \left( \frac{\int x^2 \bar{\theta}_o(x) \, dx}{\int \bar{\theta}_o(x) \, dx} \right)^{1/2} = \left( \frac{w^2 \int u^2 \bar{\theta}_o(\kappa_z(u)) \, du}{\int \bar{\theta}_o(\kappa_z(u)) \, du} \right)^{1/2} \tag{5.47}
\]

### 5.5 Evaluation of Nonwetting Phase Solution

A FORTRAN implementation of the fourth order, Runge-Kutta solution technique was adapted from Press et al. (1987) for solution of the lateral spreading width and center point relative permeability as a function of vertical distance from the source point. Source code is contained in Appendix G. The inputs to this routine were the tabulated effective properties: mean capillary pressure, mean and standard deviation of nonwetting phase volumetric content and vertical and horizontal effective permeabilities. Intermediate values were estimated by fitting a second order polynomial to the three closest points and interpolating values as necessary. Integrals are evaluated by application of Simpson’s rule, where the number of sections is used in computation of the integral is an input variable.

#### 5.5.1 Analytical Solution

The separable analytical solution described above for the case of the power law permeability function provides an opportunity to check the code developed for numerical solution of the
plume half width, \( w \). The numerical routine for estimation of plume width was adapted for the shape function as in (5.28). The integral \( \int_{-\infty}^{\infty} u^2 f(u) \, du \) in (5.21) was found for \( \nu - \mu + 1 > 0 \) to be equal to \( r^3 B \left( \frac{3}{2}, \frac{r^2+2}{2} \right) \) where \( r^2 = \frac{2\mu}{\nu-\mu+1} \) and \( B(x, y) \) is the beta function defined as (Gradshteyn and Ryzhik, 1980):

\[
B(x, y) = \int_0^1 t^{x-1} (1-t)^{y-1} \, dt; \quad [\text{Re} \, x > 0, \text{Re} \, y > 0]
\tag{5.48}
\]

(5.29).

The analytical and numerical solution for the plume half width was computed using exponents corresponding to a normalized mean capillary pressure value of 0.3 which is in the mean capillary pressure region in which the effective permeability is best approximated as a power law. The effective permeability in this region is approximated in cgs units by the power law functions:

\[
\kappa_x = (3.08 \times 10^{-63}) P_c^{14.0}
\tag{5.49}
\]

\[
\kappa_z = (4.1 \times 10^{-63}) P_c^{13.4}
\]

The analytical and numerical solution for the boundary conditions \( u_0 = 100 \text{ cm} \) and \( \kappa_{z,0} = 0.105 \) are plotted in Figure 5-3. The results of the analytical and numerical solutions are practically identical.

### 5.5.2 Kueper and Frind Characterization

Kueper and Frind (1991b) simulated DNAPL releases from the water table in a vertical, two dimensional domain. The simulations, conducted in media representing the natural heterogeneity of the Borden Aquifer, used the Brooks-Corey p-s-k functions and modified Leverett scaling as described in Section 4.4.4. The simulated source condition was that of a constant wetting phase saturation of 0.5 over a width of 0.4 m. An exact quantitative comparison between the results of their simulations and the integral solution is not possible because only a single simulation result was conducted and the narrow width of the source relative to the horizontal correlation scale of the media make it particularly sensitive to nonergodic effects. Also, the integral method solution was derived for a steady state system, while the simulations of Kueper
Figure 5-3: Analytical and numerical solution of plume half width $w$ for power law permeability-capillary pressure function with $\mu = 13.4, \nu = 14.0$
and Frind (1991b) are of a continuous source for 7.4 days.

The plume width was estimated by the integral method for the effective properties presented in Section 4.4.4 with input properties as summarized in Table 5.1, for boundary conditions \( w_o = 100 \text{ cm} \) and \( \hat{e}_{z,0} = 0.105 \). The relative permeability boundary condition was selected to produce the same average nonwetting phase specific discharge as the base case simulated by Kueper and Frind (1991b). Effective permeability for this case is plotted versus the mean capillary pressure in Figure 4.17. The plume half width, \( w \), and the square root of the second moment, \( M_2 \), are plotted in Figure 5-4a. Figure 5-4b is of the capillary pressure gradient at the center line. The gradient is at its peak at the source elevation and rapidly diminishes with depth. Note that the gravity flow assumption is not met in the zone immediately below the source since \( \delta_{pg} = 981 \text{ dynes/cm}^3 \). Gravity flow is rapidly restored within a minimal distance below the source point relative to the total domain, so the condition of nongravity flow near the source is assumed to have negligible impact. Figure 5-4c plot shows the mean and standard deviation of the nonwetting phase volumetric content on the center line and Figure 5-4d shows the mean and standard deviation of the capillary pressure, also along the center line. At a depth of 2 m, the plume half-width, \( w \), is over 11 m, while the square root of the second moment is approximately 6 m. Similarity between the simulated plume width and the width of the single realization of Kueper-Frind (1991b) is not however indicative of the accuracy of the numerical solution, as significant variability is anticipated between Monte Carlo realizations, at least in part due to the small source size relative to the simulated horizontal correlation scale.

Table 5.1: Moments of transformed Brooks-Corey parameters for representation of Borden Aquifer characterization by Kueper and Frind (1991b).

<table>
<thead>
<tr>
<th>F</th>
<th>( \sigma_f )</th>
<th>B</th>
<th>( \sigma_{g_b} )</th>
<th>( b_b )</th>
<th>L</th>
<th>( \sigma_{g_l} )</th>
<th>( b_l )</th>
<th>( \xi_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(ln cm(^2))</td>
<td>(ln dynes/cm(^2))</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>(cm)</td>
</tr>
<tr>
<td>based on Kueper and Frind (1991b)</td>
<td>-16.01</td>
<td>0.538</td>
<td>10.16</td>
<td>0.0</td>
<td>-0.65</td>
<td>0.96</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

5.5.3 Base Case and Sensitivity Analysis

**Base Case.** The simulated plume for the base case, van Genuchten, Borden Aquifer characterization with the same boundary conditions, \( w_o = 100 \text{ cm} \) and \( \hat{e}_{z,0} = 0.11 \), is shown in Figure 5-5. The parameter moments of this simulated condition and other simulated conditions from
Figure 5-4: Kueper-Frind (1991b), Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: $w_o = 100$ cm, $\kappa_{z,0} = 0.11$. 

143
this section are listed in Table 5.2. This has a reduced $\ln k$ permeability variability relative to the prior Kueper and Frind style characterization and uses the van Genuchten p-s-k functions with independent estimation of p-s-k function parameters for each soil sample.

The base case van Genuchten lateral spread is less than that found for the Kueper-Frind characterization, with Brooks-Corey p-s-k function and Leverett scaling. The simulated $\ln k$ variance of the Kueper-Frind characterization is greater, but variability of the slope parameter, $L$, is neglected in the Kueper-Frind characterization. The effective permeability anisotropy ratio of the Brooks-Corey system is insensitive to the variability of the slope parameter and approaches large magnitudes near the mean threshold pressure even in low variability systems. In conclusion, the results in these two cases suggests that the impact of Leverett scaling is less significant for systems characterized using the Brooks-Corey p-s-k function than for a comparable system characterized with the van Genuchten p-s-k function.

Rathfelder and Abriola (1998) showed that multiphase flow simulations using the Brooks-Corey characterization are sensitive to discretization, such that finer discretization increases lateral plume spreading. This finding is consistent with the effective permeability values estimated here as low mean capillary pressure values, which are resolved in numerical simulations only by increasing resolution, have associated with them extreme anisotropic values which would tend to spread a plume.

**Gaussian Shape Function.** Sensitivity to the shape function form was assessed by solving for the plume half-width with a Gaussian lateral shape function, subject to the same base case, van Genuchten, Borden Aquifer characterization. The boundary width was reduced by a factor of $4/(3\sqrt{\pi})$ so as not to change the total nonwetting phase flow from the value used with the parabolic shape function. Figure 5-6 shows the system profile for the Gaussian shape function. The center-line vertical relative permeability as a function of elevation is virtually identical for both shape functions (see Figure 5-7). Consequently, due to the condition that the vertical flow is invariant across any horizontal section and given the assumption of gravity flow, it may be easily shown that the plume width for the two shape functions are the same relative to their boundary value.

Figure 5-8 shows the vertical effective relative permeability versus lateral distance from the plume center line at a depth of 500 cm below the water table. The effective permeability
solution obtained with the Gaussian solution is slightly less at the center line, but has a fatter tail which continues at significant values for some distance beyond the zero permeability point of the parabolic shape function.

Despite the similarity of the permeability solutions, the implied distribution of the mean nonwetting phase volumetric content is significantly wider than that computed using the parabolic shape function. Figure 5-9 shows the mean nonwetting phase volumetric content plotted versus lateral distance from the plume center line at a depth of 500 cm. The lateral profile of the nonwetting phase content in the two cases is similar out to a distance approximately 1300 cm from the center line. Beyond this distance, the volumetric content of the solution with the parabolic shape function falls rapidly to zero, while the solution with the Gaussian shape function only reaches half of its center line value at approximately 1700 cm. This difference in the distribution of the nonwetting phase also shows up in differences in the second moment of the nonwetting phase content as plotted in Figure 5-10.

**Brooks-Corey.** The estimated plume width for the Brooks-Corey p-s-k function analogous to the base case van Genuchten characterization is shown in Figure 5-11. The parameter moments are specified in Table 5.2 and effective properties were estimated in Section 4.3.2. The Brooks-Corey characterization results in a diminished lateral spread despite the extreme anisotropy values occurring for mean capillary pressure approaching the mean threshold pressure. It must be noted however that two tabulated values approaching the mean threshold pressure were removed before computing the plume width solution. Beyond this point, the horizontal nonwetting phase effective permeability begins to increase with reducing capillary pressure; a physically unlikely occurrence caused by instability of the effective property solution near this limit.

**High Flow.** A high flow condition was simulated by increasing the boundary center line relative permeability a factor of 3.5 to \( \tilde{k}_{z,0} = 0.37 \). The impact of increasing flow is that the lateral spread is reduced by approximately 25 percent (see Figure 5-12). This is due to the reduced anisotropy associated with the increased mean capillary pressure which is imposed at the source. This is consistent in a qualitative sense with the flow rate dependence noted by Kueper and Frind (1991b). The issue of flow rate dependence of lateral spreading is discussed further in Chapter 6.
**Wide Source.** Sensitivity to the source width was evaluated by increasing the boundary value of the half width, \( w \), by a factor of ten to 1000 cm. Two cases were considered: in the first the center point permeability was maintained at the same value as the initial, narrow source, condition; whereas in the second case the total flow was maintained at the narrow source value by reducing the center point permeability. The results are plotted as \( w \) versus \( z \) in Figure 5-13. The growth of the half width with the same boundary permeability is reduced substantially relative to the narrow source condition, while under the constant flow condition the growth rate is approximately the same. In the first case the center point permeability is the same as in the narrow source condition, but the distance to the outer limit of the plume is increased substantially reducing the horizontal gradient which drives the lateral spreading. By reducing the center point permeability to maintain the narrow source total flow rate, the system anisotropy is increased and in this case nearly compensating for the reduced lateral gradient.

Table 5.2: Moments of transformed van Genuchten parameters for Borden Aquifer base case and alternative characterizations.

<table>
<thead>
<tr>
<th></th>
<th>( F )</th>
<th>( \sigma_f )</th>
<th>( B )</th>
<th>( \sigma_{gh} )</th>
<th>( b_b )</th>
<th>( L )</th>
<th>( \sigma_{g1} )</th>
<th>( b_l )</th>
<th>( \xi_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.119</td>
<td>-1.03</td>
<td>1.10</td>
<td>0.174</td>
<td>-0.83</td>
<td>12</td>
</tr>
<tr>
<td>Brooks Corey</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.16</td>
<td>0.096</td>
<td>-1.04</td>
<td>1.12</td>
<td>0.078</td>
<td>-0.55</td>
<td>12</td>
</tr>
<tr>
<td>Leverett Scalng</td>
<td>-16.40</td>
<td>0.346</td>
<td>10.4</td>
<td>0.0</td>
<td>-0.65</td>
<td>1.10</td>
<td>0.00</td>
<td>-0.00</td>
<td>12</td>
</tr>
<tr>
<td>Low Interfacial Tension</td>
<td>-16.40</td>
<td>0.346</td>
<td>7.90</td>
<td>0.113</td>
<td>-1.03</td>
<td>1.10</td>
<td>0.174</td>
<td>-0.83</td>
<td>12</td>
</tr>
</tbody>
</table>

**Leverett Scaling and Low Interfacial Tension.** The lateral plume width solution was applied to both the modified Leverett scaling scenario and low interfacial tension condition as initially introduced in Sections 4.4.3 and 4.4.5. The effective permeability and anisotropy for these two cases were plotted in Figures 4.14, 4.17 and 4.19. The plume width profiles for these two cases as well as the high flow and base case conditions are plotted in Figure 5-14. The parameter moments for these four cases are listed in Table 5.2. As might be anticipated from the findings of Chapter 4, the lateral spreading in the modified Leverett scaling and low interfacial cases is significantly reduced from that of the base case condition due to the relative absence of pressure dependent anisotropy in these cases. The very narrow plume found for the low interfacial tension condition is also qualitatively consistent with the results of Kueper and Frind (1991b).
In this case, Leverett scaling has a profound impact, with a plume width growth only 1/3 of the base case simulation. In the analysis of the Kueper-Frind characterization, with Leverett scaling, Brooks-Corey characterization and slightly higher ln$k$ variance, the plume width is roughly the same dimensions as in the base case, van Genuchten characterization. The difference may be attributed to the the insensitivity of the Brooks-Corey anisotropy to the variability of $L$ and the extreme anisotropy found for the Brooks-Corey characterization at low mean capillary pressure values.

5.6 Summary

The integral approach applied in this chapter reduces the governing equations to ordinary differential equations with respect to a parameterized, approximate solution. This approach was applied to evaluate the lateral plume width of a nonwetting phase, steady state plume, with mean vertical flow, through a static wetting phase. It was applied to both vertical, two-dimensional and cylindrical domains and the Runge-Kutta method was implemented to numerically solve the resulting differential equation.

A separable analytical solution was found by assuming that the effective horizontal and vertical effective permeabilities are power law functions of the mean capillary pressure. This analytical solution was used as a check of the numerical code. Moreover, the existence of a solution of this type supports the presumption that a separable solution exists for the more complicated effective permeability function.

For boundary conditions, $k_{z,0} = 0.105$, $w_0 = 100$ cm, the plume half-width of the base case, van Genuchten characterization grew from 100 cm to nearly 1300 cm at a depth of 5 m below the water table; approximately three times the half-width growth of the modified Leverett scaling system at the same depth. This is a result of a reduction of pressure dependent anisotropy in the Leverett scaling characterization due to the omission of slope parameter variability and under-representation of the variability of the log of the characteristic pressure. The Brooks-Corey characterization, with reduced sensitivity to the variability of the slope parameter, responded less forcefully to the imposition of Leverett scaling. Reducing the interfacial tension by an order of magnitude, essentially eliminates lateral spreading. Increasing nonwetting phase flow for the
Figure 5-5: Base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: \( w_o = 100 \text{ cm}, \bar{\kappa}_{z,0} = 0.11 \).
Figure 5-6: Gaussian shape function; base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: $w_o = 100$ cm, $\bar{\kappa}_{z,0} = 0.11$. 
Figure 5-7: Center line relative permeability for parabolic and Gaussian shape function for Borden, base case, van Genuchten characterization.
Figure 5-8: Vertical relative permeability versus lateral distance from plume center line for both parabolic and Gaussian shape function at 500 cm below water table.
Figure 5-9: Mean nonwetting phase volumetric content versus lateral distance from plume center line for both parabolic and Gaussian shape functions at 500 cm below water table.
Figure 5-10: Second moment of nonwetting phase volumetric content versus elevation for parabolic and Gaussian shape functions.
Figure 5-11: Brooks-Corey, Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: \( w_o = 100 \) cm, \( \kappa_{z,0} = 0.11 \).
Figure 5-12: High flow, base case Borden Aquifer characterization system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow, static water and boundary conditions: \( w_o = 100 \) cm, \( \kappa_{2,0} = 0.50 \).
Figure 5-13: Plume width profile for steady state gravity flow of nonwetting phase through static wetting phase with 1) base case, van Genuchten characterization and 2) wide source scenario ($w_o = 1000$ cm).
Figure 5-14: Plume width profile for steady state gravity flow of nonwetting phase through static wetting phase with 1) base case, van Genuchten characterization, 2) low interfacial tension, 3) high flow and 4) modified Leverett scaling.
Borden Aquifer increases the mean capillary pressure and hence reduces the anisotropy of the effective permeability field. The result is a reduction of lateral spreading relative to the base case. Increasing the source width by a factor of ten without altering the boundary center point permeability reduces the growth of the plume half width by a factor of six. On the other hand if the source width is increased by the same value, but the total flow is retained the same as for the base case then the growth of the plume width is nearly the same as for the narrow source due to the higher anisotropy of the low capillary pressure (low permeability) condition.

The next chapter contains a description of the Borden and Cape Cod Aquifers and the measured variability of the p-s-k function parameters. The plume width solution is applied to the Cape Cod Aquifer and the system behavior in that aquifer is compared to that of the Borden Aquifer.
Chapter 6

Cape Cod and Borden Aquifers: Effective Properties and Impact on Nonwetting Phase Plume Dimensions

6.1 Introduction

The Borden and Cape Cod aquifers are well suited for the purposes of this investigation due to the availability of multiple measurements of the capillary pressure-saturation relationship (Kueper and Frind, 1991b; Mace, 1994) and prior studies on the spatial variability of permeability (Sudicky, 1986; Turck and Kueper, 1996; Hess et al., 1992; Springer, 1991). Further, a field study of DNAPL flow below the water table at Borden (Kueper and Frind, 1991b) provides the opportunity for qualitative comparison with estimated effective properties and predicted flow patterns.

First the capillary pressure-saturation data for each aquifer are presented and interpretations offered for the moments of the p-s-k function parameters. Then, synthetic relative permeability data are presented to develop an understanding of the implied variability of the permeability field. Effective properties are evaluated and differences between aquifers and field
data interpretations are discussed. Integral solutions for lateral spreading developed in Chapter 5 are utilized for each aquifer—both for DNAPL and air sparging flow conditions—in order to understand the practical implications of differences in effective properties.

6.2 Evidence of Field Scale Variability

This section is a summary of the spatial variability of multiphase flow properties at the Borden and Cape Cod aquifers. For each aquifer, an overview of the geologic setting is presented, the results of studies on the variability of intrinsic permeability are summarized and the available evidence on the variability of p-s-k function parameters are presented and analyzed.

6.2.1 Borden Aquifer

Geologic Setting

The Borden aquifer soils have been described (Bolha, 1986 cited in Poulsen and Kueper, 1992) as fine to medium grained beach sands deposited in a prograding foreshore sequence. Sudicky's description of Borden aquifer soil cores (1986) is useful in providing an understanding of small scale variability.

Examination of the cores further indicated the presence of numerous lenses of coarse to silty fine-grained sand embedded in a fine- to medium-grained sand. The contact between zones having a large textural contrast was usually sharp and near-horizontal across the cores. The thickness of individual beds generally varied from a few centimetres to few tens of centimetres, with the material within each bed being relatively homogeneous in texture, although fine laminations on the order of a millimetre to a few millimetres thickness were sometimes encountered.

Permeability

Sudicky (1986) reports on the collection of thirty-two, 2 m long cores taken along two intersecting transects at a horizontal interval of 1 m. The cores were cut at intervals of 5 cm and estimates made of the saturated hydraulic conductivity using a falling head permeability test.
A follow-up study (Turek and Kueper, 1996) was undertaken to evaluate the stationarity of the \( \ln k \) moments. Turek and Kueper report on the collection of eleven, 3 m cores, taken along a transect roughly 60 m from the cores described by Sudicky (1986). Using the same analytical technique on 5 cm samples drawn from these eleven cores, they computed the moments and correlation scales of the saturated hydraulic conductivity. A summary of the findings of Sudicky (1986) and Turek and Kueper (1996) are reported in Table 6.1. The third column of Table 6.1 reports on the sample moments of a subset of the samples of Turek and Kueper (1996) which were used in later analyses of multiphase flow properties (Kueper and Frind, 1991b). The mean value of \( \ln K \) and the vertical correlation scale of the two data sets are generally the same. Some if not all of the differences in the estimated variance of \( \ln K \) and horizontal correlation scale may be attributed to inadequate sampling. Correlation scales and interval depth are not reported for the Kueper and Frind soil samples.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu_{\ln k} ) (cm/s)</td>
<td>-4.63</td>
<td>-4.96</td>
<td>5.00</td>
</tr>
<tr>
<td>( \sigma_{\ln k} )</td>
<td>0.29*</td>
<td>0.585</td>
<td>0.122</td>
</tr>
<tr>
<td>Vertical scale (m)</td>
<td>0.12</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>Horizontal scale (m)</td>
<td>2.8</td>
<td>4.8</td>
<td></td>
</tr>
<tr>
<td>Interval depth bgs (m)</td>
<td>2 - 4.5</td>
<td>3.05 - 6.10</td>
<td></td>
</tr>
</tbody>
</table>

*The raw variance of Sudicky's measurements was 0.38, but Sudicky cites a nugget effect amounting to 25 percent of the raw variance.

**Capillary Pressure Curve**

Kueper (1989) selected 7 of the 642 soil samples analyzed in Turek and Kueper (1996) for evaluation of capillary pressure-saturation curves in a tetrachloroethylene (PCE)-water system. The mean and variance of the statistical moments of \( \ln K \) for the seven soil samples is presented in Table 6.1. The \( \ln K \) sample variance of the seven samples was significantly less than that of the 642 samples from which they were selected. The criteria for selecting the seven samples is not reported, although one may presume based on the low log permeability variance of the seven
soils that either there was a biased selection procedure to represent "typical" soil behavior, or that the source locations of the seven samples were close enough to account for the reduced variability. Each of the seven samples was saturated with water and incrementally drained by the displacement of water by PCE. The capillary pressure-saturation curve for each of the seven samples is presented in Figure 6.1.

The remainder of this section describes the stochastic characterization of multiphase flow properties employed by Kueper and Frind (1991b) in their Monte Carlo aquifer simulations and an alternative characterization original to this document.

**Leverett Scaling Characterization** Kueper and Frind assume that the hydraulic conductivity is a log-normal random field with a spatial correlation model as evaluated by Sudicky (1986). They use the Brooks-Corey p-s-k functions where \( \lambda \) is constant, and the local value of \( P_d \) is a deterministic function of the local saturated permeability and the constant rescaled displacement pressure, \( P_d^* \). The functional dependence is governed by a modified form of Leverett scaling with a contact angle of zero and arbitrary exponent, \( \beta \), whereby

\[
P_d = P_d^* \sigma \left( \frac{k(x)}{n} \right)^{-\beta}
\]

(6.1)

where

\[
\begin{align*}
n & = \text{porosity} \\
\sigma & = \text{interfacial tension of fluid pair} \\
k(x) & = \text{local saturated permeability at point } x
\end{align*}
\]

Estimation of \( P_d^* \) is accomplished by

1. rescaling the measured capillary pressure according to \( P^*_c(S_c) = \frac{P_c(S_c)}{\sigma} \left( \frac{k(x)}{n} \right)^\beta \) and

2. fitting the Brooks-Corey capillary pressure-saturation function to the rescaled capillary pressure values, \( P^*_c \).

**Rescaling Capillary Pressure** Ideally, the rescaled capillary pressures will reduce to a single valued function of saturation. Figures 6-2a, 6-2b and 6-2c show the rescaled capillary
Figure 6-1: Capillary pressure versus wetting phase saturation from seven Borden Aquifer soil samples from Kueper (1991a); measured under drainage conditions for perchloroethylene-water liquid pair.
pressure curves for $\beta = 0.5$, 0.65 and 1.0, respectively, for $n = 0.35$ and $\sigma = 45$ dyne/cm. Rescaling does reduce the variability between soils, however there remains after scaling a systematic discrepancy between the rescaled curves. For $\beta = 0.5$ the original pattern of high permeability soils with reduced capillary pressure generally remains as prior to scaling. At $\beta = 0.65$ – the value selected for use by Kueper and Frind (1991b) – there are still significant deviations for high wetting phase saturation. Also, the rescaled capillary pressures of soils, which are less than the rescaled mean at high wetting phase saturation, are generally greater than the rescaled mean in the low wetting phase saturation region. Increasing the value of $\beta$ from 0.65 to 1.0 reduces the variability further for high wetting phase saturation with increased variability at the low capillary pressure end. It is beyond the scope of the present work to evaluate the utility of the Leverett scaling relationship, but the data would seem to imply the need for a scaling expression in which the $\beta$ exponent is pressure dependent. In fact the limited amount of data would suggest that the capillary pressure scales as $k^{-1/2}$ for high capillary pressure values and $k^{-1}$ for low capillary pressure. It may be that different physical processes control the local capillary pressure at low and high wetting phase saturation which would account for the different scaling exponents.

**Fitting Rescaled Capillary Pressure Data to Brooks-Corey Function** The next step is to estimate a single set of p-s-k function parameters for the rescaled capillary pressure-saturation function. The estimated Brooks-Corey parameters reported by Kueper and Frind (1991b) are given in Table 6.2. The rescaled displacement pressure, $P^*_d$, is erroneously reported to be dimensionless. It is not clear what units are in fact represented by the reported value. I repeated the exercise of rescaling the data – again using a constant $n = 0.35$ and $\sigma = 45$ dyne/cm – and estimating $P^*_d$ and $\lambda$ based on a residual volumetric wetting phase content of 0.078. The parameter estimation was performed by minimizing the sum of the squared error of the predicted $\ln P_c$, where points judged to be below the likely threshold pressure were selectively omitted prior to performing the optimization. The estimated parameter values for $\beta = 0.5$, 0.65, 0.75, and 1.0 are listed in Table 6.3 along with the implied units of $P^*_d$ computed as $cm^{2\beta-1}$. Although the numerical value of $P^*_d$ differs from that of Kueper and Frind, it is assumed that the parameter estimates are physically equivalent subject to some unspecified unit

164
Figure 6-2: Rescaled Borden aquifer capillary pressure-saturation curves using classic Leverett scaling (a) and modified Leverett scaling as in Kueper and Frind (1991b) with exponent $\beta = 0.65$ (b) and $\beta = 1.0$ (c).
conversion. The local value of $P_d$ computed using (6.1) with the local permeability equivalent to its geometric mean ($k = k_g = \exp \bar{F}$) is reported in the right-most column of Table 6.3. The value of $\lambda$ is relatively insensitive to $\beta$ as is the value of $P_d$ associated with the geometric mean of the intrinsic permeability.

Table 6.2: Keuper and Frind (1991) estimates of the Brooks-Corey parameters for the rescaled capillary pressure curve.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>95% Confidence Limits</th>
<th>Mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_d^*$</td>
<td>0.00526</td>
<td>0.0058</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>2.14</td>
<td>2.83</td>
</tr>
<tr>
<td>$\theta_r$</td>
<td>0.062</td>
<td>0.094</td>
</tr>
</tbody>
</table>

Table 6.3: Brooks-Corey parameter estimates for rescaled capillary pressure curves

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$\lambda$</th>
<th>$P_d^*$ units</th>
<th>$P_d$ at ln $k = \bar{F}$ (cm water)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.50</td>
<td>2.59</td>
<td>0.252</td>
<td>- 25.6</td>
</tr>
<tr>
<td>0.65</td>
<td>2.62</td>
<td>0.00252</td>
<td>$cm^{0.3}$ 25.8</td>
</tr>
<tr>
<td>0.75</td>
<td>2.62</td>
<td>0.000523</td>
<td>$cm^{0.5}$ 26.4</td>
</tr>
<tr>
<td>1.00</td>
<td>2.15</td>
<td>0.0000108</td>
<td>$cm$ 24.3</td>
</tr>
</tbody>
</table>

Consider three soil samples from the Borden Aquifer with intrinsic permeabilities equal to $\bar{F}$, $\bar{F} - 2\sigma_f$ and $\bar{F} + 2\sigma_f$, where as estimated for the Borden Aquifer by Sudicky (1986): $\bar{F} = -16.02 \ln cm^2$ and $\sigma_f = 0.29$. Assuming the soils are Leverett scaling then the local value of $P_d$ may be estimated for each soil from (6.1), using in this case $n = 0.35$ and $\sigma = 45$ dyne/cm and the estimated Brooks-Corey parameters of Table 6.3. Table 6.4 reports the estimated local value of $P_d$ for the three soils for both $\beta = 0.65$ and $\beta = 1.0$. Estimates of nonwetting and wetting phase permeability versus capillary pressure were computed for the three soils and plotted for $\beta = 0.65$ and $\beta = 1.0$ in Figure 6-3, where the nonwetting phase permeabilities are plotted in Figures 6-3b and 6-3d and wetting phase permeabilities are plotted in 6-3a and 6-3c. Assuming $F$ is the only spatially variable input property and has a gaussian distribution then these curves represent bounds enclosing the permeability of 95 percent of the media.

The effect of increasing the intrinsic log permeability above the mean value shows up as a shift of the nonwetting phase permeability curve toward higher permeabilities and lower capillary pressures due to the inverse dependence of $P_d$ on the permeability. The expected
permeability range is greater for $\beta = 1.0$ as shown in Figure 6-3d.

The response of the wetting phase permeability (Figures 6-3a and 6-3c) to changes in intrinsic permeability shows up as a shift toward higher permeabilities and lower capillary pressures. In this case, however this causes a crossover pattern in the wetting phase permeability whereby soils of greater intrinsic permeability have lower wetting phase permeability for high capillary pressures than soils of lesser intrinsic permeability. This is consistent with the crossover pattern observed by Yeh et al. (1985c) in the distribution of measured wetting phase permeability.

Table 6.4: Local displacement pressure (dynes/sq-cm) estimated based on modified Leverett scaling and local permeability spanning plus and minus two standard deviations from the mean

<table>
<thead>
<tr>
<th>$k = \exp F$</th>
<th>$\beta = 0.65$</th>
<th>$\beta = 1.0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-16.02</td>
<td>1908.</td>
<td>1542.</td>
</tr>
<tr>
<td>-16.60</td>
<td>2782.</td>
<td>2754.</td>
</tr>
<tr>
<td>-15.44</td>
<td>1309.</td>
<td>863.4</td>
</tr>
</tbody>
</table>

**Alternative Characterization**  The stochastic representation described in the previous section, in which the slope parameter is held constant and the characteristic pressure is a deterministic function of the local permeability, is commonly applied in Monte Carlo simulations of flow in heterogeneous media. An alternative interpretation is proposed, whereby the p-s-k function parameters are estimated independently for each soil sample and the moments of the parent population inferred based on the sample statistics. This latter interpretation is more faithful in capturing property heterogeneity than the scaling technique, enabling a comprehensive analysis of which aspects of property variability are of most importance in predicting system behavior. The value of the parameters of the Brooks-Corey and van Genuchten characterizations were estimated independently for each soil sample using the residual wetting phase saturation value reported by Kueper and Frind (1991b) of 7.8 percent. The estimated parameters are presented in Table 6.5. Physically reasonable values of $m$ are restricted to $0 < m < 1$, with values in the upper range of $m$ coinciding with the condition whereby small changes in the capillary pressure beyond some threshold pressure are associated with large changes in saturation. This would be anticipated for soils like the Borden aquifer which are well sorted in their original depositional environment, resulting in a narrow range of pore radii.

The measured capillary pressure-saturation data and the fitted characterization functions
Figure 6-3: Wetting and nonwetting phase permeability variability for Brooks-Corey characterization, with modified Leverett scaling for soils with permeability of $F \pm 2\sigma_f$ ($\sigma_f^2 = 0.29$) and (a) and (b) Leverett exponent $\beta = 0.65$ and (c) and (d) $\beta = 1.0$. 
are presented in Appendix D. The predicted nonwetting phase permeabilities for the seven soil samples based on the Brooks-Corey and van Genuchten characterizations are presented in Figures 6-4a and 6-4b. Table 6.6 presents the van Genuchten and Brooks-Corey parameter values following application of transformations defined in (2.10) and (2.14). Again, the transformations of the p-s-k function parameters are defined for the van Genuchten p-s-k functions as

\[
B = -\ln \alpha \\
L = -\ln \left( \frac{1}{m} - 1 \right)
\]

and for the Brooks-Corey p-s-k function as

\[
B = \ln P_d \\
L = \ln \lambda
\]

It is the moments of these transformed values which will be used directly in the evaluation of effective properties.

Table 6.5: Moisture Retention Parameters by Independent Evaluation of each Sample

<table>
<thead>
<tr>
<th>Sample</th>
<th>k (cm²)</th>
<th>(\frac{1}{\alpha}) (cm water)</th>
<th>m</th>
<th>(P_d) (cm water)</th>
<th>(\lambda)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.39E-07</td>
<td>17.32</td>
<td>0.71</td>
<td>13.48</td>
<td>1.91</td>
</tr>
<tr>
<td>2</td>
<td>1.04E-07</td>
<td>26.54</td>
<td>0.78</td>
<td>20.06</td>
<td>2.45</td>
</tr>
<tr>
<td>3</td>
<td>8.46E-08</td>
<td>38.49</td>
<td>0.85</td>
<td>27.26</td>
<td>2.84</td>
</tr>
<tr>
<td>4</td>
<td>6.69E-08</td>
<td>41.58</td>
<td>0.85</td>
<td>28.12</td>
<td>2.76</td>
</tr>
<tr>
<td>5</td>
<td>6.66E-08</td>
<td>38.64</td>
<td>0.80</td>
<td>29.99</td>
<td>2.78</td>
</tr>
<tr>
<td>6</td>
<td>6.23E-08</td>
<td>45.53</td>
<td>0.85</td>
<td>35.00</td>
<td>3.20</td>
</tr>
<tr>
<td>7</td>
<td>4.93E-08</td>
<td>51.42</td>
<td>0.86</td>
<td>41.36</td>
<td>3.55</td>
</tr>
</tbody>
</table>

Figures 6-5 and 6-6 are scatter plots of \(B\) versus \(\ln k\) and \(L\) versus \(\ln k\) for the van Genuchten characterization. In the case of \(B\) versus \(\ln k\), the correlation is negative, as anticipated, with a correlation of 0.96 between the two properties. The negative correlation between \(L\) and \(\ln k\) was not anticipated and is counter to the generally held notion that the magnitude of the capillary pressure-saturation curve slope is greater in low permeability soils. Figure 6-7a (same
Figure 6-4: Predicted relative permeability for seven soil samples from Borden Aquifer (based on data from Kueper and Frind, 1991b) for a) Brooks-Corey and b) van Genuchten p-s-k characterization functions.
Table 6.6: Transformed Moisture Retention Parameters by Independent Evaluation of each Sample

<table>
<thead>
<tr>
<th>Sample</th>
<th>ln k (ln cm²)</th>
<th>B (ln dyne/cm²)</th>
<th>L</th>
<th>B (ln dyne/cm²)</th>
<th>L</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-15.79</td>
<td>9.7</td>
<td>0.89</td>
<td>9.5</td>
<td>0.65</td>
</tr>
<tr>
<td>2</td>
<td>-16.08</td>
<td>10.1</td>
<td>1.28</td>
<td>9.9</td>
<td>0.89</td>
</tr>
<tr>
<td>3</td>
<td>-16.28</td>
<td>10.5</td>
<td>1.74</td>
<td>10.2</td>
<td>1.04</td>
</tr>
<tr>
<td>4</td>
<td>-16.52</td>
<td>10.6</td>
<td>1.72</td>
<td>10.2</td>
<td>1.01</td>
</tr>
<tr>
<td>5</td>
<td>-16.52</td>
<td>10.6</td>
<td>1.42</td>
<td>10.3</td>
<td>1.02</td>
</tr>
<tr>
<td>6</td>
<td>-16.59</td>
<td>10.7</td>
<td>1.76</td>
<td>10.5</td>
<td>1.16</td>
</tr>
<tr>
<td>7</td>
<td>-16.82</td>
<td>10.8</td>
<td>1.79</td>
<td>10.6</td>
<td>1.27</td>
</tr>
<tr>
<td>mean</td>
<td>-16.4</td>
<td>10.4</td>
<td>1.51</td>
<td>10.2</td>
<td>1.02</td>
</tr>
<tr>
<td>variance</td>
<td>0.12</td>
<td>0.14</td>
<td>0.113</td>
<td>0.14</td>
<td>0.039</td>
</tr>
<tr>
<td>correlation with ln k</td>
<td>-0.96</td>
<td>-0.86</td>
<td>-0.98</td>
<td>-0.96</td>
<td></td>
</tr>
<tr>
<td>regression line slope</td>
<td>-1.03</td>
<td>-0.83</td>
<td>-0.98</td>
<td>-1.68</td>
<td></td>
</tr>
</tbody>
</table>

as Figure 4.2a) shows the synthetic permeability curves for 100 random variates drawn from the stochastic model as described in Chapter 2 with moments as shown in the bottom portion of Table 6.6. Figure 6-7b shows an estimate of the envelope of permeability measurements defined as \( \exp (\bar{R} \pm 2\sigma_r) \) where \( \bar{R} \) and \( \sigma_r \) are in this context the sample statistics of the predicted nonwetting phase permeabilities.

### 6.2.2 Cape Cod Aquifer

**Geological Setting**

The Cape Cod Aquifer is largely the consequence of the region’s glacial history (LeBlanc et al., 1987). Outwash deposits carried from the terminal position of three glacial lobes generated the Mashpee Pitted Plain on top of a preexisting fine grained lacustrine aquifer. The aquifer is composed of coarse grained sand and gravel, grading to medium and fine sands towards the south. Terminal moraines were formed at the front of the stationary glaciers near the northern and western boundaries of the inner Cape. They are extremely heterogeneous with grain size varying from silts to coarse gravel to boulder erratics.
Figure 6-5: Scatter plot of $L$, transformed van Genuchten slope parameter versus $\ln k$ (ln cm$^2$) estimated for Borden aquifer soils in PCE-water system (based on data from Kueper and Frind, 1991b).
Figure 6-6: Scatter plot of $B$, transformed van Genuchten pressure normalization parameter versus $\ln k$ (ln cm$^2$) estimated for Borden aquifer soils in PCE-water system (based on data from Kueper and Frind, 1991b).
Figure 6-7: (a) Synthetic permeability curves based on base case, van Genuchten Borden Aquifer characterization with variable slope parameter. (b) Envelope of permeability variability as a function of capillary pressure defined by mean plus and minus two standard deviations for base case van Genuchten Borden Aquifer characterization.
Permeability

Analyses of the statistical variability of $\ln K$ in the lower Cape Cod, Massachusetts have been performed by Springer (1991), Hess et al., (1992). Table 6.7 summarizes the findings of these studies.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Technique</td>
<td>slug test</td>
<td>flowmeter</td>
<td>permeameter</td>
<td>permeameter</td>
</tr>
<tr>
<td>No. measurements</td>
<td>350</td>
<td>668</td>
<td>825</td>
<td>42</td>
</tr>
<tr>
<td>$K_g$ (m/d)</td>
<td>52</td>
<td>95.0</td>
<td>30.2</td>
<td>40.6</td>
</tr>
<tr>
<td>$K$ (m/d)</td>
<td>125</td>
<td>-</td>
<td>-</td>
<td>44.9</td>
</tr>
<tr>
<td>raw $\sigma_f^2$</td>
<td>2.25</td>
<td>.24</td>
<td>.14</td>
<td>0.228</td>
</tr>
<tr>
<td>residual $\sigma_f^2$</td>
<td>1.16</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$\xi_{vert}$ (m)</td>
<td>1-5</td>
<td>.19</td>
<td>.18</td>
<td>-</td>
</tr>
<tr>
<td>$\xi_{hor}$ (m)</td>
<td>250</td>
<td>2.6</td>
<td>1.2-2.0</td>
<td>-</td>
</tr>
</tbody>
</table>

Springer (1991) developed hydraulic conductivity estimates based on 350 slug tests done on wells in the US Geological Survey monitoring network for the plume from the Otis AFB sewage treatment plant. The tested wells were primarily in the coarse outwash deposits of the Mashpee Pitted Plain. A Gaussian filter was applied to remove large scale trends and the statistics of the residual values estimated. The filter length scales were 1000 m in the horizontal and 5 m in the vertical. Estimates of the correlation scale were then made by fitting an exponential curve to the variogram. Hess et al., (1991) reports the statistical variability of hydraulic conductivity estimates in the outwash deposits made using a borehole flowmeter. The mean permeability value of the lab scale test procedures performed by Hess et al. (1991) and Mace (1994) are less than the field scale tests which has been attributed to compaction of the core samples – although other factors may also be responsible including the local permeability in the region in which the samples were drawn (sampling error), or misrepresentation of the system behavior by the assumptions underlying the analytical technique. Large differences occur in estimates of the variance of $\ln k$. Leaving out the results of Mace, the variance appears to increase with the scale of the analytical technique and most likely the area over which the estimates were drawn. This increase is likely the result of scale dependence of variance estimates as the variance in ever larger features is sampled and occurs despite the under representation of high frequency
variability with large scale analytical techniques.

**Capillary Pressure-Saturation Data**

Mace (1994) performed measurements of capillary tension and saturation in 6 cores at seven 8 cm intervals along each core. Capillary pressure-saturation data for the water-air system were collected and estimates made of the parameters of the van Genuchten, Brooks Corey and Gardner characterizations. Appendix E shows the tabulated parameters and transformed parameter values for each of the 42 measurement points. Table 6.8 presents summary statistics for the van Genuchten and Brooks Corey parameter estimates, while Table 6.9 presents summary statistics for the transformed p-s-k function parameters, B and L. Many of the reported estimates of λ in the Brooks-Corey characterization were 1.005, raising some suspicions about the parameter estimation procedure and possible unreported constraints imposed on the search procedure. Graphs of the fitted functions are not contained in Mace (1994), so it is impossible to judge adequacy of fits.

<table>
<thead>
<tr>
<th></th>
<th>van Genuchten</th>
<th>Brooks-Corey</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1/α (cm water)</td>
<td>m (cm water)</td>
</tr>
<tr>
<td>mean</td>
<td>4.88</td>
<td>0.62</td>
</tr>
<tr>
<td>variance</td>
<td>2.93</td>
<td>0.012</td>
</tr>
</tbody>
</table>

Table 6.9: Statistics of transformed p-s-k parameters in Cape Cod aquifer with original estimates as reported in Mace (1994).

<table>
<thead>
<tr>
<th></th>
<th>van Genuchten</th>
<th>Brooks-Corey</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>B (ln dynes/cm²)</td>
<td>L (ln dynes/cm²)</td>
</tr>
<tr>
<td>mean</td>
<td>8.41</td>
<td>0.53</td>
</tr>
<tr>
<td>variance</td>
<td>0.15</td>
<td>0.25</td>
</tr>
<tr>
<td>correlation with ln k</td>
<td>-0.25</td>
<td>-0.12</td>
</tr>
<tr>
<td>slope of regression line vs. ln k</td>
<td>-0.22</td>
<td>-0.14</td>
</tr>
</tbody>
</table>

Scatter plots of B versus ln k and L versus ln k for the van Genuchten p-s-k functions are presented in Figures ?? and 6-9. They reveal only a weak dependence of the p-s-k function parameters on the saturated permeability. Solid lines in these figures show the results of re-
gression analysis. The predicted permeability of the nonwetting phase for all 42 samples, based on the van Genuchten parameter estimates and the nonwetting phase permeability functions (2.7) and (2.9), are plotted in Figure 6-10a. The mean and standard deviation of the log nonwetting phase permeability, \( R_o \), was computed as a function of capillary pressure over the set of 42 relative permeability predictions and \( R_o \) and \( R_o \pm 2\sigma_r \) plotted in 6-10b. It is of interest to contrast these bounds of the permeability distribution with those of the Borden Aquifer presented in Figure 6-7. In the case of the Borden Aquifer the upper bound grows nearly two orders of magnitude with diminishing capillary pressure, while the upper bound of the Cape Cod case grows only slightly. In either case it is clear that the log permeability distribution away from the near saturation condition is not well described by the mean plus and minus two standard deviations due to distribution asymmetry. Other differences between the permeability distribution of the two sites are as follows:

- greater mean intrinsic permeability at the Cape Cod Aquifer
- lesser characteristic pressure at the Cape Cod Aquifer reflected in the lower capillary pressure at which reductions in the nonwetting phase permeability are initiated
- more rapid reductions of permeability with reductions in capillary pressure at the Borden Aquifer

Each of these differences are reflected in the mean parameter values of the system’s measurable soil properties.

In order to apply these parameters to a system involving fluid pairs other than water-air it is necessary to modify the value of the displacement pressure due to differences in the interfacial tension and contact angle of different fluid pairs. One technique is to employ Leverett scaling, where the value of \( B \) for one fluid pair may be evaluated based on the value of \( B \) estimated in a second fluid pair as

\[
B^{(2)} = B^{(1)} - \ln \frac{\sigma_1}{\sigma_2}
\]

(6.4)

where in this case the impact of contact angles has been neglected. For an air-water interfacial tension of 72. dynes/cm and a PCE-water interfacial tension of 44. dynes/cm the mean value
Figure 6-8: Scatter plot of $B$, transformed van Genuchten characteristic pressure versus $\ln k$ ($\ln \text{cm}^2$) and estimated regression line for Cape Cod aquifer soils in air-water system (based on data from Mace, 1994).
Figure 6-9: Scatter plot of $L$, transformed van Genuchten slope parameter versus $\ln k$ (ln cm$^2$) and estimated regression line for Cape Cod aquifer soils in air-water system (based on data from Mace, 1994).
Figure 6-10: (a) Synthetic permeability (cm$^2$) versus capillary pressure for estimated Cape Cod Aquifer van Genuchten p-s-k parameters based on data from Mace (1994) and (b) exp(R+2$\sigma$) where $R$ and $\sigma$ are sample statistics of log permeability versus capillary pressure.
of $B$ in the tetrachloroethylene-water system would be 7.6 ln dynes/cm$^2$ for the Brooks-Corey characterization and 8.0 ln dynes/cm$^2$ for the van Genuchten characterization.

6.2.3 Discussion

The Cape Cod Aquifer is a outwash deposit, while the Borden Aquifer is derived from a lake shore depositional environment. As such, the Borden Aquifer soils are on the whole more uniform and finer grained than soils of the Cape Cod Aquifer. The relative mean value of the p-s-k function parameters is consistent with the geological description:

1. the observed mean log permeability, $\bar{F}$, is consistently greater at the Cape Cod Aquifer (see Tables 6.1 and 6.7) due to the larger grain size and the inferred relation between permeability and grain size

2. the mean log transform of the characteristic capillary pressure, $\bar{B}$, is greater at the Borden Aquifer (see Tables 6.6 and 6.9) due to the smaller pore radii and the consequential greater capillary pressure observed at a given wetting phase saturation

3. the pore scale uniformity of the Borden Aquifer soils causes the soils to drain over a diminished capillary pressure range relative to the Cape Cod aquifer. This is consistent with the significantly greater value of the mean transformed slope parameter, $\bar{L}$, observed for Borden Aquifer soils (see Tables 6.5 and 6.8).

The variability of the p-s-k function parameters is less conclusive, in part due to the larger standard error of higher moment estimators and differences in the measurement scale of the analytical procedures, the distance between samples and the dimensions of the region over which measurements were taken. Comparing the variability data for which complete p-s-k data has been collected, specifically the data sets described by Mace (1994) and Kueper and Frind (1991b) the variance of ln $k$ is greater at the Cape Cod Aquifer, while the variance of the log transform of the characteristic capillary pressure, $\sigma^2_B$, and the variance of the transformed slope parameter, $\sigma^2_{\bar{L}}$, are surprisingly consistent between the two aquifers (see Tables 6.1, 6.5, 6.6 and 6.8). Contradictory conclusions regarding the relative value of the variance of ln $k$ may be reached by considering alternative sources of information cited in Tables 6.1 and 6.6.
At the Borden Aquifer, the variability of both of the capillary pressure-saturation curve parameters was found to be strongly correlated to the log permeability. This was not observed for the Cape Cod Aquifer soils. No explanation is offered for this difference.

The variability of the permeability at a given capillary pressure was shown in Chapter 4 to be positively associated with the field scale anisotropy of the effective permeabilities. Several general observations may be made about permeability variability and differences in the same between the two soils, at least in so far as the predicted relative permeability values of the p-s-k functions accurately reflect the variability which would be observed in direct, multiple measurements of the permeability-capillary pressure relationship.

- Approaching the fully nonwetting saturated region (i.e., high capillary pressure), the variability in the predicted permeability between soils in both the Borden and Cape Cod aquifers is entirely due to the variability of the intrinsic permeability. The transition between this zone and the zone for which significantly greater variability occurs due to variability of the p-s-k parameters lies near the mean value of the van Genuchten characteristic pressure parameter.

- The variability of the predicted permeability on the low capillary pressure side of this transition is significantly greater for the Borden aquifer. This is due in part to the generally more rapid decline of nonwetting phase permeability with diminishing capillary pressure, which is itself due to the larger mean value of the transformed slope parameter, $L$, at the Borden Aquifer. Perturbations in the characteristic pressure show up as horizontal shifts in the permeability-capillary pressure curves causing greater permeability variability for the Borden Aquifer due to its sharp slope.

These differences in the distribution of the p-s-k function parameters which cause greater permeability variability at the Borden Aquifer will be shown in the next section to lead to significant difference in the anisotropy of the effective permeabilities.
6.3 Effective Properties

The effective properties of the Borden Aquifer have been evaluated in Chapters 3 and 4. This section is devoted to presenting effective properties for the Cape Cod Aquifer and describing significant differences between the two aquifers. A stochastic characterization similar to the base case Borden Aquifer characterization is developed for the Cape Cod Aquifer (i.e., van Genuchten characterization, independent estimation of p-s-k parameters, with linear correlation model between $\ln k$ and value of p-s-k parameters as described in Chapter 2).

Figure 6-11a shows the relationship between the mean capillary pressure and mean normalized saturation for the van Genuchten p-s-k functions, and parameter moments as summarized in Table 6.10. It is evaluated and presented for three conditions:

- perfectly stratified aquifer computed using (4.33)
- correlation scales as measured by Hess (1992) for Cape Cod, computed using (3.17)
- zero variance with all input properties at their mean value, $S_e (\bar{\Phi})$.

The mean values based on heterogeneous aquifers may be considered to be effective or field scale capillary pressure-saturation curves, while the zero variance function shows the discrepancy between the field scale curves and the curves obtained using the p-s-k function and the mean parameter values. Two significant differences may be observed between the field scale and capillary pressure curves plotted for the Cape Cod and Borden Aquifers in Figures 6-11 3-2 and 3-3.

- Effective Residual Saturation. This discrepancy between the homogenous and effective curves which increases with reductions in wetting phase saturation may be considered to be a field scale, residual wetting phase saturation over and above the small scale residual saturation which is included in the definition of $S_e$. The estimated effective residual saturation is greater for the Cape Cod aquifer than for the Borden Aquifer (see Figure 3-2), which is attributable to the increased vertical correlation scale at Cape Cod which facilitates the presence of a greater variance in the capillary pressure. Figure 6-11b shows for the perfect stratification condition the contributions to the mean normalized
saturation, $S_{i,j}$, first defined in Chapter 3 as

$$
\bar{S}_e = S_e(\bar{\Gamma}) + \sum_{i=1}^{n} \sum_{j=1}^{n} S_{i,j}
$$

(6.5)

$$S_{i,j} = \frac{E[\gamma_i \gamma_j]}{2} \frac{\partial^2 S_e}{\partial \Gamma_i \partial \Gamma_j}
$$

(6.6)

It is clear from inspection of this plot that the difference between the mean saturation and the homogeneous saturation is due to the persistence of capillary pressure variance at high mean capillary pressures. At the Borden Aquifer, the variance of the capillary pressure increases in this range as well, but the net impact is reduced by the even greater rate of reduction in the second derivative, $\frac{\partial^2 S_e}{\partial \Gamma_i^2}$.

- **Increase in Slope of Capillary Pressure-Saturation Relationship.** The rate of change of the effective capillary pressure relative to changes in saturation is increased relative to the homogeneous, mean condition. The same effect is seen in nonuniform soils and is due to an increase in the range of pore sizes within the sampled media.

Table 6.10: Moments of transformed van Genuchten parameters for Cape Cod Aquifer base case and modified systems.

<table>
<thead>
<tr>
<th></th>
<th>$F$</th>
<th>$\sigma_f$</th>
<th>$B$</th>
<th>$\sigma_{gb}$</th>
<th>$b_b$</th>
<th>$L$</th>
<th>$\sigma_{gl}$</th>
<th>$b_l$</th>
<th>$\xi_1$ (cm)</th>
<th>$\xi_2$ (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perfect stratification</td>
<td>-14.43</td>
<td>0.480</td>
<td>7.98</td>
<td>0.38</td>
<td>-0.22</td>
<td>0.53</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Measured cor. scale</td>
<td>-14.43</td>
<td>0.480</td>
<td>7.98</td>
<td>0.38</td>
<td>-0.22</td>
<td>0.53</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>260</td>
</tr>
<tr>
<td>Homogeneous</td>
<td>-14.43</td>
<td>0.000</td>
<td>7.98</td>
<td>0.00</td>
<td>0.00</td>
<td>0.53</td>
<td>0.50</td>
<td>0.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Modification 1</td>
<td>-14.43</td>
<td>0.480</td>
<td>10.40</td>
<td>0.38</td>
<td>-0.22</td>
<td>1.00</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Modification 2</td>
<td>-14.43</td>
<td>0.480</td>
<td>10.40</td>
<td>0.38</td>
<td>-0.22</td>
<td>1.00</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Modification 3</td>
<td>-14.43</td>
<td>0.480</td>
<td>10.40</td>
<td>0.38</td>
<td>-0.22</td>
<td>1.00</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>$\infty$</td>
</tr>
<tr>
<td>Modification 4</td>
<td>-14.43</td>
<td>0.480</td>
<td>7.98</td>
<td>0.38</td>
<td>-0.22</td>
<td>1.00</td>
<td>0.50</td>
<td>-0.14</td>
<td>19</td>
<td>$\infty$</td>
</tr>
</tbody>
</table>

Figure 6-12 shows the mean and standard deviation of the nonwetting phase volumetric content versus mean normalized wetting phase saturation where the moments of the nonwetting phase content are computed using (2.68), (2.70) and (2.79). The moments of the nonwetting phase volumetric content are in this case evaluated assuming zero porosity variance and zero residual saturation variance although analytical results for nonzero variance are available. The

184
deviation of the mean from a straight line is in this case is an artifact of the transformation of the normalized saturation used in computation of the volumetric content moments. The variance approaches zero at both full wetting phase and nonwetting phase saturation with a peak approximately midway between these extremes. The relationship between mean normalized saturation and the moments of the nonwetting phase volumetric content will be employed to illustrate the spatial distribution of nonwetting phase liquid within a plume in section 6.4 where the lateral spreading of a nonwetting phase plume is estimated.

Figure 6-13 shows the partial derivatives of the log transform of the nonwetting phase permeability \( R_o \) used for evaluation of the effective permeability of the base case case, van Genuchten characterization of Cape Cod soils. The vertical and horizontal effective permeabilities and the homogeneous permeabilities, \( \kappa_m (= \exp (R(\bar{\Theta} - \bar{F})) \) and \( \kappa_v (= \exp (\bar{\Theta} - \bar{F})) \), as defined previously in (4.34), are plotted versus the normalized mean capillary pressure in Figure 6-14. The value of \( \kappa_m \) is greater than the horizontal or vertical effective permeabilities over the entire range of capillary pressures for which the values were estimated. Of even greater interest, the vertical and horizontal effective permeabilities are nearly indistinguishable at the plotted scale. Figure 6-15 shows the effective horizontal and vertical effective permeability and the homogeneous permeability \( \kappa_m \) evaluated for the mean parameter values versus the mean normalized wetting phase saturation. The ratio of horizontal to vertical effective permeability, plotted in Figure 6-16 versus the mean capillary pressure, shows that the anisotropy in the effective permeability is not dependent on the mean capillary pressure for the Cape Cod soils. By contrast pressure dependent, effective permeability anisotropy ratios at the Borden Aquifer peak at values greater than 100.

Contributions to anisotropy, \( A_{ij} \), defined in (4.39) are plotted versus the mean capillary pressure in Figure 6-17 for the Cape Cod Aquifer case under examination. As expected, approaching nonwetting phase saturation the variability of the log of the intrinsic permeability has the only significant contribution. Approaching wetting phase saturation, the contribution to anisotropy due to the variance of \( L \) has a minor contribution. This is in direct contrast to the large degree of anisotropy found in the effective permeabilities of the Borden Aquifer. In that case, significant contributions to anisotropy occurred due to the variance of \( B \), the variance of \( L \), as well as the covariance of \( B \) and \( L \). The absence of anisotropy at Cape Cod is largely due
to differences in the value of partial derivatives with respect to \( R_o \) in the two aquifers.

From (4.31) we know that the anisotropy, \( A \), of the effective nonwetting phase permeabilities in a perfectly stratified aquifer with uniform, vertical flow through a static wetting phase is given by

\[
A = \exp \left[ \frac{\left( b_i b_j \sigma_j^2 + \delta_{i,j} \sigma_g^2 \right) \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j}}{(|\varepsilon| + 1)} \right]
\]

(6.7)

where \( \varepsilon = \xi_1 J_{01} \frac{\partial R_o}{\partial \zeta_c} \). Defining \( B_{i,j} \) as

\[
A_{i,j} = \exp \left( \frac{B_{i,j}}{|\varepsilon| + 1} \right)
\]

(6.8)

\[
B_{i,j} = \left( b_i b_j \sigma_j^2 + \delta_{i,j} \sigma_g^2 \right) \frac{\partial R_o}{\partial \Phi_i} \frac{\partial R_o}{\partial \Phi_j} (2 - \delta_{i,j})
\]

and \( A = \exp \left( \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{B_{i,j}}{|\varepsilon| + 1} \right) \right) \). It is apparent that the magnitude of \( B_{i,j} \) relative to the value of \(|\varepsilon| + 1\) determines whether a parameter pair covariance will make a significant contribution to the anisotropy of the effective permeabilities. Figures 6-18 and 6-19 show the value of \( B_{i,j} \) and \(|\varepsilon| + 1\) versus normalized mean capillary pressure for the base case Cape Cod and Borden Aquifer characterizations. The value of \(|\varepsilon| + 1\) is significantly greater than every value of \( B_{i,j} \) for the Cape Cod Aquifer conditions due both to the generally low values of \( \frac{\partial R_o}{\partial \zeta_c} \) relative to \( \frac{\partial R_o}{\partial \Phi_i} \) and \( \xi_1 \) in these soils. By contrast, the value of \(|\varepsilon| + 1\) for Borden Aquifer is approximately one-tenth of the Cape Cod value, while the values of \( B_{i,j} \) are generally greater for the Borden Aquifer than for the Cape Cod Aquifer – illustrating why the Borden aquifer is more anisotropic than the Cape Cod Aquifer.

In order to isolate the role of the mean parameters in the estimated permeability anisotropy, the base case conditions for the Cape Cod Aquifer were systematically altered by modifying the mean value of the p-s-k parameters to the values estimated for the Borden Aquifer and the value of the permeability anisotropy estimated in each case. Figure 6-20 shows the permeability anisotropy for the base case and modified systems. See Table 6.10 for the parameter values used in the base case and modified systems. Note that the value of \( \bar{L} \) was set to an intermediate value, rather than the exact Borden Aquifer value, because physically unreasonable effective permeabilities resulted when the mean value of \( L \) was set to the Borden value; the physically
unreasonable values were of the type discussed in Chapter 4 where the horizontal effective nonwetting phase permeability increased with falling capillary pressures over some range. It is apparent from the anisotropy in the base case and the modified cases that modifying $\bar{L}$ by itself has little effect, while increasing the mean value $\bar{B}$ by itself or $\bar{B}$ with $\bar{L}$ increases the permeability anisotropy substantially.
Figure 6-11: a) Mean normalized saturation versus mean capillary pressure for both perfectly stratified condition and measured correlation scale ratio and normalized saturation at mean parameters, $S_e (\bar{\Gamma})$ and b) contributions to mean normalized saturation for base case, van Genuchten characterization of Cape Cod aquifer.
Figure 6-12: Mean and standard deviation of nonwetting phase volumetric content for base case, Cape Cod aquifer, van Genuchten characterization with zero porosity variance and zero residual saturation variance.
<table>
<thead>
<tr>
<th></th>
<th>Pc'</th>
<th>B</th>
<th>L</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Graph" /></td>
<td><img src="image2" alt="Graph" /></td>
<td><img src="image3" alt="Graph" /></td>
<td><img src="image4" alt="Graph" /></td>
<td></td>
</tr>
<tr>
<td><img src="image5" alt="Graph" /></td>
<td><img src="image6" alt="Graph" /></td>
<td><img src="image7" alt="Graph" /></td>
<td><img src="image8" alt="Graph" /></td>
<td></td>
</tr>
</tbody>
</table>

Figure 6-13: First and second partial derivatives of $R_o$ with respect to $\hat{P}_c (= \alpha_g P_c)$, $B$, $L$, and $F$ for variable slope parameter, van Genuchten characterization at Cape Cod aquifer versus normalized capillary pressure $\hat{P}_c$. 

190
Figure 6-14: Effective horizontal and vertical relative permeability, $\kappa_h$ and $\kappa_v$, and homogeneous relative permeability, $\kappa_g = \exp(\bar{R})$ and $\kappa_m = \exp(\bar{\Gamma})$, versus normalized mean capillary pressure, evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.
Figure 6-15: Effective relative permeability, $\kappa_u$ and $\kappa_h$, and homogeneous permeability, $\kappa_m = \exp R_o (\bar{S}_e)$ versus mean normalized saturation; evaluated for base case, van Genuchten Cape Cod aquifer characterization with perfect stratification.
Figure 6-16: Ratio of horizontal to vertical effective permeabilities versus mean normalized capillary pressure, evaluated for base case Cape Cod aquifer conditions.
Figure 6-17: Contributions to horizontal - vertical permeability ratio, $A_{i,j}$, versus normalized mean capillary pressure, where anisotropy is product of individual contributions at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.
Figure 6-18: Contributions to horizontal - vertical permeability ratio, $B_{i,j} = (|\varepsilon| + 1) \ln A_{ij}$, versus normalized mean capillary pressure, where anisotropy is, $\exp \left( \frac{\sum B}{(|\varepsilon|+1)} \right)$, exponential of sum of individual contributions divided by $(|\varepsilon| + 1)$ at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Cape Cod aquifer with perfect stratification.
Figure 6-19: Contributions to horizontal - vertical permeability ratio, $B_{i,j} = (|\varepsilon| + 1) \ln A_{ij}$, versus normalized mean capillary pressure, where anisotropy is, $\exp \left( \frac{\sum B}{(|\varepsilon| + 1)} \right)$, exponential of sum of individual contributions divided by $(|\varepsilon| + 1)$ at given mean capillary pressure. Evaluated for van Genuchten, variable slope, characterization of Borden aquifer with perfect stratification.
Figure 6-20: Ratio of horizontal to vertical effective permeability for Cape Cod base case characterization and selected modifications to mean parameters.
6.4 Lateral Spreading of Nonwetting Phase Plumes in the Cape Cod and Borden Aquifers

The length scale of the lateral spreading of density driven, nonwetting phase flow, with static wetting phase, was estimated using the integral technique discussed in Chapter 5 for both the Cape Cod and Borden Aquifers. Two cases are considered.

1. Steady state PCE release at the water table ($\rho_o = 1.6$, $\sigma = 45$ dynes/cm, $\mu_o = 0.01$ g/cm²/sec²) in vertical, two dimensional domain with boundary conditions as follows: center line relative permeability $\tilde{k}_{r,0} = 0.105$ and initial plume length scale, $w_0 = 100$ cm. Note, the represented source area is of infinite extent in the direction perpendicular to the solution domain.

2. Continuous air sparging ($\rho_o = 0.0012$, $\sigma = 73$ dynes/cm, $\mu_o = 0.00018$ g/cm²/sec²) below the water table from circular, horizontal source, with base case boundary conditions as follows: center line relative permeability $\tilde{k}_{r,0} = 0.80$ and plume radius, $r_0 = 250$ cm. Air sparging simulations neglect the compressibility effects accompanying injection of air flow below the water table and the impact of the water table itself.

The value of $B$ was modified as a function of the ratio of the interfacial tension (see Section 2.2.3) of the fluid pair in which the p-s-k parameters were estimated and the interfacial tension of the simulated system.

6.4.1 DNAPL

Figure 6-21 (same as Figure 5.2) shows the system profile of the simulated DNAPL release for the base case Borden aquifer. Figure 6-22 shows the system profile for the same boundary conditions for base case Cape Cod Aquifer. The plume width in the Cape Cod Aquifer expands less due to the absence of pressure dependent anisotropy as found at Borden.

6.4.2 Air Sparging

The air sparging solution was evaluated for both the Borden and Cape Cod aquifer conditions and the system profiles are represented in Figures 6-23 and 6-24. In this case, the plume is
assumed to be axisymmetric and the lateral radial extent, \( R \), is defined for \( f(u) = f(r/R) \). The air sparging simulations do not explicitly represent the water table or the pressure dependence of air density, however the reduction of accuracy is acceptable given the narrow goal of estimating the sensitivity of system response to differences in effective properties. There is significantly greater lateral spreading under Borden Aquifer conditions implying the need for more closely spaced sparge points in the Cape Cod Aquifer than at Borden; however the air content is greater and more smoothly distributed in the Cape Cod than at the Borden Aquifer, as reflected in the higher mean nonwetting phase content and lesser nonwetting phase content variance – two desirable properties for air sparging remediation systems.

The rate of air flow was increased for both aquifers by increasing the source point, center line, relative permeability as high as 0.8 and repeating the estimation of lateral plume half-width. Figure 6-25 shows the plume half width, \( w \), versus elevation under Borden Aquifer conditions for \( \kappa_{r,0} = 0.2, 0.4, \) and \( 0.8 \). In the Borden Aquifer increases in flow reduced the lateral spreading of the plume. This response occurs in part due to the increase of source point capillary pressure and the associated reduction in the magnitude of pressure dependent anisotropy. Figure 6-26 shows the plume width dependence on flow rate at Cape Cod. The rate of flow has the reverse impact at the Cape Cod aquifer, where increases in the rate of air flow increase the lateral spreading of the nonwetting phase plume. This occurs due to the absence of significant, pressure dependent anisotropy in the Cape Cod effective permeabilities and increases in lateral gradients which accompany increases in the center line, source point relative permeability.

### 6.5 Summary

Cape Cod and Borden aquifers were used as prototypes to examine effective properties in different aquifers. The Cape Cod aquifer contains more coarse grained materials than Borden due to the different depositional environment of the two aquifers. Estimates of the Brooks-Corey and van Genuchten function parameters for capillary pressure data sets for the two aquifers were described, including for the Borden aquifer alternative interpretations of the variability of soil properties.
Figure 6-21: DNAPL release at Borden aquifer; system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Borden van Genuchten characterization, with variable slope parameter; boundary conditions: $w_0 = 100$ cm, $\kappa_{z,0} = 0.105$ (same as Figure 5.2).
Figure 6-22: DNAPL release at Cape Cod aquifer; system profile for steady state simulation of DNAPL release at water table, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Cape Cod van Genuchten characterization, with variable slope parameter. Boundary conditions: \( w_o = 100cm, \kappa_{z,0} = 0.105 \).
Figure 6-23: Air sparging at Borden aquifer; system profile for steady state simulation of air sparging, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Borden van Genuchten characterization, with variable slope parameter; boundary conditions: \( w_0 = 250 \text{ cm}, \kappa_{z,0} = 0.80 \).
Figure 6-24: Air sparging at Cape Cod Aquifer; system profile for steady state simulation of air sparging, subject to gravity flow based on nonwetting phase effective properties, for uniform mean flow and static water and Cape Cod, van Genuchten characterization, with variable slope parameter. Boundary conditions: \( w_o = 250 \text{ cm}, \, \kappa_{z,0} = 0.80 \).
Figure 6-25: Flow rate dependence of lateral spreading at Borden aquifer; nonwetting phase, lateral plume length scale for $\kappa_{r,0} = 0.2, 0.4,$ and 0.8 for base case characterization and $w_o = 250$ cm.
Figure 6.26: Flow rate dependence of lateral spreading at Cape Cod aquifer; nonwetting phase, lateral plume length scale for $\bar{r}_x,0 = 0.2, 0.4, \text{ and } 0.8$ for base case characterization and $w_o = 250 \text{ cm.}$
The estimated effective permeability of the Cape Cod Aquifer is less anisotropic than at the Borden Aquifer, largely the result of the greater correlation scale and lower characteristic pressure of the Cape Cod Aquifer.

Integral solutions of the nonwetting phase, plume half-width are presented for cases of DNAPL and air sparging. In both cases, not surprisingly given the anisotropy of the effective permeabilities at the Borden Aquifer, lateral spreading was significantly greater at the Borden Aquifer. Increasing nonwetting phase flow rate increased lateral spreading at the Cape Cod Aquifer due to increases in lateral pressure gradients. Conversely, increasing flow rate reduced lateral spreading at the Borden Aquifer due to the capillary pressure dependence of the effective permeability anisotropy.
Chapter 7

Summary of Findings and Concluding Remarks

This chapter is a discussion of the principal contributions of this work, including its place in the context of prior investigations, a summary of significant findings and the implications for future work in this area.

7.1 Overview

Natural variability has a profound impact on the nature of flow through porous media. The impact of heterogeneity on multiphase flow is explored using a spectral perturbation technique employing a stationary, stochastic representation of the spatial variability of soil properties. A derivation of the system's effective properties - nonwetting phase moisture content, capillary pressure, normalized saturation and permeability - was developed which is not specific as to the form of the permeability dependence on saturation or capillary pressure; enabling evaluation and comparison of effective properties with differing characterization forms and encompassing prior work on unsaturated flow and multiphase systems. Conventional characterization techniques are employed to parameterize the saturation, capillary pressure, relative permeability relationships and applied to the Cape Cod and Borden aquifers.

An approximate solution for the characteristic width of a dense nonaqueous phase liquid (DNAPL) plume or air sparging contributing area is derived to evaluate the sensitivity of system
behavior to properties of input processes. Significant nonwetting phase, capillary pressure dependent, anisotropy is predicted for uniform, vertical flow in the Borden Aquifer consistent with both prior experimental observations and Monte Carlo simulations. Similar levels of anisotropy are not found in the case of the Cape Cod aquifer; the difference is attributed largely to the mean value of the log of the characteristic pressure which is shown to control the rate of return to asymptotic permeability and hence system uniformity. Reduction of anisotropy with reductions in interfacial tension were observed, consistent with prior numerical simulations. Positive dependence of lateral spreading on input flow rate is predicted for Cape Cod Aquifer with reverse response at Borden Aquifer due to capillary pressure dependent anisotropy of Borden Aquifer. The effective permeability for horizontal flow with core scale heterogeneity was found to be velocity dependent with features qualitatively similar to experimental observations and numerical experiments. Application of Leverett scaling as generally implemented in Monte Carlo simulations found to was significantly under represent aquifer heterogeneity and for Borden Aquifer, van Genuchten characterization reduces system anisotropy by several orders of magnitude. Anisotropy of the effective properties proved to be less sensitive to Leverett scaling if the Brooks-Corey characterization was used due to insensitivity in this case to the variance of the slope parameter.

7.2 Context of Prior Investigations

Field scale experimentation and Monte Carlo simulations point to the importance of understanding the role of heterogeneity in order to make reliable and accurate forecasts of multiphase flow in natural systems. Even if a "complete" mapping of soil properties were physically possible, practical limits on the discretization of numerical models will not permit representation of small scale heterogeneity. The goal of this work is to develop an understanding of the impact of natural variability, such that effective field scale properties might be specified which accurately reflect the important characteristics of subgrid heterogeneity. Important, qualitative evidence of the impact of correlation scale, interfacial tension, flow rate, and variance magnitude have been gained in Monte Carlo investigations of heterogeneous multiphase systems. The lessons are not however, readily transferable to other aquifers. An initial investigation using analytical,
stochastic techniques has highlighted the promise of the technique, but failed to illuminate the impact of natural variability due to inaccurate representation of system anisotropy and less than complete evaluation of the significant engineering issues.

7.3 Methodology

The present work may be seen methodologically as an extension of the unsaturated flow investigations of Yeh et al. (1985 a,b,c) to include both the wetting and nonwetting phases. This technique employs a perturbation analysis of the continuity equation of each of the two flowing phases. A spectral representation of the perturbation and system parameters is introduced, subject to the assumption of local stationarity, enabling solution of the moments of pressure, capillary pressure and saturation. The effective permeability is expressed as a function of the output moments by the application of the expectation operator to the multiphase form of the Darcy equation. The exponential generalization approximation of the effective permeabilities was adopted, as in Gelhar and Axness (1983), Yeh et al. (1985a) and elsewhere, whereby the result was regarded to be a truncated Taylor expansion of an exponential function; this prevents the occurrence of negative effective permeabilities in the case of high variability systems.

As is typical in investigations of multiphase flow, functions describing the relationship between capillary pressure, saturation and permeability are specified to complete the mathematical representation of the system. The effective property derivations are general in that the derivatives of the relative permeability functions are left in an unevaluated form until the time when the properties were to be estimated. In this way effective properties can be evaluated for any p-s-k function form. In principal, the effective property findings are general for any flow / aquifer configuration; however, closed form analytical expressions for estimation of the effective properties were derived for the case of uniform flow parallel to one of the principal axes or nonuniform flow in an arbitrary direction in a perfectly stratified aquifer – other more complicated conditions require numerical integration of the spectral functions.
7.4 Findings

7.4.1 Capillary Pressure Sensitive Anisotropy

Although scalar forms were assumed for local representation of the relative and intrinsic permeabilities, the predicted effective permeabilities are anisotropic. The saturated effective permeabilities, wetting and nonwetting phases, were consistent with prior findings on the effective permeability of heterogeneous systems. The relative permeability of a given phase is in general increasingly anisotropic with reductions in that phase’s volumetric content. The nature of the anisotropy of the relative permeability is a function of the mean and variance of soil properties as well as the pressure gradient, the correlation scale and the partial derivative of the relative permeability with respect to the capillary pressure.

In gravity driven, uniform nonwetting phase flow, the anisotropy is directly proportional to the exponent of the variability of ln $k$ over a representative set of soils at a given capillary pressure. Increases in vertical correlation scale or in the partial derivative of the log permeability with respect to capillary pressure will however reduce anisotropy and it is the relative magnitude of the variability of ln $k$ and the input properties which determines the magnitude of the anisotropy of the effective permeability. Analogous results for unsaturated flow may be found in Yeh et al. (1985b).

**Anisotropy magnitude dependent on both mean and variance of p-s-k parameters.** The anisotropy ratio, the ratio of the horizontal to vertical effective permeabilities, predicted for the Borden aquifer reaches a peak near 4000 despite relatively low log permeability variance. This high anisotropy is consistent with field experiments and Monte Carlo simulations of multiphase flow in the Borden aquifer in which large lateral spreading occurred or was predicted for DNAPL flow below the water table. By contrast, the effective permeability anisotropy for the Cape Cod aquifer was relatively low, despite variability of the same relative magnitude as the Borden Aquifer. Several factors were responsible for the high anisotropy of the Borden aquifer including a smaller correlation scale, greater measured correlation between the p-s-k function parameters and a smaller partial derivative of the relative permeability with respect to the capillary pressure. The magnitude of this derivative is a function of the mean values of the characteristic pressure and slope parameters, whose values in the case of the Bor-
den Aquifer are characteristic of soils which dewater at higher capillary pressures, but then reach residual saturation values over a relatively small capillary pressure range — as would be expected in a uniform, medium to fine grained soil.

Inverse dependence of anisotropy on interfacial tension. Effective properties and lateral spreading are sensitive to the value of the interfacial tension, represented by modification of the mean of the characteristic pressure parameter. Reducing interfacial tension reduces system anisotropy and therefore lateral spreading because of the characteristic pressure dependence of the partial derivative of the log permeability with respect to capillary pressure. This effect is consistent with Monte Carlo simulations which demonstrate significant dependence of lateral spreading on the magnitude of the interfacial tension.

7.4.2 Effective Residual Wetting Phase Saturation

The rate of approach of the mean normalized wetting phase saturation to zero with increasing capillary pressure is diminished relative to the homogeneous capillary pressure-saturation function. The mean normalized saturation in some cases persists to capillary pressures of sufficient magnitude as to be interpreted as an effective residual wetting phase saturation. The effective residual saturation increases with increasing horizontal and vertical correlation scales.

7.4.3 Impact of p-s-k Characterization Form

Leverett Scaling misrepresents system variability. Imposition of Leverett scaling, whereby the local characteristic pressure is a deterministic function of the local permeability and the slope parameter is held constant, produces substantial errors in the effective permeability and significantly underestimates the field scale anisotropy. The anisotropy of the Borden Aquifer effective permeability using the Leverett scaling stochastic model was several orders of magnitude less than in the alternative interpretation representing the measured system variability.

Further, there was little impact of the form of the characteristic pressure variability. That is, effective permeabilities evaluated for the case of uncorrelated characteristic pressure variability were nearly the same as when the characteristic pressure was assumed to be a deterministic function of the local permeability.

Brooks-Corey / van Genuchten. Effective properties were estimated for multiphase
flow based on both the van Genuchten and Brooks-Corey characterizations. The predicted anisotropy of heterogeneous systems in which the relative permeability is governed by the Brooks-Corey functions approaches extremely large values for mean capillary pressures approaching the threshold pressure. Some caution is warranted in interpreting these results due to discontinuities in the derivative of the relative permeability at the threshold pressure. Reported problems with discretization dependence of numerical simulations in Brooks-Corey systems (Rathfelder and Abriola, 1998) may be in part due to high anisotropies reached within a narrow capillary pressure range – regions which are resolved only with high levels of discretization.

7.4.4 Velocity Dependent Relative Permeability Effects

Effective permeabilities, evaluated for horizontal flow systems are sensitive to the flow velocity, in a manner qualitatively consistent with prior experimental and analytical investigations.

Issues of scale and heterogeneity appear even at the core scale. Undisturbed cores and even cores which are by intent homogenized contain internal structure which effect system response. Prior experimental and numerical investigations indicate that steady state relative permeability measurements are sensitive to flow velocity and that the form of the dependence on velocity depends in part on the system heterogeneity.

Relative permeability measurements sensitive to flow rate. The velocity dependence of effective properties in laminated soils was qualitatively consistent with prior observations, whereby increases in the capillary number (i.e., ratio of viscous to capillary forces) is associated with increases of the nonwetting phase effective permeability. Increasing capillary number had mixed effects in the wetting phase, increasing the wetting phase permeability for low wetting phase saturations and reducing the wetting phase permeability for high wetting phase saturations.

End point permeability positive function of total flow rate. End point permeabilities were estimated as the nonwetting phase permeability coinciding with a wetting phase relative permeability of 1 percent. Velocity dependence of end point permeabilities was found which is qualitatively similar to that observed in relative permeability measurement experiments, such that greater total velocity is positively related to the end point nonwetting phase permeability

212
and inversely related to the effective residual wetting phase saturation.

7.4.5 Implications for Lateral Spreading in Natural Aquifers

Integral method applied to estimate nonwetting phase lateral spread. The integral method was applied to derive the ordinary differential equation for the characteristic width of a steady state, nonwetting phase plume with mean, vertical flow and static wetting phase. In order to simplify the analysis, the component of vertical flow due to vertical capillary pressure gradients was assumed to be small relative to the gravity flow component. The derivative of the characteristic plume width with respect to elevation was found to be proportional to the Kirchoff transform averaged over the plume width. A numerical solution was implemented and applied to the cases of DNAPL and air sparging at both the Borden and Cape Cod aquifers. Lateral spreading was significantly greater at the Borden Aquifer due to the relatively high levels of pressure dependent anisotropy.

Impact of flow rate on lateral plume width is aquifer dependent. At the Borden Aquifer the estimated plume width was a negative function of the rate of flow. Increasing flow, accomplished by an increase in the source point capillary pressure, reduced anisotropy and consequently lateral flow. Conversely, at the Cape Cod aquifer, with minimal pressure dependent anisotropy effects, increases in source point permeability increase lateral flows due to the impact of greater horizontal gradients.

7.5 Recommendations for Future Investigations

Recommendations for future research fall into two broad categories. The first stems from a sense that improvements in the description of the local scale problem of relating permeability, saturation and capillary pressure are desirable. The techniques in common practice are empirical or first order physical models representing initial attempts to grapple with these difficult problems, which involve local scale representations due to pore scale physics in complex domains. The second broad category of recommendations deals with direct extensions to the current work to further our understanding of field scale properties and extend these results to deal with problems of dissolution and efficient air sparging design.
7.5.1 Local Scale Representation

This research effort has provided insight into the impact of characterization form and the interplay of the mean hydraulic properties and their spatial variability. This has lead to a corroboration and physical understanding of the Monte Carlo findings of other researchers. We can with some confidence predict the impact of modifying correlation scale, or the statistical moments of the parameters of the p-s-k functions on numerical simulations of flow in heterogeneous media. Extension of these predictions to natural systems is however uncertain due to shortcomings in the predictive capacity of commonly used p-s-k functions and the still not well understood sensitivity of relative permeability measurements to experimental conditions.

A profound source of frustration is derived from the sense that the findings and the analysis in general are true only in so far as they apply to the world of simulated flow. The foundation of the techniques employed both here and commonly in simulations of heterogeneous media rely on models of pore connectivity that enable predictions of the permeability as a function of capillary pressure and saturation, based on measurements of capillary pressure and saturation during soil drainage. Despite mixed successes in predictions of wetting phase permeability, the engineering and scientific community have adopted these techniques for the nonwetting phase with even less substantial experimental support.

Nonwetting phase relative permeability measurements that have been performed do not support the prevailing model of relative permeability. A common and still not fully understood phenomena is the occurrence of end point nonwetting phase permeabilities less than half the intrinsic permeability, even with wetting phase content at what seem to be residual levels. This has given rise to additional ad-hoc techniques to salvage the p-s-k functions by introducing still another parameter which represents the end point nonwetting phase permeability achieved at wetting phase residual saturation. Even this property has been shown to be a function of the drainage history and fluid velocity (Demond and Roberts, 1993).

The concept of relative permeability itself, unchanged since its introduction over 60 years ago, raises serious questions. While generally treated as a single valued function of saturation, both experimental and theoretical findings, including this document, suggest that the property is a complex function of the flow conditions, soil properties and system heterogeneity. Core scale heterogeneities impart to relative permeability measurements a sensitivity to the experimental
conditions under which the measurements were taken; the relevant conditions include drainage history, fluid viscosity, fluid pair interfacial tension and measured velocity. It is important not to forget that flow occurs in a tortuous domain of interconnected pores and that the dynamic process of drainage and the associated measurements of relative permeability are a function of the physical attributes of drained pores and the continuity of liquid phases between pores. Relative permeability expressed as a function of either capillary pressure or saturation is principally an empirical concept which attempts to lump the impacts of pore scale processes, but with a less firm statistical, empirical or physical grounding than is the case for saturated flow.

Finally, Leverett scaling and other similar scaling relationships are often invoked to relate pressure scale parameters as deterministic functions of the local permeability; but the reliability of these scaling practices remains not thoroughly examined. The soil samples from the Borden Aquifer reflect the uniformity of the aquifer, but even here Leverett scaling and modifications of Leverett scaling introduce systematic errors in the rescaled capillary pressure curves. For the Borden soils, the capillary pressure curves appear to scale as $k^{-1/2}$ for high capillary pressures, but to scale as $k^{-1}$ for lower capillary pressures raising the possibility of a pressure dependent scaling exponent or the definition of scaling regimes defined based on a reexamination of the pore scale dynamics during drainage.

It is likely that improvements in representation of the local scale problem will require cooperation between experimentalists and hydrodynamicists, and should draw also on the experience of the stochastic hydrologists who have addressed upscaling problems of the type that needs to be achieved to extend the understanding of pore scale fluid mechanics to improvements in local scale characterization.

### 7.5.2 Direct Extensions of Current Work

One of the strongest findings of this document is the substantial difference in the effective anisotropy of Cape Cod and Borden Aquifers. Strongly anisotropic behavior observed at the Borden Aquifer is consistent with findings of this document and related Monte Carlo type investigations. By contrast, the Cape Cod aquifer has virtually no predicted pressure dependent anisotropy. A field investigation is recommended which will ideally involve the emplacement
of DNAPL's at the water table in the Cape Cod Aquifer as was done previously at the Borden Aquifer. Controlled lab scale experimentation in two-dimensional systems with replicated natural soil conditions might also be used to resolve the question with somewhat less certainty.

The direction of future analytical and numerical investigations should draw on similar experiences in the investigation of unsaturated flow. In that area numerical simulations in heterogeneous media and "equivalent" homogeneous media with effective properties were performed to validate the predicted effective properties and their application for domains where the characteristic length of mean properties approaches the correlation scale of input properties. The same type of investigation is a worthy effort for the multiphase flow problem. The objectives ought to be:

1. verification of effective properties, including effective permeability, moments of capillary pressure, and moments of nonwetting phase volumetric content for the assumptions in which they were derived - low amplitude variability and separation of scales

2. test extension of effective property estimates into systems of high variability and rapid variation in mean properties

3. expand understanding of the distribution of nonwetting phase saturation to develop sense of sensitivity of dissolution of nonwetting phase to flow and media properties

4. simulation of lab scale investigations including soil drainage and relative permeability measurements to understand the dynamics of the drainage process and the impact of core scale heterogeneity on the measured relative permeability, capillary pressure and residual saturation

The effective permeabilities predicted for some range of mean parameter values and high variability as found at Borden Aquifer were found to be physically unreasonable. Future investigations are warranted to explore methods of addressing this limitation. This might include improved linearization or implementation of approximations in such a way to ameliorate this problem.

Nonwetting phase dissolution may also be amenable to investigation by analytical, stochastic techniques. In this case, the results from the current investigation of the moments of the
nonwetting phase volumetric content might be extended to compute the correlation scales of
the nonwetting phase and used as input properties to the analysis and estimation of effective
dissolution kinetics in heterogeneous aquifers. A similar technique to that used in estimation
of sorption kinetics in heterogeneous aquifers (Miralles-Wilhelm and Gelhar, 1996) might be
employed in this case.

The correlation scale of the nonwetting phase volumetric content is an important measure
impacting both the rate of DNAPL dissolution and effectiveness of air sparging, as it may
effect the distances required for the diffusion of dissolved compounds to a flowing air phase
or dissolution and transport of DNAPL. The correlation scale may be estimated directly by
integration of the spectral density of the nonwetting phase or alternatively, approximations of
the correlation scale may be made by assuming a form for the output process correlation model.
Bibliography


221


Appendix A

Notation

\(\alpha\) \hspace{1em} \text{characteristic pressure of Van Genuchten characterization}

\(\beta\) \hspace{1em} \text{modified Leverett Scaling exponent (also phase index)}

\(\delta_p\) \hspace{1em} \text{difference between nonwetting and wetting phase liquid density}

\(\varepsilon\) \hspace{1em} \text{composite variable \((= \frac{J_0 \xi_1 \partial R_a}{\partial c})\)}

\(\Phi\) \hspace{1em} \text{parameter set \(\{B, L, F\}\)}

\(\Gamma\) \hspace{1em} \text{parameter set \(\{P, \Phi\}\)}

\(\kappa_{\beta}\) \hspace{1em} \text{relative permeability of \(\beta\) phase}

\(\kappa_g\) \hspace{1em} \text{exponent of mean log relative permeability \((\exp \bar{R})\)}

\(\kappa_m\) \hspace{1em} \text{relative permeability for zero variance evaluated for mean parameter values}

\(\lambda\) \hspace{1em} \text{slope parameter of Brooks-Corey characterization}

\(\mu_{\beta}\) \hspace{1em} \text{dynamic viscosity of phase \(\beta\)}

\(\sigma\) \hspace{1em} \text{interfacial tension}

\(\theta_o\) \hspace{1em} \text{nonwetting phase volumetric content}

\(\theta_r\) \hspace{1em} \text{irreducible wetting phase residual volumetric content}

\(\theta_w\) \hspace{1em} \text{wetting phase volumetric content}

\(\rho\) \hspace{1em} \text{ratio of correlation scales \(\xi_2/\xi_1\)}

\(\rho_{\beta}\) \hspace{1em} \text{density of phase \(\beta\)}

\(\omega, \omega_j\) \hspace{1em} \text{wave number vector and \(j\) component of wave number}

\(\xi_i\) \hspace{1em} \text{correlation scale in \(i\) direction}
$A_{ij}$ contribution to effective permeability anisotropy ratio, where ratio is product of contributions

$B$ log of p-s-k function characteristic pressure ($= -\ln \alpha, \ln P_d$)

$F$ natural logarithm intrinsic permeability ($= \ln k$)

$g$ downward pointing vector with magnitude of gravitational acceleration

$j$ direction index

$J_{\beta}$ negative of pressure gradient plus gravitational force vector

$k$ intrinsic permeability

$L$ transformed p-s-k function slope parameter ($= \ln \frac{m}{1-m}, \ln \lambda$)

$m$ slope parameter of Van Genuchten characterization

$n$ porosity

$P_{\beta}$ pressure of phase $\beta$

$P_c$ capillary pressure

$P_d$ displacement pressure of Brooks-Corey characterization

$q_{\beta}$ specific discharge vector of $\beta$ phase

$q_{\beta,j}$ component of $\beta$ phase specific discharge in $j$ direction

$Q_t$ total nonwetting phase flow

$R_{\beta}$ log permeability of wetting phase

$S_e$ normalized wetting phase saturation

$S_{ij}$ contribution to mean saturation

$(\bar{\circ})$ mean

$(\circ)'$ perturbation

$(\bar{\circ})$ effective property

$(\bar{\circ})$ center line value
Appendix B

Summary of Multiphase Monte Carlo Simulation References

This Appendix contains a single table summarizing many of the numerical simulations of multiphase flow in heterogeneous media in the water resources literature. The table describes the simulated domain, the p-s-k functions, the numerical discretization and the characteristics of the random field. This table is an overview of each of the references, but is not intended to completely characterize the model or all of the simulated domains or scenarios. The reader is strongly encouraged to consult the original references to complement the information provided in this table.

The appendix is intended to be read as a single table where the first four pages make up the upper half of the table and the latter four pages the bottom half of the table as shown in the figure below.

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Authors</td>
<td>Year</td>
<td>Title</td>
<td>domain</td>
</tr>
<tr>
<td>----------------------------------------</td>
<td>------</td>
<td>----------------------------------------------------------------------</td>
<td>--------</td>
</tr>
<tr>
<td>Abin, A., J.J. Kaluarachchi, M.W. Kemblowski and C.-M. Chang</td>
<td>1996</td>
<td>Stochastic analysis of multi-phase flow in porous media: II Numerical Simulations</td>
<td>1D</td>
</tr>
<tr>
<td>Brown, C.L., G.A. Pope, L.M. Abriola and K. Sepehrnoor</td>
<td>1994</td>
<td>Stimulation of surfactant-enhanced aquifer remediation</td>
<td>2D</td>
</tr>
<tr>
<td>Chang, C.-M., Kemblowski, M.W. Kaluarachchi, J.J. and A. Abdin</td>
<td>1995b</td>
<td>Stochastic analysis of two-phase flow in porous media: II. Comparison between perturbation and Monte Carlo results</td>
<td>1D</td>
</tr>
<tr>
<td>Dekker, T.J. and L.M. Abriola</td>
<td>unpub</td>
<td>The influence of field-scale heterogeneity on the infiltration and entrapment of dense nonaqueous phase liquids in saturated formations</td>
<td>2D</td>
</tr>
<tr>
<td>Kueper, B.H. and E.O. Frind</td>
<td>1991b</td>
<td>Two-phase flow in heterogeneous porous media: 2. Model application</td>
<td>2D</td>
</tr>
<tr>
<td>Kueper, B.H. and J.J. Gerhard</td>
<td>1995</td>
<td>Variability of point source infiltration rates for two-phase flow in heterogeneous porous media</td>
<td>3D</td>
</tr>
<tr>
<td>units</td>
<td>Relative Permeability</td>
<td>Hysteresis</td>
<td>Capillary Pressure</td>
</tr>
<tr>
<td>-------</td>
<td>-----------------------</td>
<td>------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>5 g/cm/s</td>
<td>$k_{r,w} = \bar{S}_w^n$</td>
<td>no</td>
<td>$\bar{s}<em>w = \exp\left(\frac{-\alpha \beta</em>{sw} p_{sw}}{n}\right)$</td>
</tr>
<tr>
<td></td>
<td>$k_{r,nw} = \bar{S}_n^n - \bar{S}_w^n$</td>
<td></td>
<td>$\bar{s}<em>t = \exp\left(\frac{-\alpha \beta</em>{sw} p_{sw}}{n}\right)$</td>
</tr>
<tr>
<td>2</td>
<td>$k_{r1} = k_{r1}^0 (S_{n1})^{r1}$</td>
<td>no</td>
<td>$S_n = (P_s / P_s)^{1/k}$</td>
</tr>
<tr>
<td></td>
<td>$k_{r2} = k_{r2}^0 (1 - S_{n1})^{r2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k_{r3} = k_{r3}^0 (S_{n3})^{r3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 g/cm/s</td>
<td>$k_{r,w} = \exp(-\Gamma P_s)$</td>
<td>no</td>
<td>Saturation not explicitly modeled</td>
</tr>
<tr>
<td></td>
<td>$k_{r,nw} = 1 - \exp(-\Gamma P_s)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 g/cm/s</td>
<td>$k_{r,w} = \bar{S}_w^{1/2} \left[ 1 - (1 - \bar{S}_w^{1/m})^{1/m} \right]^2$</td>
<td>no</td>
<td>$S_s = \frac{\theta_s - \theta_{sw,i}}{\phi - \theta_{sw,i}}$</td>
</tr>
<tr>
<td></td>
<td>$k_{r,nw} = \left(1 - \bar{S}_w\right)^{1/2} \left(1 - \bar{S}_w^{1/m}\right)^{1/m}$</td>
<td></td>
<td>$= \left[ 1 + \left(\sigma (k) P_s\right)^n \right]^m$</td>
</tr>
<tr>
<td></td>
<td>$\bar{S}<em>w = S_w + S</em>{sw}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 g/cm/s</td>
<td>$k_{r,w} = S_s^{2/\lambda + 3}$</td>
<td>no, drainage not simulated</td>
<td>$S_s = \frac{\theta_s - \theta_{sw,i}}{\phi - \theta_{sw,i}}$</td>
</tr>
<tr>
<td></td>
<td>$k_{r,nw} = (1 - S_s)^2(1 - S_s^{2/\lambda + 1})$</td>
<td></td>
<td>$= \left[ \frac{P_s}{P_s \sigma (\phi / k)} \right]^{1/\lambda}$</td>
</tr>
<tr>
<td>6 g/cm/s</td>
<td>$k_{r,w} = S_s^{2/\lambda + 3}$</td>
<td>no, drainage not simulated</td>
<td>$S_s = \frac{\theta_s - \theta_{sw,i}}{\phi - \theta_{sw,i}}$</td>
</tr>
<tr>
<td></td>
<td>$k_{r,nw} = (1 - S_s)^2(1 - S_s^{2/\lambda + 1})$</td>
<td></td>
<td>$= \left[ \frac{P_s}{P_s \sigma (\phi / k)} \right]^{1/\lambda}$</td>
</tr>
<tr>
<td>Random Parameters</td>
<td>mean</td>
<td>std. deviation</td>
<td>cross correlation</td>
</tr>
<tr>
<td>-------------------</td>
<td>------</td>
<td>----------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>1 in k α</td>
<td>-18.3</td>
<td>0.0001366 cm·s⁻²/g</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.00001366</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 in k</td>
<td>8.5 x 10⁻¹³ - 4.8 x 10⁻¹⁰ m²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3 in k Γ</td>
<td>-18.3</td>
<td>0.00037 cm·s⁻²/g</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>0.000037</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4 in Kw (ln k)</td>
<td>-4.62</td>
<td>Borden</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-4.62 -</td>
<td>sqrt(0.24) = .49</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LN(1000·9.8/0.001/100) = 16.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Jussel</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>5 in Kw (ln k)</td>
<td>-4.68</td>
<td>.51 = sqrt(0.26)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>-4.68 -</td>
<td>= -</td>
<td></td>
</tr>
<tr>
<td></td>
<td>LN(1000·9.8/0.001/100) = 16.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6 in Kw (ln k)</td>
<td>-4.55 - -4.65</td>
<td>sqrt(1.9) - sqrt(2.1)</td>
<td>1.36 - 1.45</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.86</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.86</td>
<td></td>
</tr>
<tr>
<td>Domain</td>
<td>h (m)</td>
<td>r (m)</td>
<td>nw Source</td>
</tr>
<tr>
<td>--------</td>
<td>-------</td>
<td>-------</td>
<td>-----------</td>
</tr>
<tr>
<td>1 NA</td>
<td>10</td>
<td></td>
<td>specified flow</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td>specified flow</td>
</tr>
<tr>
<td>3 NA</td>
<td>10</td>
<td></td>
<td>specified flow</td>
</tr>
<tr>
<td>4 10</td>
<td>5</td>
<td>75 L at 15 L/d **3 width of source area not specified - looks like point source - simulation continues until redistribution of nw phase is complete (approx. 40-120 days)</td>
<td>zero flow @ horizontal bdys, spec pressure @vertical bdys horizontal Jw = 1E-06 m/m</td>
</tr>
<tr>
<td>5 9</td>
<td>3.5</td>
<td>constant NAPL source at top - mid 40 cm of top bdy, constant wetting phase pressure = 0.0 and wetting phase saturation of 0.50 - elapsed time on order 5x10^5 seconds (6 days)</td>
<td>- zero flow @ horizontal bdys, - spec pressure @vertical bdy, hydrostatic for aqueous phase, value not specified for nonaqueous phase (looks like Pnw = Pw)</td>
</tr>
<tr>
<td>6 50</td>
<td>20</td>
<td>+2100 Pa capillary pressure at two nodes along top bdy + wide source spans 50 nodes</td>
<td></td>
</tr>
<tr>
<td>Authors</td>
<td>Year</td>
<td>Title</td>
<td>domain</td>
</tr>
<tr>
<td>----------------------</td>
<td>------</td>
<td>----------------------------------------------------------------------</td>
<td>--------</td>
</tr>
<tr>
<td>Mayer, A.S. and C.T. Miller</td>
<td>1996</td>
<td>The influence of mass transfer characteristics and porous media heterogeneity on nonaqueous phase dissolution</td>
<td>2D</td>
</tr>
<tr>
<td>Sleep, B.E. and J.F. Sykes</td>
<td>1993a</td>
<td>Compositional simulation of groundwater contamination by organic compounds: 1. Model development and verification</td>
<td>2D</td>
</tr>
<tr>
<td>Tjolosen, C.B. and E. Damseth</td>
<td>1991</td>
<td>A model for the simultaneous generation of core-controlled stochastic absolute and relative permeability fields</td>
<td>3D</td>
</tr>
<tr>
<td>Units</td>
<td>Relative Permeability</td>
<td>Hysteresis</td>
<td>Capillary Pressure</td>
</tr>
<tr>
<td>-----------</td>
<td>-----------------------</td>
<td>------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>7 g/cm/s</td>
<td>( k_{rw} = S_r^2 \left[ 1 - \left( 1 - S_r^{1/m} \right)^m \right]^2 )</td>
<td>yes, Luckner (1989)</td>
<td>( S_s = \frac{\theta_s - \theta_w}{\theta_m - \theta_o} \left[ 1 + \left( \frac{\theta_m - \theta_w}{\theta_m - \theta_o} \right)^m \right] )</td>
</tr>
<tr>
<td>8</td>
<td>( k_{r,w} = S_{rw}^{2/3} )</td>
<td>no</td>
<td>( S_s = \frac{\phi - \theta_{w,1}}{\phi - \theta_{w,1}} \left[ \frac{p_s}{p_d} \left( \frac{\phi}{k} \right)^{a - 1} \right] )</td>
</tr>
<tr>
<td>9 g/cm/s</td>
<td>( k_{rw} = k_{rw} \left( S_{rw} \right)^{a - 1} \left( \frac{S_{rw} - S_{sw}}{1 - S_{sw}} \right) )</td>
<td>no</td>
<td>( P_c = 0 )</td>
</tr>
<tr>
<td>Random Parameters</td>
<td>mean</td>
<td>std. deviation</td>
<td>cross correlation</td>
</tr>
<tr>
<td>-------------------</td>
<td>------</td>
<td>----------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>7 ln k</td>
<td></td>
<td>0.538516481</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8 multiple indicator knitting conditional simulation, 3 soil types</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9 lnkh</td>
<td>5.26 mD</td>
<td>0.89</td>
<td></td>
</tr>
<tr>
<td>Snr</td>
<td>.266</td>
<td>0.049</td>
<td></td>
</tr>
<tr>
<td>Swi</td>
<td>.221</td>
<td>0.074</td>
<td></td>
</tr>
<tr>
<td>\phi</td>
<td>.214</td>
<td>0.022</td>
<td></td>
</tr>
<tr>
<td>ln(no)</td>
<td>1.11</td>
<td>0.19</td>
<td></td>
</tr>
<tr>
<td>ln(nw)</td>
<td>0.89</td>
<td>0.37</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>corr. = 0.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>8</td>
<td>24 - 24</td>
<td></td>
</tr>
<tr>
<td>Domain</td>
<td>h (m)</td>
<td>v (m)</td>
<td>Boundary Conditions</td>
</tr>
<tr>
<td>--------</td>
<td>-------</td>
<td>-------</td>
<td>---------------------</td>
</tr>
<tr>
<td></td>
<td>7.1341</td>
<td>3.57</td>
<td>constant NAFL source at top between x = 6.12 and 6.57 m</td>
</tr>
<tr>
<td></td>
<td>8.200</td>
<td>11</td>
<td>- hydrostatic aqeous phase on vertical boyls. - no flow for both phase on horizontal boyls.</td>
</tr>
<tr>
<td></td>
<td>9.720x720</td>
<td>96</td>
<td>wetting phase source at one corner and extraction at opposite corner, 5% of pore volume per year</td>
</tr>
</tbody>
</table>

235
Appendix C

Evaluation of Integrals

C.1 \[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\pi^2 (1+u_1^2+u_2^2+u_3^2)^2} \left( \frac{u_1^2 du_1 du_2 du_3}{(\rho^2 u_1^2+u_2^3+u_3^2)^2+u_1^4 \xi_1^2} \right) \]

Convert to polar coordinates by making the change of variables \( u_1 = r \cos \phi \), \( u_2 = r \sin \phi \sin \theta \), \( u_3 = r \sin \phi \cos \theta \):

\[
I_1 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{(r \cos \phi)^2 |\sin \phi| r^2}{\pi^2 \left( 1 + (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2 \right)^2} \frac{1}{\left( \rho^2 (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2 \right)^2 + \rho^4 \xi_1^2 (r \cos \phi)^2} dr d\phi d\theta
\]

(C.1)

\[
I_1 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \cos^2 \phi \left| \frac{\sqrt{1 - \cos^2 \phi}}{r^2} \right| \frac{1}{\pi^2 (1 + r^2)^2} \frac{1}{\left( r^2 (\rho^2 \cos^2 \phi + 1 - \cos^2 \phi)^2 + \rho^4 \xi_1^2 \cos^2 \phi \right)^2} dr d\phi d\theta
\]

(C.2)

\[
I_1 = 2 \int_0^{\pi} \int_0^\infty \cos^2 \phi \left| \frac{\sqrt{1 - \cos^2 \phi}}{r^2} \right| \frac{1}{\pi (1 + r^2)^2} dr d\phi
\]

(C.3)
\[
\frac{1}{(r^2 ((\rho^2 - 1) \cos^2 \phi + 1)^2 + \rho^4 \xi_1^2 \cos^2 \phi)} \, dr \, d\phi
\]

Substitute \(t\) for \(\cos \phi\)

\[
I_1 = 2 \int_{-1}^{1} \int_{0}^{\infty} t^2 \left| \sqrt{1 - t^2} \right| \frac{r^2}{\pi (1 + r^2)^2} \frac{1}{\rho^4 \xi_1^2 \left( r^2 (\rho^2 - 1) t^2 + 1 \right)^2 + t^2} \frac{1}{\sqrt{1 - t^2}} \, dr \, dt
\]  \hspace{1cm} (C.4)

Substitute \(a = \rho^2 - 1\) and \(b = \rho^2 |\xi_1|\)

\[
I_1 = 2 \int_{-1}^{1} \int_{0}^{\infty} t^2 \left| \sqrt{1 - t^2} \right| \frac{r^2}{\pi (1 + r^2)^2} \frac{1}{b^2 t^2 \left( (at^2 + 1)^2 + 1 \right)} \frac{1}{\sqrt{1 - t^2}} \, dr \, dt
\]  \hspace{1cm} (C.5)

\[
I_1 = \frac{2}{4} \int_{-1}^{1} \frac{1}{b^2 t^2 \left( \left| \frac{1}{bt} (at^2 + 1) \right| + 1 \right)^2} \frac{t^2}{\sqrt{1 - t^2}} \, dt
\]  \hspace{1cm} (C.6)

\[
I_1 = \int_{0}^{1} \frac{t^2}{b^2 \left( \left| \frac{1}{bt} (at^2 + 1) \right| + t \right)^2} \, dt
\]  \hspace{1cm} (C.7)

\[
I_1 = \int_{0}^{1} \frac{t^2}{(at^2 + |b| t + 1)^2} \, dt
\]  \hspace{1cm} (C.8)

For \(\int_{0}^{1} \frac{x^2}{(a_1 x^2 + a_2 x + a_3) ^2} \, dx\) and \(\Delta = 4a_1 a_3 - a_2^2\) the solution is

\[
\begin{align*}
\left\{
\begin{array}{ll}
-\frac{4a_3 \arctan \left( \frac{2a_1 + a_2}{\Delta} \right)}{\Delta} + \frac{4a_3 \arctan \left( \frac{a_2}{\sqrt{\Delta}} \right)}{-\Delta \sqrt{\Delta}} + \frac{2a_3 + a_2}{\Delta (a_1 + a_2 + a_3)^2} ; & \Delta > 0 \\
- \frac{2}{2a_1 + a_2} + \frac{2}{a_2} ; & \Delta = 0 \\
\frac{4a_3 \tanh^{-1} \left( \frac{2a_1 + a_2}{\sqrt{-\Delta}} \right)}{\Delta \sqrt{-\Delta}} - \frac{4a_3 \tanh^{-1} \left( \frac{\sqrt{-\Delta}}{2a_1 + a_2} \right)}{-\Delta \sqrt{-\Delta}} - \frac{2a_3 + a_2}{\Delta (a_1 + a_2 + a_3)^2} ; & \Delta < 0
\end{array}
\right.
\end{align*}
\]

Based on the identity (1.622 of Gradshteyn and Ryzhik)

\[
\tanh^{-1} z = \frac{1}{2} \ln \frac{1 + z}{1 - z}
\]

and for \(\Delta = 4a - b^2\) \((a_1 = a, a_3 = 1, a_2 = |b|)\)

237
\[
\frac{4 \tanh^{-1} \left( \frac{2a + b}{\sqrt{-\Delta}} \right)}{\Delta \sqrt{-\Delta}} - \frac{4 \tanh^{-1} \left( \frac{b}{\sqrt{-\Delta}} \right)}{\Delta \sqrt{-\Delta}} = \frac{2}{(-\Delta)^{3/2}} \left( \ln \frac{1 + \frac{2a + |b|}{\sqrt{-\Delta}}}{1 - \frac{2a + |b|}{\sqrt{-\Delta}}} - \ln \frac{1 + \frac{|b|}{\sqrt{-\Delta}}}{1 - \frac{|b|}{\sqrt{-\Delta}}} \right)
\]
\[
= \frac{2}{(-\Delta)^{3/2}} \left( \ln \frac{\sqrt{-\Delta + 2a + |b|}}{\sqrt{-\Delta - 2a - |b|}} - \ln \frac{\sqrt{-\Delta + |b|}}{\sqrt{-\Delta - |b|}} \right)
\]
\[
= \frac{2}{(-\Delta)^{3/2}} \left( \ln \frac{\sqrt{-\Delta + 2a + |b|} \left( -\sqrt{-\Delta + |b|} \right)}{(-\sqrt{-\Delta + 2a + |b|}) \left( \sqrt{-\Delta + |b|} \right)} \right)
\]

\[
I_1 = \begin{cases} 
- \frac{4 \tan^{-1} \left( \frac{2a + b}{\sqrt{-\Delta}} \right)}{-\Delta \sqrt{-\Delta}} + \frac{4 \tan^{-1} \left( \frac{|b|}{\sqrt{-\Delta}} \right)}{-\Delta \sqrt{-\Delta}} - \frac{2 + |b|}{\Delta (a + |b| + 1)}; & \Delta > 0 \\
- \frac{2}{2a + |b|} + \frac{2}{|b|}; & \Delta = 0 \\
- \frac{2 + |b|}{\Delta (a + |b| + 1)} + \frac{2}{(-\Delta)^{3/2}} \ln \left( \frac{\left( 2a + |b| + \sqrt{-\Delta} \right) \left( |b| + \sqrt{-\Delta} \right)}{\left( 2a + |b| - \sqrt{-\Delta} \right) \left( |b| - \sqrt{-\Delta} \right)} \right); & \Delta < 0
\end{cases}
\]

For \( a = 0 \)

\[
I_1 = \int_0^1 \frac{t^2 \, dt}{(|b| \, t + 1)^2} \quad \text{(C.9)}
\]
\[
= \frac{|b| (|b| + 2) - 2 (|b| + 1) \ln (|b| + 1)}{|b|^3 (|b| + 1)}
\]

and for \( a = 0 \) and \( b = 0 \)

\[
I_1 = \frac{1}{3}
\]

238
\[ C.2 \quad \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{u_1^4 du_1 du_2 du_3}{\pi^2 (1+u_1^2+u_2^2+u_3^2)^2 \left( (\rho^2 u_1^2+u_2^2+u_3^2)^2 + \rho^4 \xi_1^2 u_1^2 \right)} \]

Convert to polar coordinates by making the change of variables \( u_1 = r \cos \phi, u_2 = r \sin \phi \sin \theta, u_3 = r \sin \phi \cos \theta \):

\[ I_2 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{(r \cos \phi)^4 |\sin \phi|}{\pi^2 \left(1 + (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2\right)^2} \]

\[ \frac{1}{\left(\rho_1^2 (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2\right)} \]

\[ \frac{1}{\left(\rho^2 (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2\right)^2 + \rho^4 \xi_1^2 (r \cos \phi)^2} \]

\[ dr \, d\phi \, d\theta \]

\[ I_2 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{\cos^4 \phi |\sin \phi| \, r^6}{\pi^2 \left(1 + r^2 (\cos^2 \phi + \sin^2 \phi \sin^2 \theta + \sin^2 \phi \cos^2 \theta)\right)^2} \]

\[ \frac{1}{\rho^2 \cos^2 \phi + \sin^2 \phi \sin^2 \theta + \sin^2 \phi \cos^2 \theta} \]

\[ \frac{1}{r^2 \left(\rho^2 \cos^2 \phi + \sin^2 \phi \sin^2 \theta + \sin^2 \phi \cos^2 \theta\right)^2 + \rho^4 \xi_1^2 \cos^2 \phi} \]

\[ dr \, d\phi \, d\theta \]

\[ I_2 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{\cos^4 \phi |\sin \phi| \, r^2}{\pi^2 (1 + r^2)^2} \]

\[ \frac{1}{(\rho^2 \cos^2 \phi + \sin^2 \phi) \left(\rho^2 \cos^2 \phi + \sin^2 \phi\right)^2 + \rho^4 \xi_1^2 \cos^2 \phi} \]

\[ dr \, d\phi \, d\theta \]

\[ I_2 = \int_0^\pi \int_0^\infty \frac{2 \cos^4 \phi |\sin \phi| \, r^2}{\pi (1 + r^2)^2} \]

\[ \frac{1}{(\rho^2 \cos^2 \phi + \sin^2 \phi) \left(\rho^2 \cos^2 \phi + \sin^2 \phi\right)^2 + \rho^4 \xi_1^2 \cos^2 \phi} \]

\[ dr \, d\phi \]
\[ I_2 = \int_0^\infty \int_0^{\infty} \frac{2 \cos^4 \phi \left( \sqrt{1 - \cos^2 \phi} \right) r^2}{\pi (1 + r^2)^2} \frac{1}{(\rho^2 \cos^2 \phi + 1 - \cos^2 \phi) \left( r^2 (\rho^2 \cos^2 \phi + 1 - \cos^2 \phi)^2 + \rho^4 \xi_1^2 \cos^2 \phi \right)} dr d\phi \]  

(C.14)

Substitute \( t \) for \( \cos \phi \)

\[ I_2 = -\int_1^{-1} \int_0^{\infty} \frac{2t^4 \left( \sqrt{1 - t^2} \right) r^2}{\pi (1 + r^2)^2 \sqrt{1 - t^2} (\rho^2 t^2 + 1 - t^2)} \frac{1}{\left( r^2 (\rho^2 t^2 + 1 - t^2)^2 + \rho^4 \xi_1^2 t^2 \right)} dr dt \]  

(C.15)

\[ I_2 = \frac{2}{\rho^4 g^2} \int_{-1}^{1} \frac{t^4}{t^2 (t^2 \rho^2 - 1) + 1} \left[ \int_0^{\infty} \frac{r^2}{\pi (1 + r^2)^2} \frac{1}{\left( r^2 \left( t^2 (\rho^2 - 1) + 1 \right)^2 + \frac{1}{\rho^4 \xi_1^2} \right)} dr \right] dt \]  

(C.16)

Evaluate integral with respect to \( r \) using integration routine in Maple V

\[ I_2 = \frac{2}{\rho^4 g^2} \int_{-1}^{1} \frac{t^4}{t^2 (t^2 \rho^2 - 1) + 1} \frac{1}{4 \left( \left( \frac{1}{\rho^4 \xi_1^2 t^2} \right) + 1 \right)^2} dt \]  

(C.17)

Symmetric with respect to \( t \) so rewrite with integral over \([0, 1]\)

\[ I_2 = \frac{1}{\rho^4 g^2} \int_{0}^{1} \frac{t^4}{t^2 (t^2 \rho^2 - 1) + 1} \frac{1}{\left( \left( \frac{1}{\rho^4 \xi_1} + t \right) \right)^2} dt \]  

(C.18)

Substitute \( a = \rho^2 - 1, b = \rho^2 \xi_1 \)

\[ I_2 = \frac{1}{b^2} \int_{0}^{1} \frac{t^4}{(t^2 a + 1) \left( \left( \frac{1}{b} \right) + t \right)^2} dt \]  

(C.19)

\[ I_2 = \int_{0}^{1} \frac{t^4}{(t^2 a + 1) \left( at^2 + b |t + 1|^2 \right)^2} dt \]  

(C.20)

Evaluate with Maple where for \( \Delta = 4a - b^2 \)
\[ I_2 = \begin{cases} 
\frac{8}{b^2 \Delta^{3/2}} \left( \tan^{-1} \left( \frac{2a + |b|}{\sqrt{\Delta}} \right) - \tan^{-1} \left( \frac{|b|}{\sqrt{\Delta}} \right) \right) - \frac{\tan^{-1}(\sqrt{\alpha})}{a^{3/2} b^2} - \frac{|b| + b^2 - 2a}{a \Delta b ((1 + a) + |b|)} & \Delta \geq 0 \\
\frac{8\Delta}{b^2 (-\Delta)^{3/2}} \left( \tanh^{-1} \left( \frac{b}{\sqrt{-\Delta}} \right) - \tanh^{-1} \left( \frac{2a + b}{\sqrt{-\Delta}} \right) \right) - \frac{\tan^{-1}(\sqrt{\alpha})}{a^{3/2} b^2} - \frac{b - 2a + b^2}{ab \Delta (1 + a + b)} & \Delta < 0 
\end{cases} \]

(C.21)

Finally, for \( a = 0 \)

\[ I_2 = \int_0^1 \frac{t^4}{(|b| t + 1)^2} \, dt \]  

(C.22)

\[ I_2 = \int_0^1 \frac{t^4}{(|b| t + 1)^2} \, dt = \frac{1}{3} \frac{12 |b| + |b|^4 - 2 |b|^3 + 6 |b|^2 - 12 \ln (|b| + 1) (1 + |b|)}{|b|^5 (|b| + 1)} \]
\[ C.3 \quad \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{u_1^2 du_1 du_2 du_3}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2 (\rho^2 u_1^2 + u_2^2 + u_3^2)} \]

Convert to polar coordinates by making the change of variables \( u_1 = r \cos \phi, u_2 = r \sin \phi \sin \theta, \)

\[ I_3 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{(r \cos \phi)^2 |\sin \phi| r^2}{\pi^2 \left(1 + (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2\right)^2} \]

\[ dr d\phi d\theta \]

\[ \left(\rho^2 (r \cos \phi)^2 + (r \sin \phi \sin \theta)^2 + (r \sin \phi \cos \theta)^2\right) \]

This simplifies to

\[ I_3 = \int_0^{2\pi} \int_0^\pi \int_0^\infty \frac{\cos^2 \phi |\sin \phi| r^2}{\pi^2 (1 + r^2)^2} \frac{dr d\phi d\theta}{((\rho^2 - 1) \cos^2 \phi + 1)} \]

Following integration with respect to \( \theta \) and then \( r \)

\[ I_3 = \frac{2}{4} \int_0^\pi \frac{\cos^2 \phi |\sin \phi| d\phi}{((\rho^2 - 1) \cos^2 \phi + 1)} \]

Substitute \( \cos \phi = t \)

\[ I_3 = \int_0^1 \frac{t^2 dt}{((\rho^2 - 1) t^2 + 1)} \]

Let \( \frac{s}{\sqrt{\rho^2 - 1}} = t \),

\[ I_3 = \frac{1}{(\rho^2 - 1)^{3/2}} \int_0^{\sqrt{\rho^2 - 1}} \frac{s^2 ds}{(s^2 + 1)} \]

resulting in

\[ I_3 = \frac{\sqrt{\rho^2 - 1} - \arctan \sqrt{\rho^2 - 1}}{(\rho^2 - 1)^{3/2}} \]

where for the case where \( \rho = 1 \) this result reduces to \( 1/3 \).
C.4 \[ \int_{-\infty}^{\infty} \frac{(u_1^2 + a_1) du_1}{\pi(u_1^2 - r_2)(u_1^2 - r_3)} \]

Analytical solution has been derived in Appendix of Mantoglou and Gelhar (1987b). Derivation repeated here for completeness and clarity.

For \( r_2 \) and \( r_3 \) real and negative

\[
I_4 = \frac{1}{\pi (r_2 - r_3)} \int_{-\infty}^{\infty} \left[ \frac{r_2 + a_1}{u_1^2 - r_2} - \frac{r_3 + a_1}{u_1^2 - r_3} \right] du_1
\]

\[
I_4 = \frac{1}{(r_2 - r_3)} \left[ \frac{r_2 + a_1}{\sqrt{-r_2}} - \frac{r_3 + a_1}{\sqrt{-r_3}} \right]
\]

For \( r_2 \) and \( r_3 \) complex conjugate pairs

\[
I_4 = \int_{-\infty}^{\infty} \frac{(u_1^2 + a_1) du_1}{\pi (u_1^4 - (r_2 + r_3) u_1^2 + r_2 r_3)}
\]

\[
I_4 = 2 \int_{0}^{\infty} \frac{(u_1^2 + a_1) du_1}{\pi (u_1^4 - (r_2 + r_3) u_1^2 + r_2 r_3)}
\]

Let \( u_1^2 = t \)

\[
I_4 = 2 \int_{0}^{\infty} \frac{(t + a_1) dt}{\pi \sqrt{t} (t^2 - (r_2 + r_3) t + r_2 r_3)}
\]

\[
I_4 = 2 \int_{0}^{\infty} \frac{(t^{1/2} + a_1 t^{-1/2}) dt}{\pi (t^2 - (r_2 + r_3) t + r_2 r_3)}
\]

Now, since \( r_2 = r_3^* \)

\[
I_4 = 2 \int_{0}^{\infty} \frac{(t^{1/2} + a_1 t^{-1/2}) dt}{\pi \left( t^2 - 2 \text{Re} (r_2) t + (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)}
\]

243
From equation 3.252.12 of Gradshteyn and Ryzhik (1980)

\[ \int_0^\infty \frac{x^{\mu-1}}{x^2 + 2ax \cos \tau + a^2} \, dx = -\pi a^{\mu-2} \csc(\gamma) \csc(\mu \pi) \sin((\mu - 1) \tau) \]

for

\[ a > 0 \]
\[ 0 < |\tau| < \pi \]
\[ 0 < \text{Re} \mu < 2 \]

Rewrite the integral as

\[ I_4 = 2 \int_0^\infty \frac{(t^{1/2} + a_1 t^{-1/2}) \, dt}{\pi \left( t^2 + 2 \left( (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)^{1/2} t \frac{(-\text{Re}(r_2))}{(\text{Re} r_2)^2 + (\text{Im} r_2)^2} + \left( (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)^{1/2} \right)} \]

\[ I_4 = -2 \left[ (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right]^{3/2 - 2} \frac{\csc(\gamma) \csc \left( \frac{\pi}{2} \right) \sin \left( \frac{3}{2} - 1 \right) \tau}{2 \left[ (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right]^{1/2 - 2} \frac{\csc(\gamma) \csc \left( \frac{\pi}{2} \right) \sin \left( \frac{1}{2} - 1 \right) \tau}{\csc(\gamma) \csc \left( \frac{\pi}{2} \right) \sin \left( \frac{1}{2} - 1 \right) \tau}} \]

where

\[ \cos \tau = \frac{(-\text{Re}(r_2))}{(\text{Re} r_2)^2 + (\text{Im} r_2)^2}^{1/2} \]

\[ I_4 = 2 \left( (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)^{-1/4} \sin \left( \frac{\tau}{2} \right) \]
\[ -2 \left( (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)^{-3/4} \sin \left( \frac{-\tau}{2} \right) \sin \left( \frac{\tau}{2} \right) \]

Given the identity

\[ \sin \tau = 2 \sin \left( \frac{\tau}{2} \right) \cos \left( \frac{\tau}{2} \right) \]

\[ I_4 = 2 \left( (\text{Re} r_2)^2 + (\text{Im} r_2)^2 \right)^{-1/4} \cos \left( \frac{\tau}{2} \right) \]

244
\[ +2 \left( (\text{Re} \, r_2)^2 + (\text{Im} \, r_2)^2 \right)^{-3/4} \cos \left( \frac{\tau}{2} \right) \]

Further since

\[
\cos \left( \frac{\tau}{2} \right) = \left[ \frac{1}{2} \left( 1 + \cos \tau \right) \right]^{1/2}
= \left[ \frac{1}{2} \left( 1 + \frac{-\text{Re}(r_2)}{(\text{Re} \, r_2)^2 + (\text{Im} \, r_2)^2}^{1/2} \right) \right]^{1/2}
\]

and

\[
I_4 = \sqrt{2} \left( 1 - \frac{\text{Re}(r_2)}{(\text{Re} \, r_2)^2 + (\text{Im} \, r_2)^2}^{1/2} \right)^{1/2}
\left[ (\text{Re} \, r_2)^2 + (\text{Im} \, r_2)^2 \right]^{-1/4} + \left[ (\text{Re} \, r_2)^2 + (\text{Im} \, r_2)^2 \right]^{-3/4}
\]
\[ C.5 \quad \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{du_2 du_3}{\pi^2 (1 + u_1^2 + u_2^2 + u_3^2)^2} \]

Convert to cylindrical coordinates

\[ I_5 = \int_0^{2\pi} \int_0^{\infty} \frac{r dr d\theta}{\pi^2 (1 + u_1^2 + r^2)^2} \]

Evaluate outer integral

\[ I_5 = 2 \int_0^{\infty} \frac{r dr}{\pi (1 + u_1^2 + r^2)^2} \]

Substitute \( r^2 = t \)

\[ I_5 = \int_0^{\infty} \frac{dt}{\pi (1 + u_1^2 + t)^2} \]

whereby from inspection

\[ I_5 = -\left. \frac{1}{\pi (1 + u_1^2 + t)} \right|_0^{\infty} \]

and on substitution of the limits

\[ I_5 = \frac{1}{\pi (1 + u_1^2)} \]
C.6  \[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{(u_1^4 + a_4 u_1^2 + a_5) du_1 du_2 du_3}{\pi^2 (u_1^4 + a_1 u_1^2 + a_2 u_1^2 + a_3) (1 + u_1^2 + u_2^2 + u_3^2)^2} \]

\[ I_6 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{u_1^4 + a_4 u_1^2 + a_5}{\pi^2 (u_1^4 + a_1 u_1^2 + a_2 u_1^2 + a_3) (1 + u_1^2 + u_2^2 + u_3^2)^2} \]
\[ = \int_{-\infty}^{\infty} \frac{u_4^4 + a_4 u_4^2 + a_5}{\pi (u_4^6 + a_1 u_4^4 + a_2 u_4^2 + a_3) (1 + u_4^2)} \]

\[ I_6 = \int_{-\infty}^{\infty} \frac{u_1^4 + a_4 u_1^2 + a_5}{\pi (u_1^2 - r_1) (u_1^2 - r_2) (u_1^2 - r_3) (1 + u_1^2)} \]

for \( r_1 \) real and negative and \( r_2, r_3 \) real or complex

\[ I_6 = \frac{r_1^2 + a_5 + a_4 r_1}{\pi (r_1 + 1) (r_1 - r_3) (r_1 - r_2)} \int_{-\infty}^{\infty} \frac{du_1}{u_1^2 - r_1} \]
\[ - \int_{-\infty}^{\infty} \frac{((r_1 + r_3 r_2) a_4 + (1 + r_3 + r_2 - r_1) a_5 + ((r_3 + 1) r_2 + r_3) r_1 - r_3 r_2) u_1^2}{\pi (u_1^2 - r_2) (u_1^2 - r_3)} \]
\[ + (r_1 r_3 r_2 - r_3 r_2^2 - r_2 r_3 (1 + r_3)) a_4 + ((1 + r_3 + r_2) r_1 - r_2^2 - (r_3 + 1) r_2 - r_3 (1 + r_3)) a_5 \]
\[ - \frac{u_2^2 - r_1 r_2 r_3}{\pi (u_1^2 - r_2) (u_1^2 - r_3)} \]
\[ [((r_3 + 1) r_2 + r_3 + 1) r_1^2 + ((-r_3 - 1) r_2^2 + (-r_3^2 - 1 - 2r_3) r_2 - r_3 - r_3^2) r_1 \]
\[ + (1 + r_3) (r_2 + 1) r_2]^{-1} \]
\[ + a_5 + 1 - a_4 \]
\[ \int_{-\infty}^{\infty} \frac{du_1}{(1 + u_1^2)} \]

\[ I_6 = \frac{r_1^2 + a_5 + a_4 r_1}{(r_1 + 1) (r_1 - r_3) (r_1 - r_2) \sqrt{-r_1}} \]
\[ - \int_{-\infty}^{\infty} \frac{[((r_1 + r_3 r_2) a_4 + (1 + r_3 + r_2 - r_1) a_5 + ((r_3 + 1) r_2 + r_3) r_1 - r_3 r_2) u_1^2}{\pi (u_1^2 - r_2) (u_1^2 - r_3)} \]
\[ + (r_1 r_3 r_2 - r_3 r_2^2 - r_2 r_3 (1 + r_3)) a_4 + ((1 + r_3 + r_2) r_1 - r_2^2 - (r_3 + 1) r_2 - r_3 (1 + r_3)) a_5 \]
\[ - \frac{u_2^2 - r_1 r_2 r_3}{\pi (u_1^2 - r_2) (u_1^2 - r_3)} \]
\[ [((r_3 + 1) r_2 + r_3 + 1) r_1^2 + ((-r_3 - 1) r_2^2 + (-r_3^2 - 1 - 2r_3) r_2 - r_3 - r_3^2) r_1 \]
\[ + (1 + r_3) (r_2 + 1) r_2]^{-1} \]

247
\[ \begin{align*}
&= \frac{\pi \left( \frac{u_1^2}{(r_3^2 + r_1) (r_2^2 + r_1) (r_3 + 1)} \right) \frac{du_1}{u_1^2 - r_2} \left( \frac{1}{(r_2 + 1)(r_1 - r_2)(r_1 - r_3)} \right)}{a_5 + 1 - a_4}
&\quad - \int_{-\infty}^{\infty} \left[ \left( (r_1 + r_3 r_2) a_4 + (1 + r_3 + r_2 - r_1) a_5 + r_3 r_2 r_1 + r_2 r_1 + r_3 r_1 - r_3 r_2 \right) u_1^2 \right. \\
&\quad + r_3 r_2 (r_1 - r_2 - 1 - r_3) a_4 + \left( r_2 (r_1 - r_2) + (r_1 - r_2 - r_3) (1 + r_3) \right) a_5 \\
&\quad - \left. \frac{\pi}{\pi} \frac{1}{u_1^2 - r_2} \left( \frac{u_1^2 - r_3}{r_3 + 1} \right) \frac{1}{(r_2 + 1)(r_1 - r_2)(r_1 - r_3)} \right]
&\quad - \frac{a_5 + 1 - a_4}{(r_1 + 1)(r_2 + 1)(r_3 + 1)}
\end{align*} \]
\[ I_7 = \int_{-\infty}^{\infty} \frac{(u_1^4 + a_4 u_1^4 + a_5 u_1^2 + a_6) \, du_1}{\pi (u_1^2 - r_1) (u_1^2 - r_2) (u_1^2 - r_3) (u_1^2 + a_7^2) (1 + u_1^2)} \]

\[ I_7 = \frac{a_4 r_1^2 + r_2^3 + r_1 a_5 + a_6}{\pi (1 + r_1) (r_1 + a_7^2) (r_2 + r_3) (r_1 - r_2)} \int_{-\infty}^{\infty} \frac{1}{(u^2 - r_1)} \, du 
- \frac{1}{\pi (1 + r_2) (1 + r_3) (r_1 - r_2) (r_2 + r_3) (a_7^2 + r_2) (a_7^2 + r_3)} \int_{-\infty}^{\infty} B_1 u^2 + B_2 (u^2 - r_3) \, du 
\]

\[ a_4 r_1^2 + r_2^3 + r_1 a_5 + a_6 \]

\[ r_1 a_5 + a_6 \]

\[ 1 \]

\[ 1 \]

\[ 1 \]

\[ 1 \]

\[ 1 \]

\[ 1 \]

where

\[ B_1 = \left[ (r_1 r_2 r_3 - r_3 r_2 + r_1 r_3 + r_1 r_2) a_7^2 + r_3 r_2 (r_2 r_3 + 1) \right] a_4 
+ \left[ (r_3 r_2 + r_1) a_7^2 - r_3 r_2 (-r_2 - r_3 + r_1 - 1) \right] a_5 
+ \left[ (r_2 + r_3 - r_1 + 1) a_7^2 - r_1 + r_3 r_2 - r_1 r_3 - r_1 r_2 + r_2^3 + r_3 + r_2 + r_2 \right] a_6 
+ \left( r_1 r_2^2 + r_1 r_2 r_3 - r_3 r_2^2 + r_1 r_3^2 - r_3 r_2^2 - r_3 r_2 r_1 + r_3 r_2 r_2 \right) a_7^2 
+ r_2 r_3 (r_1 r_2 r_3 - r_3 r_2 + r_1 r_3 + r_1 r_2) \]

\[ B_2 = \left[ -r_3 r_2 (r_2 r_3 + r_1) a_7^2 + r_3 r_2^2 (-r_2 - r_3 + r_1 - 1) \right] a_4 
+ \left[ (-r_2 - r_3 + r_1 - 1) a_7^2 - r_2^2 - r_3 r_2 - r_2 + r_1 r_2 - r_3 - r_3 + r_1 r_3 + r_1 \right] r_3 r_2 a_5 
+ \left( -r_2^2 - r_3 r_2 - r_2 + r_1 r_2 - r_3 - r_3 r_2 + r_1 r_3 + r_1 \right) a_6 a_7^2 + 
\left[ -r_3 r_2 + r_1 r_2^2 + r_1 r_3 + r_1 r_3 r_2 + r_1 r_2 + r_1 r_2^2 - r_3 r_2^2 - r_3 - r_3 r_2 - r_3 - r_3 r_2 \right] a_6 
- r_3 r_2 (r_1 r_2 r_3 - r_3 r_2 + r_1 r_3 + r_1 r_2) a_7^2 - r_3 r_2^2 (r_3 r_2 + r_1) \]

249
\[ I_7 = \frac{a_4 r_1^2 + r_1^3 + r_1 a_5 + a_6}{(1 + r_1) (r_1 + a_7^2) (r_1 - r_3) (r_1 - r_2) \sqrt{-r_1}} \frac{1}{\pi (1 + r_3) (1 + r_2) (r_1 - r_3) (r_1 - r_2) (a_7^2 + r_2) (a_7^2 + r_3) \int_{-\infty}^{\infty} \frac{B_1 u^2 + B_2}{(u^2 - r_2) (u^2 - r_3)} \, du} \]

\[ + \frac{(-a_7^6 + a_7^4 a_4 - a_7^2 a_5 + a_6)}{(a_7^2 - 1) (a_7^2 + r_2) (a_7^2 + r_3) (r_1 + a_7^2) |a_7|} \frac{1}{(a_6 + a_4 - a_5 - 1)} \]

\[ - \frac{1}{(a_7^2 - 1) (1 + r_1) (1 + r_3) (1 + r_2)} \]
C.8 \[ \int_{-\infty}^{\infty} \frac{1}{\pi(1+u_1^2)} \frac{(u_1^2 + A_1)}{(u_1^2 + A_2^2)} \, du_1 \]

\[ I_8 = \int_{-\infty}^{\infty} \frac{(A_1 u_1^2 + 1)}{\pi (u_1^4 + (1 + A_2^2) u_1^2 + A_2^2)} \, du_1 \]

\[ I_8 = (1 - A_1) \arctan u_1 - \left( \frac{1}{A_2} - A_1 A_2 \right) \arctan \left( \frac{u_1}{A_2} \right) \bigg|_{-\infty}^{\infty} \]

\[ I_8 = \frac{(-1 + |A_2|) - A_1 |A_2| (1 + |A_2|)}{(-1 + A_2^2) |A_2|} \]
Appendix D

Borden Aquifer p-s-k Function Parameters
van Genuchten Parameter Estimation

<table>
<thead>
<tr>
<th>Sr</th>
<th>m^o g</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.8</td>
<td>981</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Se</th>
<th>Pc</th>
<th>Pcest</th>
<th>ln(Pcest)-ln(Pc)</th>
<th>Pd</th>
<th>1698.9 028620</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sw</td>
<td>Pc (cm h20)</td>
<td>k</td>
<td>1.21E-02</td>
<td>m</td>
<td>0.709535</td>
</tr>
<tr>
<td>11.85</td>
<td>67.97</td>
<td>0.044</td>
<td>66677</td>
<td>60821</td>
<td>0.008452</td>
</tr>
<tr>
<td>13.50</td>
<td>57.42</td>
<td>0.062</td>
<td>56331</td>
<td>52795</td>
<td>0.004201</td>
</tr>
<tr>
<td>17.02</td>
<td>43.36</td>
<td>0.100</td>
<td>42536</td>
<td>43108</td>
<td>0.000178</td>
</tr>
<tr>
<td>22.42</td>
<td>35.35</td>
<td>0.159</td>
<td>34680</td>
<td>35304</td>
<td>0.000318</td>
</tr>
<tr>
<td>28.05</td>
<td>29.69</td>
<td>0.220</td>
<td>29123</td>
<td>30464</td>
<td>0.000227</td>
</tr>
<tr>
<td>35.56</td>
<td>26.56</td>
<td>0.301</td>
<td>26058</td>
<td>26174</td>
<td>0.000020</td>
</tr>
<tr>
<td>39.55</td>
<td>24.22</td>
<td>0.344</td>
<td>23759</td>
<td>24430</td>
<td>0.000775</td>
</tr>
<tr>
<td>50.12</td>
<td>21.29</td>
<td>0.459</td>
<td>20885</td>
<td>20760</td>
<td>0.000301</td>
</tr>
<tr>
<td>55.28</td>
<td>19.34</td>
<td>0.515</td>
<td>18969</td>
<td>19288</td>
<td>0.000279</td>
</tr>
<tr>
<td>62.09</td>
<td>17.58</td>
<td>0.589</td>
<td>17244</td>
<td>17510</td>
<td>0.000233</td>
</tr>
<tr>
<td>71.24</td>
<td>15.82</td>
<td>0.688</td>
<td>15520</td>
<td>15276</td>
<td>0.000251</td>
</tr>
<tr>
<td>77.35</td>
<td>14.84</td>
<td>0.754</td>
<td>14562</td>
<td>13793</td>
<td>0.002945</td>
</tr>
<tr>
<td>82.98</td>
<td>14.06</td>
<td>0.815</td>
<td>13795</td>
<td>12546</td>
<td>0.012315</td>
</tr>
<tr>
<td>97.30</td>
<td>8.59</td>
<td>0.971</td>
<td>8430</td>
<td>6801</td>
<td>0.046140</td>
</tr>
</tbody>
</table>

0.011259

<table>
<thead>
<tr>
<th>k</th>
<th>9.10E-03</th>
<th>m</th>
<th>0.783129</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.38</td>
<td>84.18</td>
<td>0.039</td>
<td>82580</td>
</tr>
<tr>
<td>13.50</td>
<td>60.94</td>
<td>0.062</td>
<td>59780</td>
</tr>
<tr>
<td>17.96</td>
<td>48.83</td>
<td>0.110</td>
<td>47900</td>
</tr>
<tr>
<td>23.12</td>
<td>41.41</td>
<td>0.166</td>
<td>40620</td>
</tr>
<tr>
<td>38.62</td>
<td>32.23</td>
<td>0.334</td>
<td>31614</td>
</tr>
<tr>
<td>47.30</td>
<td>29.69</td>
<td>0.428</td>
<td>29123</td>
</tr>
<tr>
<td>54.58</td>
<td>28.13</td>
<td>0.507</td>
<td>27591</td>
</tr>
<tr>
<td>62.79</td>
<td>25.78</td>
<td>0.596</td>
<td>25291</td>
</tr>
<tr>
<td>68.66</td>
<td>24.22</td>
<td>0.660</td>
<td>23759</td>
</tr>
<tr>
<td>74.53</td>
<td>22.27</td>
<td>0.724</td>
<td>21843</td>
</tr>
<tr>
<td>82.75</td>
<td>20.90</td>
<td>0.813</td>
<td>20501</td>
</tr>
<tr>
<td>89.55</td>
<td>19.53</td>
<td>0.887</td>
<td>19160</td>
</tr>
</tbody>
</table>

0.017514

<table>
<thead>
<tr>
<th>k</th>
<th>7.38E-03</th>
<th>m</th>
<th>0.850068</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.45</td>
<td>85.35</td>
<td>0.029</td>
<td>83730</td>
</tr>
<tr>
<td>12.09</td>
<td>77.15</td>
<td>0.047</td>
<td>75683</td>
</tr>
<tr>
<td>14.67</td>
<td>68.55</td>
<td>0.075</td>
<td>67252</td>
</tr>
<tr>
<td>16.55</td>
<td>62.70</td>
<td>0.095</td>
<td>61504</td>
</tr>
<tr>
<td>24.53</td>
<td>43.24</td>
<td>0.181</td>
<td>47326</td>
</tr>
<tr>
<td>33.92</td>
<td>44.53</td>
<td>0.283</td>
<td>43685</td>
</tr>
<tr>
<td>47.77</td>
<td>39.26</td>
<td>0.434</td>
<td>38512</td>
</tr>
<tr>
<td>54.58</td>
<td>35.55</td>
<td>0.507</td>
<td>34871</td>
</tr>
<tr>
<td>66.55</td>
<td>33.98</td>
<td>0.637</td>
<td>33339</td>
</tr>
<tr>
<td>72.18</td>
<td>31.05</td>
<td>0.698</td>
<td>30465</td>
</tr>
<tr>
<td>77.58</td>
<td>29.69</td>
<td>0.757</td>
<td>29123</td>
</tr>
<tr>
<td>85.56</td>
<td>27.93</td>
<td>0.843</td>
<td>27399</td>
</tr>
<tr>
<td>99.41</td>
<td>24.80</td>
<td>0.994</td>
<td>24333</td>
</tr>
</tbody>
</table>

0.195411

253
van Genuchten Parameter Estimation

<table>
<thead>
<tr>
<th>k</th>
<th>Pd</th>
<th>(5.84E-03)</th>
<th>m</th>
<th>(0.848491)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.15</td>
<td>88.26</td>
<td>0.036</td>
<td>86604</td>
<td>73495</td>
</tr>
<tr>
<td>12.79</td>
<td>75.39</td>
<td>0.054</td>
<td>73958</td>
<td>68311</td>
</tr>
<tr>
<td>19.37</td>
<td>60.35</td>
<td>0.125</td>
<td>56205</td>
<td>58284</td>
</tr>
<tr>
<td>26.64</td>
<td>52.15</td>
<td>0.204</td>
<td>51158</td>
<td>52603</td>
</tr>
<tr>
<td>37.91</td>
<td>46.29</td>
<td>0.327</td>
<td>45410</td>
<td>47515</td>
</tr>
<tr>
<td>79.46</td>
<td>32.23</td>
<td>0.777</td>
<td>31614</td>
<td>34727</td>
</tr>
<tr>
<td>91.43</td>
<td>29.86</td>
<td>0.907</td>
<td>29315</td>
<td>29649</td>
</tr>
<tr>
<td>98.71</td>
<td>24.41</td>
<td>0.986</td>
<td>23950</td>
<td>21953</td>
</tr>
</tbody>
</table>

\[0.026142\]

<table>
<thead>
<tr>
<th>k</th>
<th>Pd</th>
<th>(5.81E-03)</th>
<th>m</th>
<th>(0.804577)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.85</td>
<td>94.73</td>
<td>0.044</td>
<td>92927</td>
<td>80624</td>
</tr>
<tr>
<td>13.73</td>
<td>83.27</td>
<td>0.064</td>
<td>78748</td>
<td>73321</td>
</tr>
<tr>
<td>16.55</td>
<td>69.73</td>
<td>0.095</td>
<td>68402</td>
<td>66439</td>
</tr>
<tr>
<td>21.24</td>
<td>59.38</td>
<td>0.146</td>
<td>58247</td>
<td>59381</td>
</tr>
<tr>
<td>28.29</td>
<td>51.17</td>
<td>0.222</td>
<td>50200</td>
<td>52861</td>
</tr>
<tr>
<td>35.27</td>
<td>45.70</td>
<td>0.309</td>
<td>44835</td>
<td>47888</td>
</tr>
<tr>
<td>49.88</td>
<td>41.02</td>
<td>0.456</td>
<td>40236</td>
<td>41804</td>
</tr>
<tr>
<td>63.03</td>
<td>37.30</td>
<td>0.599</td>
<td>36596</td>
<td>37056</td>
</tr>
<tr>
<td>77.35</td>
<td>33.79</td>
<td>0.754</td>
<td>33147</td>
<td>31988</td>
</tr>
<tr>
<td>87.44</td>
<td>29.69</td>
<td>0.864</td>
<td>29213</td>
<td>27664</td>
</tr>
</tbody>
</table>

\[0.018866\]

<table>
<thead>
<tr>
<th>k</th>
<th>Pd</th>
<th>(5.44E-03)</th>
<th>m</th>
<th>(0.853314)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.26</td>
<td>89.65</td>
<td>0.059</td>
<td>87945</td>
<td>72205</td>
</tr>
<tr>
<td>15.14</td>
<td>74.80</td>
<td>0.080</td>
<td>73382</td>
<td>68470</td>
</tr>
<tr>
<td>19.84</td>
<td>65.04</td>
<td>0.131</td>
<td>63803</td>
<td>62490</td>
</tr>
<tr>
<td>27.11</td>
<td>57.03</td>
<td>0.209</td>
<td>55948</td>
<td>56956</td>
</tr>
<tr>
<td>33.89</td>
<td>53.52</td>
<td>0.281</td>
<td>52499</td>
<td>53517</td>
</tr>
<tr>
<td>41.67</td>
<td>49.22</td>
<td>0.367</td>
<td>48294</td>
<td>50252</td>
</tr>
<tr>
<td>50.82</td>
<td>46.48</td>
<td>0.467</td>
<td>45601</td>
<td>47133</td>
</tr>
<tr>
<td>66.08</td>
<td>41.99</td>
<td>0.632</td>
<td>41194</td>
<td>42491</td>
</tr>
<tr>
<td>77.82</td>
<td>38.28</td>
<td>0.759</td>
<td>37554</td>
<td>38763</td>
</tr>
<tr>
<td>86.38</td>
<td>35.55</td>
<td>0.874</td>
<td>34871</td>
<td>34470</td>
</tr>
<tr>
<td>94.72</td>
<td>32.70</td>
<td>0.943</td>
<td>32572</td>
<td>32037</td>
</tr>
<tr>
<td>99.65</td>
<td>29.88</td>
<td>0.996</td>
<td>29315</td>
<td>20213</td>
</tr>
</tbody>
</table>

\[0.015767\]

<table>
<thead>
<tr>
<th>k</th>
<th>Pd</th>
<th>(4.30E-03)</th>
<th>m</th>
<th>(0.657101)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.26</td>
<td>88.67</td>
<td>0.059</td>
<td>86987</td>
<td>80360</td>
</tr>
<tr>
<td>16.08</td>
<td>79.69</td>
<td>0.090</td>
<td>78173</td>
<td>74717</td>
</tr>
<tr>
<td>22.89</td>
<td>68.75</td>
<td>0.164</td>
<td>67444</td>
<td>66960</td>
</tr>
<tr>
<td>29.83</td>
<td>61.91</td>
<td>0.240</td>
<td>60738</td>
<td>62097</td>
</tr>
<tr>
<td>41.67</td>
<td>55.08</td>
<td>0.367</td>
<td>54032</td>
<td>56516</td>
</tr>
<tr>
<td>50.59</td>
<td>53.32</td>
<td>0.464</td>
<td>52307</td>
<td>53184</td>
</tr>
<tr>
<td>57.86</td>
<td>51.17</td>
<td>0.543</td>
<td>50200</td>
<td>50714</td>
</tr>
<tr>
<td>70.07</td>
<td>47.46</td>
<td>0.675</td>
<td>46559</td>
<td>46668</td>
</tr>
<tr>
<td>82.75</td>
<td>43.75</td>
<td>0.813</td>
<td>42919</td>
<td>41807</td>
</tr>
<tr>
<td>90.73</td>
<td>39.26</td>
<td>0.899</td>
<td>38512</td>
<td>37750</td>
</tr>
<tr>
<td>98.00</td>
<td>35.94</td>
<td>0.978</td>
<td>35255</td>
<td>29916</td>
</tr>
</tbody>
</table>

\[0.005961\]
## Brooks-Corey Parameter Estimation

### Parameter Table

<table>
<thead>
<tr>
<th>Sr</th>
<th>mo&quot;g</th>
<th>-16.05684869</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.8</td>
<td>981</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sw</th>
<th>Pc (cm h⁻²)</th>
<th>k</th>
<th>1.21E⁻²</th>
<th>lambda</th>
<th>Pd</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.85</td>
<td>67.97</td>
<td>0.044</td>
<td>66677</td>
<td>67773</td>
<td>13220.6205</td>
</tr>
<tr>
<td>13.50</td>
<td>57.42</td>
<td>0.062</td>
<td>56331</td>
<td>56723</td>
<td>4.80496E⁻⁵</td>
</tr>
<tr>
<td>17.02</td>
<td>43.36</td>
<td>0.100</td>
<td>42536</td>
<td>44099</td>
<td>0.001303292</td>
</tr>
<tr>
<td>22.42</td>
<td>35.35</td>
<td>0.159</td>
<td>34680</td>
<td>34649</td>
<td>7.92257E⁻⁷</td>
</tr>
<tr>
<td>28.05</td>
<td>29.69</td>
<td>0.220</td>
<td>29123</td>
<td>29216</td>
<td>1.03486E⁻⁵</td>
</tr>
<tr>
<td>35.56</td>
<td>26.55</td>
<td>0.301</td>
<td>26058</td>
<td>24771</td>
<td>0.0005638832</td>
</tr>
<tr>
<td>39.55</td>
<td>24.22</td>
<td>0.344</td>
<td>23759</td>
<td>23091</td>
<td>0.000813425</td>
</tr>
<tr>
<td>50.12</td>
<td>21.29</td>
<td>0.459</td>
<td>20865</td>
<td>19870</td>
<td>0.000242547</td>
</tr>
<tr>
<td>55.28</td>
<td>19.34</td>
<td>0.515</td>
<td>18969</td>
<td>18708</td>
<td>0.000191430</td>
</tr>
<tr>
<td>62.09</td>
<td>17.58</td>
<td>0.589</td>
<td>17244</td>
<td>17442</td>
<td>0.000129574</td>
</tr>
<tr>
<td>71.24</td>
<td>15.82</td>
<td>0.888</td>
<td>15520</td>
<td>18076</td>
<td>0.00124038</td>
</tr>
<tr>
<td>77.35</td>
<td>14.84</td>
<td>0.754</td>
<td>14562</td>
<td>15322</td>
<td>0.002589193</td>
</tr>
<tr>
<td>82.98</td>
<td>14.06</td>
<td>0.815</td>
<td>13795</td>
<td>14710</td>
<td>0.004121882</td>
</tr>
<tr>
<td>97.30</td>
<td>8.59</td>
<td>0.971</td>
<td>8430</td>
<td>13428</td>
<td>0.216663607</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>k</th>
<th>9.10E⁻³</th>
<th>lambda</th>
<th>2.448825225</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.38</td>
<td>84.18</td>
<td>0.039</td>
<td>82580</td>
</tr>
<tr>
<td>13.50</td>
<td>60.94</td>
<td>0.062</td>
<td>59780</td>
</tr>
<tr>
<td>17.96</td>
<td>48.83</td>
<td>0.110</td>
<td>47900</td>
</tr>
<tr>
<td>23.12</td>
<td>41.41</td>
<td>0.166</td>
<td>40620</td>
</tr>
<tr>
<td>38.62</td>
<td>32.23</td>
<td>0.334</td>
<td>31614</td>
</tr>
<tr>
<td>47.30</td>
<td>29.69</td>
<td>0.426</td>
<td>29123</td>
</tr>
<tr>
<td>54.58</td>
<td>28.13</td>
<td>0.507</td>
<td>27591</td>
</tr>
<tr>
<td>62.79</td>
<td>25.78</td>
<td>0.596</td>
<td>25291</td>
</tr>
<tr>
<td>68.66</td>
<td>24.22</td>
<td>0.660</td>
<td>23759</td>
</tr>
<tr>
<td>74.53</td>
<td>22.27</td>
<td>0.724</td>
<td>21843</td>
</tr>
<tr>
<td>82.75</td>
<td>20.90</td>
<td>0.813</td>
<td>20501</td>
</tr>
<tr>
<td>89.55</td>
<td>19.53</td>
<td>0.887</td>
<td>19160</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>k</th>
<th>7.38E⁻³</th>
<th>lambda</th>
<th>2.837690638</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.45</td>
<td>85.35</td>
<td>0.029</td>
<td>83730</td>
</tr>
<tr>
<td>12.09</td>
<td>77.15</td>
<td>0.047</td>
<td>75683</td>
</tr>
<tr>
<td>14.67</td>
<td>68.55</td>
<td>0.075</td>
<td>67252</td>
</tr>
<tr>
<td>16.55</td>
<td>62.70</td>
<td>0.095</td>
<td>61504</td>
</tr>
<tr>
<td>24.53</td>
<td>48.24</td>
<td>0.181</td>
<td>47326</td>
</tr>
<tr>
<td>33.92</td>
<td>44.53</td>
<td>0.283</td>
<td>43685</td>
</tr>
<tr>
<td>47.77</td>
<td>39.26</td>
<td>0.434</td>
<td>38512</td>
</tr>
<tr>
<td>54.58</td>
<td>35.55</td>
<td>0.507</td>
<td>34871</td>
</tr>
<tr>
<td>66.55</td>
<td>33.98</td>
<td>0.837</td>
<td>33339</td>
</tr>
<tr>
<td>72.18</td>
<td>31.05</td>
<td>0.698</td>
<td>30465</td>
</tr>
<tr>
<td>77.58</td>
<td>29.69</td>
<td>0.757</td>
<td>29123</td>
</tr>
<tr>
<td>86.56</td>
<td>27.93</td>
<td>0.843</td>
<td>27399</td>
</tr>
<tr>
<td>99.41</td>
<td>24.80</td>
<td>0.994</td>
<td>24333</td>
</tr>
<tr>
<td>100.82</td>
<td>22.85</td>
<td>1.009</td>
<td>22417</td>
</tr>
</tbody>
</table>
## Brooks-Corey Parameter Estimation

<table>
<thead>
<tr>
<th>Pd</th>
<th>27582.0290</th>
<th></th>
<th>5.84E-03</th>
<th>lambda</th>
<th>2.758524899</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>11.15</td>
<td>8.828</td>
<td>0.026</td>
<td>86604</td>
<td>91732</td>
</tr>
<tr>
<td></td>
<td>12.79</td>
<td>7.539</td>
<td>0.054</td>
<td>73956</td>
<td>79376</td>
</tr>
<tr>
<td></td>
<td>19.37</td>
<td>6.355</td>
<td>0.125</td>
<td>59205</td>
<td>58539</td>
</tr>
<tr>
<td></td>
<td>26.64</td>
<td>5.215</td>
<td>0.204</td>
<td>51158</td>
<td>49046</td>
</tr>
<tr>
<td></td>
<td>37.91</td>
<td>4.629</td>
<td>0.327</td>
<td>45410</td>
<td>41382</td>
</tr>
<tr>
<td></td>
<td>79.46</td>
<td>3.223</td>
<td>0.777</td>
<td>31614</td>
<td>30221</td>
</tr>
<tr>
<td></td>
<td>91.43</td>
<td>2.988</td>
<td>0.907</td>
<td>29515</td>
<td>29575</td>
</tr>
<tr>
<td></td>
<td>98.71</td>
<td>24.41</td>
<td>0.866</td>
<td>23950</td>
<td>27723</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pd</th>
<th>29422.65419</th>
<th></th>
<th>5.81E-03</th>
<th>lambda</th>
<th>2.782927669</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>11.85</td>
<td>94.73</td>
<td>0.044</td>
<td>92927</td>
<td>90412</td>
</tr>
<tr>
<td></td>
<td>13.73</td>
<td>80.57</td>
<td>0.054</td>
<td>78746</td>
<td>78855</td>
</tr>
<tr>
<td></td>
<td>16.55</td>
<td>69.73</td>
<td>0.095</td>
<td>68402</td>
<td>68579</td>
</tr>
<tr>
<td></td>
<td>21.24</td>
<td>59.38</td>
<td>0.146</td>
<td>58247</td>
<td>58770</td>
</tr>
<tr>
<td></td>
<td>28.29</td>
<td>51.17</td>
<td>0.222</td>
<td>50200</td>
<td>50515</td>
</tr>
<tr>
<td></td>
<td>36.27</td>
<td>45.70</td>
<td>0.309</td>
<td>48835</td>
<td>48883</td>
</tr>
<tr>
<td></td>
<td>49.86</td>
<td>41.02</td>
<td>0.456</td>
<td>40236</td>
<td>39001</td>
</tr>
<tr>
<td></td>
<td>63.03</td>
<td>37.30</td>
<td>0.599</td>
<td>36596</td>
<td>35372</td>
</tr>
<tr>
<td></td>
<td>77.35</td>
<td>33.79</td>
<td>0.754</td>
<td>33147</td>
<td>32560</td>
</tr>
<tr>
<td></td>
<td>87.44</td>
<td>29.69</td>
<td>0.864</td>
<td>29123</td>
<td>31012</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pd</th>
<th>34338.89025</th>
<th></th>
<th>5.44E-03</th>
<th>lambda</th>
<th>3.203488784</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>13.26</td>
<td>89.65</td>
<td>0.058</td>
<td>87945</td>
<td>82966</td>
</tr>
<tr>
<td></td>
<td>15.14</td>
<td>74.80</td>
<td>0.080</td>
<td>73383</td>
<td>75655</td>
</tr>
<tr>
<td></td>
<td>19.84</td>
<td>65.04</td>
<td>0.131</td>
<td>63803</td>
<td>64836</td>
</tr>
<tr>
<td></td>
<td>27.11</td>
<td>57.03</td>
<td>0.209</td>
<td>55948</td>
<td>55938</td>
</tr>
<tr>
<td></td>
<td>33.69</td>
<td>53.52</td>
<td>0.291</td>
<td>52499</td>
<td>51050</td>
</tr>
<tr>
<td></td>
<td>41.67</td>
<td>49.22</td>
<td>0.367</td>
<td>48284</td>
<td>49492</td>
</tr>
<tr>
<td></td>
<td>50.82</td>
<td>46.48</td>
<td>0.467</td>
<td>45601</td>
<td>43564</td>
</tr>
<tr>
<td></td>
<td>66.08</td>
<td>41.99</td>
<td>0.632</td>
<td>41194</td>
<td>39625</td>
</tr>
<tr>
<td></td>
<td>77.82</td>
<td>38.28</td>
<td>0.759</td>
<td>37554</td>
<td>37420</td>
</tr>
<tr>
<td></td>
<td>88.38</td>
<td>35.55</td>
<td>0.874</td>
<td>34871</td>
<td>35814</td>
</tr>
<tr>
<td></td>
<td>94.72</td>
<td>33.20</td>
<td>0.943</td>
<td>32572</td>
<td>34977</td>
</tr>
<tr>
<td></td>
<td>99.65</td>
<td>29.88</td>
<td>0.996</td>
<td>29315</td>
<td>34380</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Pd</th>
<th>40579.3265</th>
<th></th>
<th>4.30E-03</th>
<th>lambda</th>
<th>3.548253815</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>13.26</td>
<td>88.67</td>
<td>0.059</td>
<td>86987</td>
<td>89990</td>
</tr>
<tr>
<td></td>
<td>16.08</td>
<td>79.69</td>
<td>0.090</td>
<td>78173</td>
<td>80038</td>
</tr>
<tr>
<td></td>
<td>22.89</td>
<td>68.75</td>
<td>0.164</td>
<td>67444</td>
<td>67586</td>
</tr>
<tr>
<td></td>
<td>29.93</td>
<td>61.91</td>
<td>0.240</td>
<td>60738</td>
<td>60669</td>
</tr>
<tr>
<td></td>
<td>41.87</td>
<td>55.08</td>
<td>0.367</td>
<td>54032</td>
<td>53813</td>
</tr>
<tr>
<td></td>
<td>50.59</td>
<td>53.32</td>
<td>0.464</td>
<td>52307</td>
<td>50382</td>
</tr>
<tr>
<td></td>
<td>57.86</td>
<td>51.17</td>
<td>0.543</td>
<td>50200</td>
<td>48200</td>
</tr>
<tr>
<td></td>
<td>70.07</td>
<td>47.46</td>
<td>0.675</td>
<td>46559</td>
<td>45325</td>
</tr>
<tr>
<td></td>
<td>82.75</td>
<td>43.75</td>
<td>0.813</td>
<td>42919</td>
<td>43019</td>
</tr>
<tr>
<td></td>
<td>90.73</td>
<td>39.26</td>
<td>0.899</td>
<td>38512</td>
<td>41810</td>
</tr>
<tr>
<td></td>
<td>98.00</td>
<td>35.94</td>
<td>0.978</td>
<td>35255</td>
<td>40630</td>
</tr>
</tbody>
</table>

0.006525842 1.000000000 0.000000000 0.000000000 0.000000000

0.012160058 1.000000000 0.000000000 0.000000000 0.000000000

0.011114223 1.000000000 0.000000000 0.000000000 0.000000000

0.001111423 1.000000000 0.000000000 0.000000000 0.000000000

256
Appendix E

Cape Cod Moisture Retention
Curve Parameters

Appendix F

Evaluation of Analytical Solution of Plume Half Width

This appendix describes the derivation of an analytical solution of separable form for the non-wetting phase plume half width with static wetting phase, gravity flow of wetting phase in a homogeneous aquifer. First, the functional form of the function, $f$, describing the lateral distribution of the vertical relative permeability is found for a power law representation of the relative permeability as a function of the capillary pressure. Then the analytical solution for the plume half width $w$ is found corresponding to the derived form of $f$. Then an closed form solution of the integral $\int_{-\infty}^{\infty} u^2 f(u) du$ is found for use in the evaluation of the integral method solution. Lastly, an closed form solution is found for the integral of the Kirchhoff transform. This was used in a preliminary check of the numerical integration routine and is included merely to document that work.

F.1 Find $f$ Function with Separable Solution

The steady state flow equation is given by

$$k_z \frac{\partial}{\partial x} \left( \kappa_z \frac{\partial P_c}{\partial x} \right) + k_z \frac{\partial}{\partial z} \left( \kappa_z \frac{\partial P_c}{\partial z} \right) + \delta \rho g k_z \frac{\partial \kappa_z}{\partial z} = 0 \quad (F.1)$$

259
where neglecting vertical flow due to the capillary pressure gradient

\[ k_x \frac{\partial}{\partial x} \left( \kappa_x \frac{\partial P_c}{\partial x} \right) + \delta g k_z \frac{\partial \kappa_z}{\partial z} = 0 \] (F.2)

Neglecting flow due to the capillary pressure gradient is essentially equivalent to the assumption commonly employed in analysis of the advection dispersion equation, where dispersive flow in the direction of the mean flow is assumed to not contribute significantly to the total flux in the direction of flow. This assumption simplifies the analysis by reducing the complexity of the boundary conditions and the ultimate numerical solution.

\[ \kappa_z = \tilde{k}_z(z) f \left( \frac{x}{w(z)} \right) \] (F.3)

\[ = \tilde{k}_z(z) f(u(x,z)) \]

Assume a power law function for \( \kappa_x \) and \( \kappa_z \):

\[ \kappa_x = a P_c^m \] (F.4)

\[ \kappa_z = b P_c^m \]

or

\[ P_c = \left( \frac{\kappa_x}{a} \right)^{1/n} = \left( \frac{\kappa_z}{b} \right)^{1/m} \] (F.5)

\[ \frac{\partial P_c}{\partial \kappa_z} = \frac{1}{bm} \left( \frac{\kappa_z}{b} \right)^{1/m-1} \]

The strategy employed in finding a valid function \( f \) is to write \( \frac{\partial P_c}{\partial x} \), \( \frac{\partial}{\partial z} \left( \kappa_x \frac{\partial P_c}{\partial z} \right) \) and \( \frac{\partial \kappa_x}{\partial z} \) as functions of the independent variables \( \tilde{k}_z \), \( w \) and to substitute those expressions back into the flow equation:

\[ \frac{\partial P_c}{\partial x} = \frac{\partial P_c}{\partial \kappa_z} \frac{\partial \kappa_z}{\partial x} \]

\[ = \frac{1}{bm} \left( \frac{\kappa_z}{b} \right)^{1/m-1} \tilde{k}_z \frac{\partial f}{\partial u} \]

\[ = \frac{1}{bm} \left( \frac{f}{b} \right)^{1/m-1} \tilde{k}_z^{1/m} \frac{\partial f}{\partial w} \]

260
Now, find $\kappa_x \frac{\partial P_c}{\partial x}$

$$
\kappa_x \frac{\partial P_c}{\partial x} = \left(a P^n \right) \frac{1}{b m} \left( \frac{f}{b} \right)^{1/m-1} \frac{\kappa_x^{1/m} \partial f}{w} \frac{\partial f}{\partial u}
$$

$$
= a \left( \frac{\kappa_x}{b} \right)^{n/m} \frac{1}{b m} \left( \frac{f}{b} \right)^{1/m-1} \frac{\kappa_x^{1/m} \partial f}{w} \frac{\partial f}{\partial u}
$$

$$
= a \left( \frac{\kappa_x}{b} \right)^{n/m} \frac{1}{b m} \left( \frac{f}{b} \right)^{1/m-1} \frac{\kappa_x^{1/m} \partial f}{w} \frac{\partial f}{\partial u}
$$

$$
= \frac{a \kappa_x^{(n+1)/m} f^{(n-m+1)/m} \partial f}{m w b^{(n+1)/m}} \frac{\partial f}{\partial u}
$$

and $\frac{\partial}{\partial x} \left( \kappa_x \frac{\partial P_c}{\partial x} \right)$ with respect to $\tilde{\kappa}_z$, $w$

$$
\frac{\partial}{\partial x} \left( \kappa_x \frac{\partial P_c}{\partial x} \right) = \frac{a \kappa_x^{(n+1)/m}}{m w b^{(n+1)/m}} \frac{\partial f}{\partial x} \left( f^{(n-m+1)/m} \frac{\partial f}{\partial u} \right)
$$

$$
= \frac{a \kappa_x^{(n+1)/m}}{m w b^{(n+1)/m}} \frac{\partial u}{\partial x} \frac{\partial f}{\partial x} \left( f^{(n-m+1)/m} \frac{\partial f}{\partial u} \right)
$$

$$
= \frac{a \kappa_x^{(n+1)/m}}{m w b^{(n+1)/m}} \frac{\partial}{\partial u} \left( f^{(n-m+1)/m} \frac{\partial f}{\partial u} \right)
$$

Do the same for $\frac{\partial \kappa_x}{\partial z}$

$$
\frac{\partial \kappa_x}{\partial z} = \frac{\partial f \tilde{\kappa}_z}{\partial z}
$$

$$
= f \frac{\partial \kappa_x}{\partial z} + \tilde{\kappa}_z \frac{df}{du} \frac{\partial u}{\partial z}
$$

$$
= f \frac{\partial \kappa_x}{\partial z} - \tilde{\kappa}_z \frac{df}{w} \frac{\partial w}{du} \frac{\partial z}{\partial u}
$$

Given the gravity flow assumption noted earlier, the assumed separability of the permeability solution and continuity of vertical flow the product of the centerline permeability and the half width $w$ must remain at their boundary condition value

$$
\tilde{\kappa}_z w = C_1
$$

$$
\frac{\partial \tilde{\kappa}_z w}{\partial z} = 0
$$

$$
\frac{\partial \tilde{\kappa}_z}{\partial z} = -\frac{\tilde{\kappa}_z \partial w}{w} \frac{\partial z}{\partial u}
$$

261
Therefore

\[
\frac{\partial \kappa_z}{\partial z} = -f \frac{\tilde{\kappa}_z \partial w}{w \partial z} - \tilde{\kappa}_z u \frac{df}{du} \frac{\partial w}{\partial z} = -\frac{\tilde{\kappa}_z \partial w}{w \partial z} \left( f + u \frac{df}{du} \right)
\]

and the continuity equation with respect to \( f \) and \( w \) is

\[
0 = -\delta_\rho g k_z \frac{\tilde{\kappa}_z \partial w}{w \partial z} \left( f + u \frac{df}{du} \right) + k_z \frac{a \kappa_z^{(n+1)/m}}{m w^2 b^{(n+1)/m}} \frac{d}{du} \left( f^{(n-m+1)/m} \frac{df}{du} \right)
\]

If \( f \) is to be a function of only \( u \), the \( z \)-dependent coefficients must satisfy

\[
\delta_\rho g k_z \frac{\tilde{\kappa}_z \partial w}{w \partial z} = C_2 k_z \frac{a \kappa_z^{(n+1)/m}}{m w^2 b^{(n+1)/m}}
\]

and taking \( C_2 = 1 \),

\[
\left( f + u \frac{df}{du} \right) + \frac{d}{du} \left( f^{(n-m+1)/m} \frac{df}{du} \right) = 0
\]

For \( f, \frac{df}{du} \to 0 \) as \( u \to \pm \infty \) and \( f = 1 \) at \( u = 0 \) it is possible to show that

\[
f = \left( 1 - \frac{(n-m+1) u^2}{2m} \right)^{m/(n-m+1)}
\]

**F.2 Develop Analytical Solution for \( W \)**

With \( C_2 = 1 \), the differential equation for the width is then

\[
-\delta_\rho g k_z \frac{\tilde{\kappa}_z \partial w}{w \partial z} = k_z \frac{a \kappa_z^{(n+1)/m}}{m w^2 b^{(n+1)/m}}
\]

and substituting \( \frac{c_1}{w} \) for \( \tilde{\kappa}_z \)

\[
-\delta_\rho g k_z \frac{c_1}{w^2} \frac{\partial w}{\partial z} = k_z \frac{a c_1^{(n+1)/m}}{m w^{2+(n+1)/m} b^{(n+1)/m}}
\]
\[ w^{(n+1)/m} \frac{\partial w}{\partial z} = \frac{k_x a c_1^{(n-m+1)/m}}{b^{(n+1)/m} \delta_p g k_z m} \]

For boundary condition \( w(0) = w_o \)

\[ \frac{m}{m + n + 1} w^{1+(n+1)/m} \bigg|_{w_o} = -\frac{k_x a c_1^{(n-m+1)/m}}{b^{(n+1)/m} \delta_p g k_z m} z \]

\[ w^{1+(n+1)/m} = w_o^{1+(n+1)/m} - \frac{(m + n + 1) k_x a c_1^{(n-m+1)/m}}{b^{(n+1)/m} \delta_p g k_z m^2} z \]

resulting in the analytical solution for the width:

\[ w = \left( w_o^{1+(n+1)/m} - \frac{(m + n + 1) k_x a b_1^{(n-m+1)/m} c_1^{(n-m+1)/m}}{\delta_p g k_z m^2} z \right)^{m/(n+1+m)} \]

**F.3 Evaluate \( \int_{-\infty}^{\infty} u^2 f(u) \, du \)**

For \( r^2 = \frac{2m}{n-m+1} \), evaluate

\[ \int_{-\infty}^{\infty} u^2 f(u) \, du = \int_{-r}^{r} u^2 \left( 1 - \frac{u^2}{r^2} \right) \, du \]

where specified limits so as to integrate over \( u \) space where \( f > 0 \). Let \( tr = u \)

\[ \int_{-\infty}^{\infty} u^2 f(u) \, du = r^3 \int_{-1}^{1} t^2 \left( 1 - t^2 \right)^{\frac{r^2}{2}} \, dt \]

Let \( t = \sin \theta \)

\[ \int_{-\infty}^{\infty} u^2 f(u) \, du = 2r^3 \int_{0}^{\frac{\pi}{2}} \sin^2 \theta \cos^{\frac{r^2}{2}} \theta \cos \theta d\theta = 2r^3 \int_{0}^{\frac{\pi}{2}} \sin^2 \theta \cos^{r^2+1} \theta d\theta \]

From 3.621 of Gradshteyn and Ryzik

263
\[ \int_0^{\frac{\pi}{2}} \sin^{\mu-1} \theta \cos^{\nu-1} \theta d\theta = \frac{1}{2} B \left( \frac{\mu}{2}, \frac{\nu}{2} \right) \text{ where } \Re(\mu) > 0, \Re(\nu) > 0 \]

Therefore

\[ \int_{-\infty}^{\infty} u^2 f(u) \, du = r^3 B \left( \frac{3}{2}, \frac{r^2 + 2}{2} \right) \]

**F.4 Evaluate** \( \int_{-\infty}^{\infty} \int_{0}^{P_c(u)} \kappa_x (P_c) \, dP_c du \)

\[
\int_{-\infty}^{\infty} \int_{0}^{P_c(u)} \kappa_x (P_c) \, dP_c du = \int_{-r}^{r} \int_{0}^{P_c(u)} a P_c^n dP_c du \\
= \int_{-r}^{r} \frac{a}{n+1} P_c^{n+1} \bigg|_{0}^{P_c(u)} du \\
= \int_{-r}^{r} \frac{a}{n+1} P_c(u)^{n+1} du \\
= \int_{-r}^{r} \frac{a}{n+1} \left( \frac{\tilde{K}_2(f)}{b} \right)^{(n+1)/m} du \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} \int_{-r}^{r} f^{(n+1)/m} du \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} \int_{-r}^{r} \left( 1 - \frac{u^2}{r^2} \right)^{r^2(n+1)/2m} du \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} 2r \int_{0}^{1} \left( 1 - t^2 \right)^{r^2(n+1)/2m} dt \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} 2r \int_{0}^{\frac{\pi}{2}} (\cos \theta)^{r^2(n+1)/m} \cos \theta d\theta \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} 2r \int_{0}^{\frac{\pi}{2}} (\cos \theta)^{r^2(n+1)+m} d\theta \\
= \frac{a}{n+1} \left( \frac{\tilde{K}_2}{b} \right)^{(n+1)/m} r B \left( \frac{1}{2}, \frac{r^2(n+1) + m}{m} + 1 \right) \]
Appendix G

Code for Evaluation of Integral Solution to Lateral Spreading of Nonwetting Phase Plume
c width3

c Evaluates approximate integral solution to lateral spreading of
 c nonwetting phase plume through static wetting phase.
 c Utilizes implementation of Runge-Kutta solution algorithm and
 c driver routine from Numerical Recipes, Press et al.

c Input files:
 c 1. Tabulated effective permeabilities as contained in output
 c from maple routine 'summary' in moments.mws.
 c 2. Specification of boundary conditions, step size, accuracy
 c control, domain

c W0  - plume width scale boundary condition
 c KAPZ0 - centerline relative permeability boundary condition

c KAPX - horizontal relative permeability vector
 c KAPZ - vertical relative permeability vector
 c PC  - mean capillary pressure vector
 c SPC - standard deviation of capillary pressure vector
 c THO - mean nonwetting phase volumetric content vector
 c N   - dimension of tabulated data vectors

c KSX - saturated horizontal permeability
 c A  - ratio of horizontal to vertical saturated permeability
 c FRM - functional form of f(u) (P, parabolic/G, gaussian
 c    / A, analytic solution)
 c DOMAIN - specifies radial or planar domain (R, radial /
 c        / P, planar)

c for function form A:
 c
 c KAPX = AA * PC**N
 c KAPZ = BB * PC**M

c MEXP - exponent of vertical permeability function
 c NEXP - exponent of horizontal permeability function
 c AA
 c BB

c N2 - number of segments in evaluation of Kirchoff integral

COMMON /PARAMS/ W0, KAPX, KAPZ, PC, SPC, THO, STHO, KAPZ0, A,
 c QT, KSX, N2, N, FRM, DOMAIN
COMMON /EXPON/ AA, BB, MEXP, NEXP
COMMON /PATH/ DXSAV
COMMON /PATH2/ KMAX, KOUNT
COMMON /DENSE/ DELRHO, G
CHARACTER*132 INFILE, OUTFILE, INFIL1, PROGNAME
CHARACTER*12 STRING
CHARACTER*1 FRM, DOMAIN
CHARACTER*1 T_
INTEGER ARGC, ARGLEN
DOUBLE PRECISION YSTART(3),
 * W0, DELZ, RNW, RW, MUNW,
 * KSZ, KSX, QT, KAPZ0,
 * PC(100), KAPZ(100), KAPX(100), THO(100),
WIDTH3.FOR

09/25/98

* SPC(100), STHO(100),
61 * A, DELRHO, G,
62 * DXSAV,
63 * AA, BB, MEXP, NEXP, R, ARG1, ARG2
64
65 T_ = CHAR(9)
66 G = 981.
67
68 ARGC = IARGC()
69 ARGLEN = IGETARG( 0, PROGNAME )
70 PRINT *, 'Program name is ', PROGNAME(1:ARGLEN)
71 IF(ARGC.GE.2) THEN
72    ARGLEN = IGETARG( 1, INFILE1 )
73    PRINT '(A, 2A)', 'INPUT FILE',
74    INFILE1(1:ARGLEN)
75 ELSE
76    C
77    IF(ARGLEN .EQ. 0 ) THEN
78       print *, 'enter input file name'
79       READ(5, '(A)') INFILE1
80    ENDIF
81
82 OPEN(3,FILE=INFILE1,FORM='FORMATTED',STATUS='OLD')
83 READ(3,'(A)') INFIL
84 READ(3,'(A)') OUTFILE
85 READ(3,* ) W0,KAPZ0
86 READ(3,'(A1)') FRM
87 READ(3,'(A1)') DOMAIN
88 READ(3,* ) N2,NDIM,EPS
89
90 IF ( FRM .EQ. 'A' ) THEN
91    READ(3,* ) BB, MEXP, AA,NEXP
92 ENDIF
93
94 OPEN(1, FILE=INFILE1, FORM='FORMATTED', STATUS='OLD')
95 OPEN(2, FILE=OUTFILE, FORM='FORMATTED' )
96 OPEN(999, FILE='TO.OUT', FORM='FORMATTED')
97
98 WRITE(2,(''''''))
99 WRITE(2,('''INFILE''',A1,A))T_,INFILE
100 WRITE(2,('''OUTFILE''',A1,A))T_,OUTFILE
101 WRITE(2,('''W0, KAPZ0''',3(A1,F12.2))) T_,W0,T_,KAPZ0
102 WRITE(2,('''FORM''',A1,A)) T_,FRM
103 WRITE(2,('''FORM''',A1,A)) T_,DOMAIN
104
105 WRITE(2,('''Z2,DELZ''',A1,F12.2))
106 T_,Z2,T_,DELZ
107 WRITE(2,('''N2,NDM,EPS''',A1, I6, A1, I6, A1, E12.6'))
108 T_,N2,T_,NDIM,T_,EPS
109
110 DO I = 1, 17
111    READ( 1, * )
112 END DO
113
114 READ(1,'(A)') STRING
115 PRINT *, STRING
116 READ(STRING(9:18), '(F10.0)') RW
117
118 READ(1,'(A)') STRING

267
WIDTH3.FOR

09/25/98

119 C PRINT *, STRING
120 READ(STRING(12:21),'(F10.0)')RNW
121 READ(STRING(23:32),'(F10.0)') MUNW
122 READ(STRING(56:66),'(F11.0)')KSZ
123 READ(STRING(68:78),'(F11.0)')KXS
124
125 PRINT *, ' RNW,RNW ', RNW
126 PRINT *, ' MUNW ', MUNW
127 PRINT *, ' KSZ, KXS ', KSZ
128
129 DELRHO = RNW - RNW
130
131 IF ( FRM.EQ.'A') THEN
132 WRITE(2,'( '' BB,MEXP,AA,NEXP ',' (E14.6,'','','') )')MEXP,NEXP
133 ELSE
134 DO I = 1, 4
135 READ( 1, * )
136 END DO
137
138 DO I = 1, 100
139 READ(1,'(A)',END=100) STRING
140 IC = 0
141 DO J = 11, 132
142 IF(ICHAR(STRING(J)))) .EQ.9) THEN
143 IC = IC+1
144 IF(IIC.EQ.4) J1 = J
145 IF(IIC.EQ.5) J2 = J
146 ENDIF
147 IF(IIC.EQ.8) GO TO 2
148 END DO
149 N = I
150 READ(STRING(1:10),'(F10.0)') PC(I)
151 READ(STRING(12:21),'(F10.0)') SPC(I)
152 READ(STRING(J1+1:J1+8),'(F8.0)') THO(I)
153 READ(STRING(J2+1:J2+8),'(F8.0)') STHO(I)
154 READ(STRING(J+1:J+11),'(F11.0)') KAPZ(I)
155 READ(STRING(J+13:J+24),'(F11.0)') KAPX(I)
156 PRINT *, PC(I), KAPZ(I), KAPX(I)
157 END DO
158
159 100 CONTINUE
160 CLOSE (1)
161 ENDIF
162 A = KSZ / KSZ
163 YSTART(I) = W0
164 NVAR = 1
165 X1 = 0.0
166 X2 = 22
167 C EPS = .01
168 H1 = DELZ
169 HMIN = DELZ / 100.
170 C PATH COMMON BLOCK VARIABLES
171 KMAX = 200
172 DXSAV = DELZ
173 QT = KAPZ0 * KSZ * DELRHO * G * W0

268
09/25/98

WIDTH3.FOR

178   QTOT = QT / MNUMW
179
180   C MULTIPLY QT BY INT(U^2 F(U), U=-INF..INF)
181   C MULTIPLY QTOT BY INT( F(U), U=-INF..INF)
182
183     IF (DOMAIN .EQ. 'P') THEN
184       IF (FM .EQ. 'G') THEN
185         QT = QT * SQRT(3.14159)/2.
186         QTOT = QTOT * SQRT(3.14159)
187       ELSEIF (FM .EQ. 'P') THEN
188         QT = QT * 4. / 15.
189         QTOT = QTOT * 4. / 3.
190       ELSEIF (FM .EQ. 'A') THEN
191         R = SQRT(2.0*D0*MEXP/((NEXP-MEXP+1.0*D0))
192         ARG1 = 1.5D0
193         ARG2 = (R**2 + 2.0)/2.0
194         QT = QT * R*3 * BETA(ARG1,ARG2)
195         ARG1 = 0.5D0
196         QTOT = QTOT * R * BETA(ARG1,ARG2)
197     ELSE
198       PRINT *, ' WHAT FORM IS BEING USED ? ',FM
199       ENDF
200   ELSE
201     QT = QT * W0 / 2.
202     IF (FM .EQ. 'G') THEN
203       QT = QT * 1. / 2.
204     ENDIF
205     QTOT = QTOT * 3.14159
206     ELSEIF (FM .EQ. 'P') THEN
207       QT = QT * 1. / 12.
208       QTOT = QTOT * 3.14159 / 2.
209     ELSEIF (FM .EQ. 'A') THEN
210       PRINT *, ' not programmed '
211       STOP
212     ENDIF
213     QT = QT *
214     QTOT = QTOT *
215   ELSE
216     PRINT *, ' FORM NOT DEFINED: ',FM
217     STOP
218     ENDF
219
220     WRITE(2, (''QTOT '',A1,F15.7)) T_,QTOT
221     WRITE(2, (''' '''))
222     WRITE(2, (''Z'',A1,''W'',A1,''S(X)'',A1,''ZC'',A1,
223         ''DKZC_DZ'',A1,''PC'',A1,''SPC'',A1,
224         ''DPCC_DZ'',A1,''TO'',A1,''STO'',A1,''Z''))
227     CALL ODEINT(YSTART,NVAR,X1,X2,EPS,H1,HMIN,NOK,
228         *   NBAD)
229     STOP
230     END
231
232
C =======================================================================
233
234   SUBROUTINE DERIVS(X,Y,DYDX)
235   DOUBLE PRECISION X, Y(1), DYDX(1)
236
COMMON /PARAMS/ W0, KAPX, KAPZ, PC, SPC, THC, STHO, KAPZ0, A,
                   & QT, KSX, N2, N, FRM, DOMAIN
DOUBLE PRECISION C4, C4_,
DOUBLE PRECISION W, A, QT, KSX
DOUBLE PRECISION PC(100), KAPX(100), KAPZ(100), THO(100),
                   & SPC(100), STHO(100),
                   & W0,KAPZ0
CHARACTER*1 FRM, DOMAIN

W = Y(1)
C4_ = C4(FRM, DOMAIN, W, W0, KAPZ0, PC, KAPX, KAPZ, N2, N)
IF (DOMAIN.EQ. 'P') THEN
   DYDX(1) = -KSX * C4_ / QT
ELSE
   DYDX(1) = -KSX * W * C4_ / QT
ENDIF
RETURN

C======================================================================

DOUBLE PRECISION FUNCTION GETDZ(W,DWDZ,KZ)
DOUBLE PRECISION W, A, QT, KSX, DWDZ, KZ
DOUBLE PRECISION PC(100), KAPX(100), KAPZ(100), THO(100),
                   & SPC(100), STHO(100),
                   & W0,KAPZ0
CHARACTER*1 FRM, DOMAIN
IF (DOMAIN.EQ. 'P') THEN
   GETDZ = - KZ / W * DWDZ
ELSE
   GETDZ = - 2 * KZ / W * DWDZ
ENDIF
RETURN

C======================================================================

DOUBLE PRECISION FUNCTION GETKZ(W)
DOUBLE PRECISION W, A, QT, KSX
DOUBLE PRECISION PC(100), KAPX(100), KAPZ(100), THO(100),
                   & SPC(100), STHO(100), W0,KAPZ0
CHARACTER*1 FRM, DOMAIN
IF (DOMAIN.EQ. 'P') THEN
   GETKZ = W0 * KAPZ0 / W
ELSE
   GETKZ = W0**2 * KAPZ0 / W**2
ENDIF
RETURN

C======================================================================

DOUBLE PRECISION FUNCTION GETDKDP(KZ)
DOUBLE PRECISION KZ, DK,
* COF(4), PD(2)
CHARACTER*1 FRM, DOMAIN
DOUBLE PRECISION A, QT, KSX
DOUBLE PRECISION PC(100), KAPX(100), KAPZ(100), THO(100),
& SPC(100), STHO(100), W0, KAPZ0, MEXP, NEXP,
& AA, BB, PP
COMMON /PARAMS/ W0, KAPX, KAPZ, PC, SPC, THO, STHO, KAPZ0, A,
& QT, KSX, N2, N, FRM, DOMAIN
COMMON /EXPON/ AA, BB, MEXP, NEXP
SAVE J

IF (FRM.EQ.'A') THEN
  PP = (KZ/BB)**(1/MEXP)
  GETDKDP = MEXP * BB * PP**(MEXP-1)
ELSE
  IF (J.EQ.0 .OR. ((KAPZ(J).GT.KZ).EQV.(KAPZ(J+1).GT.KZ)))
  * CALL LOCATE(KAPZ, N, KZ, J)
  IF (J .EQ. 0) THEN
    PAUSE 'OUT OF RANGE IN EVALKAPZ'
    KZ = -999999999.
    DK = -999999999.
  ELSEIF (J .EQ. N) THEN
    PAUSE '+ OUT OF RANGE IN EVALKAPZ'
    KZ = 0.
    DK = 0.
  ELSE
    IF (J .EQ. 1) THEN
      JJ = 1
      N1 = 3
    ELSEIF (J .EQ. N-1) THEN
      JJ = J-1
      N1 = 3
    ELSE
      JJ = J - 1
      N1 = 3
    ENDIF
  CALL POLCOE(KAPZ(JJ), PC(JJ), N1, COF)
  CALL DDPOLY( COF, N1, KZ, PD, 2)
  KZ = PD(2)
  GETDKDP = 1 / PD(2)
ENDIF
ENDIF
ENDIF
RETURN
END

C ===================================================================================

DOUBLE PRECISION FUNCTION
& C4(FRM, DOMAIN, W, W0, KAPZ0, PC, KAPX, KAPZ, N2, N)
DOUBLE PRECISION W, PC(100), KAPX(100), KAPZ(100), INVF
CHARACTER*1 FRM, DOMAIN
DOUBLE PRECISION SUM, HI, HO, TI1, TI2, TI3, PP, P, U, W0,
& KAPZ0, PC0, KAPZ0, INTERP
DOUBLE PRECISION AA, BB, MEXP, NEXP, R, ARG1, ARG2, CC4
DOUBLE PRECISION AA2, BB2
COMMON /EXPON/ AA, BB, MEXP, NEXP
.wp 355	KAPZ_ = W0 * KAPZ0 / W
356
357	C ANALYTICAL SOLUTION OF INTEGRAL
358	  IF (FRM.EQ. 'A') THEN
359	    R = SQRT (2.*MEXP/(NEXP-MEXP+1.))
360	    ARG1 = 0.5D0
361	    ARG2 = (R**2*(NEXP+1)/MEXP+2.) / 2.
362	    CC4 = AA/(NEXP+1.) * (KAPZ_/BB)**((NEXP+1.)/MEXP)
363	    *R*BETA(ARG1,ARG2)
364	    C4 = CC4
365
366	C RETURN
367
368	ENDIF
369
370	SUM = 0.0D0
371	HO = 1./(N2-1.)
372
373	IF (FRM.EQ. 'A') THEN
374	  PC_ = ( KAPZ_/ / BB )**(1./MEXP)
375	  AA2 = AA * PC_**NEXP
376	  BBZ = BB * PC_**MEXP
377	  IF (AA2.GT.1.0) THEN
378	    PRINT *, ' CHECK INPUT DATA '
379	    PRINT *, ' REL PERM > 0 '
380	    PAUSE
381	  ENDIF
382	  PC_ = 1.0
383	ELSE
384	  PC_ = INTERP(KAPZ, PC, KAPZ_, N)
385	ENDIF
386
387	T13 = 0.0
388	P = 0.0
389	HI = PC_ / (N2-1)
390	DO II = 1,N2-1
391	  T11 = T13
392	  P = (II-1) * HI
393	  IF (FRM.EQ. 'A') THEN
394	    PP = BBZ * (P)**MEXP / KAPZ_
395	    U = INVF (PP, FRM)
396	    TI2 = 2 * U * AA2 * (P)**NEXP
397	  ENDIF
398	  PP = BBZ * (P+HI)**MEXP / KAPZ_
399	  U = INVF (PP, FRM)
400	  T13 = 2 * U * AA2 * (P+HI)**NEXP
401
402	SUM = SUM + TI2 + T13
403
404	ELSE
405	  IF (DOMAIN.EQ. 'P') THEN
406	    U = INVF (INTERP (PC, KAPZ, P+HI/2., N) / KAPZ_, FRM)
407	    TI2 = INTERP (PC, KAPX, P+HI/2., N) * 2 * U
408	  ELSE
409	    PP = INTERP (PC, KAPZ, P+HI/2., N) / KAPZ_
410	    U = INVF (PP, FRM)
411	    TI2 = INTERP (PC, KAPX, P+HI/2., N) * U**2 / 2.
412
413	ENDIF
414
415	IF (DOMAIN.EQ. 'P') THEN
WIDTH3.FOR

09/25/98

414 \quad U = \text{INVF}( \text{INTERP}( \text{PC}, \text{KAPZ}, \text{P}+\text{HI}, \text{N}) / \text{KAPZ}_- , \text{FRM} ) \\
415 \quad T13 = \text{INTERP}( \text{PC}, \text{KAPX}, \text{P}+\text{HI}, \text{N}) * 2 * U \\
416 \quad \text{ELSE} \\
417 \quad \quad PP = \text{INTERP}( \text{PC}, \text{KAPZ}, \text{P}+\text{HI}, \text{N}) / \text{KAPZ}_- \\
418 \quad \quad U = \text{INVF}( PP , \text{FRM} ) \\
419 \quad \quad T13 = \text{INTERP}( \text{PC}, \text{KAPX}, \text{P}+\text{HI}, \text{N}) * U^{**2} / 2. \\
420 \quad \text{ENDIF} \\
421 \quad \text{ENDIF} \\
422 \quad \quad \text{SUM} = \text{SUM} + T11 + 4. * T12 + T13 \\
423 \quad \quad P = P + \text{HI} \\
424 \quad \text{ENDIF} \\
425 \quad \text{END DO} \\
426 \quad \text{IF}(\text{FRM.EQ.'A'})\text{THEN} \\
427 \quad \quad CC4 = \text{SUM} * \text{HI} * ( \text{KAPZ}_- / \text{BB} )^{**(1/MEXP)} / 2. \\
428 \quad \text{ELSE} \\
429 \quad \quad CC4 = \text{SUM} * \text{HI} / 6. \\
430 \quad \text{ENDIF} \\
431 \quad \quad C4 = CC4 \\
432 \quad \text{RETURN} \\
433 \quad \text{END} \\

\text{================================================} \\
434 \quad \text{DOUBLE PRECISION FUNCTION INVF(F,FRM)} \\
435 \quad \text{DOUBLE PRECISION F} \\
436 \quad \text{DOUBLE PRECISION AA,BB,M, N} \\
437 \quad \text{COMMON /EXFON/ AA,BB,M, N} \\
438 \quad \text{CHARACTER*1 FRM} \\
439 \quad \text{C IF(F.GT.1.0) THEN} \\
440 \quad \text{C PRINT *, ' F > 1 IN INVF',F} \\
441 \quad \text{C STOP} \\
442 \quad \text{C ELSE} \\
443 \quad \text{IF(F.GT.1.0) F = 1.0} \\
444 \quad \text{IF(FRM .EQ. 'G')THEN} \\
445 \quad \quad \text{INVF = SQRT( -LOG(F) )} \\
446 \quad \text{ELSEIF(FRM.EQ.'P')THEN} \\
447 \quad \quad \text{IF( F .LE.0.0 ) THEN} \\
448 \quad \quad \quad \text{INVF = 1} \\
449 \quad \quad \quad \text{ELSE} \\
450 \quad \quad \quad \quad \text{INVF = SQRT(1-F)} \\
451 \quad \quad \quad \text{ENDIF} \\
452 \quad \quad \text{ELSEIF(FRM.EQ.'A')THEN} \\
453 \quad \quad \quad \text{IF( F .LT. 0.0 ) THEN} \\
454 \quad \quad \quad \quad \text{INVF = SQRT(2*M/(N-M+1))} \\
455 \quad \quad \quad \text{ELSE} \\
456 \quad \quad \quad \quad \text{INVF = SQRT(((1-F**(N-M+1)/M))2*M/(N-M+1))} \\
457 \quad \quad \quad \text{ENDIF} \\
458 \quad \quad \text{ELSE} \\
459 \quad \quad \quad \text{PRINT *, ' INVALID FORM ', FRM} \\
460 \quad \quad \quad \text{STOP} \\
461 \quad \quad \text{ENDIF} \\
462 \quad \quad \text{C ENDIF} \\
463 \quad \quad \text{C print *, ' invf ',invf} \\
464 \quad \text{RETURN} \\
465 \quad \text{END} \\

273
C DOUBLE PRECISION FUNCTION MOMENTTO(W,KAPZ_C)
        COMMON /PARAMS/ W0, KAPX, KAPZ, PC, SPC, THO, STHO, KAPZ0, A,
        & QT, KSX, N2, N, FRM, DOMAIN
        COMMON /EXPON/ AA, BB, MEXP, NEXP

        DOUBLE PRECISION PC(100), THO(100), KAPX(100), KAPZ(100),
        * SPC(100), STHO(100),
        * A, KAPZ_C, W, W0, KAPZ0, QT, KSX,
        * T12, T13, K1, K2, K, F, U1, U2, U3,
        * INTERP, LIM, MEXP, NEXP, AA, BB
        CHARACTER*1 FRM, DOMAIN
        CHARACTER*132 OUT

        U3 = 0.0
        TO = 0.0
        T2 = 0.0

        IF(FRM.EQ.'P')THEN
            LIM = 1.0
        ELSEIF(FRM.EQ.'G')THEN
            LIM = 5.0
        ELSEIF(FRM.EQ.'A')THEN
            PRINT *, ' A FORM IN MOMENTTO '
            STOP
        ENDIF

        H = LIM / (N2-1)
        U1 = 0
        K = KAPZ_C * F(U1, FRM)
        T13 = INTERP( KAPZ, THO, K, N )
        WRITE(999,*)
        DO II = 1,N2-1
            T11 = T13
            U1 = U3
            U2 = U1 + H / 2.
            IF(II.EQ. N2-1) THEN
                U3 = LIM
            ELSE
                U3 = U1 + H
            ENDIF

            K1 = KAPZ_C * F(U2, FRM)
            K2 = KAPZ_C * F(U3, FRM)
            T12 = INTERP( KAPZ, THO, K1, N )
            T13 = INTERP( KAPZ, THO, K2, N )
            IF(MOD(II-1,2).EQ.0) WRITE(999,9999)U1*W, T11
               print *, 'U1,u2,u3,p,p1,p2',u1,u2,u3,p,p1,p2
        c IF(DOMAIN.EQ.'P')THEN
            TO = TO + T11 + 4. * T12 + T13
            T2 = T2 + U1**2*T11 + 4. * U2**2*T12 + U3**2*T13
        ELSE
            TO = TO + U1 * T11 + 4. * U2 * T12 + U3 * T13
            T2 = T2 + U1**3*T11 + 4. * U2**3*T12 + U3**3*T13
        ENDIF
        K = K2
        END DO
        MOMENTTO =SQRT( W**3 * T2 / (W * TO))
RETURN
END

C=====================================================================
C Given tabulated function Y(X), find Y1=Y(X1) using C polynomial fitted to nearest 4 points. If X1 is C between the first or last two data points in X then C only 3 points are used.
C Caution:
C 1. X data points must be monotonically increasing C or decreasing
C 2. If X1 is out of range at end of series,
C Y1 is extrapolated using the last 3 points
C 3. For X1 out of range at beginning of series,
C the program is stopped.

DOUBLE PRECISION FUNCTION INTERP( X, Y, X1, N )
DOUBLE PRECISION X(100), Y(100), X1, DY, Y1

SAVE J

IF(J.EQ.0 .OR. ((X(J).GT.X1).EQV.(X(J+1).GT.X1)))
* CALL LOCATE(X, N, X1, J)
IF ( J .EQ. 0 ) THEN
PRINT *, 'BELOW RANGE IN INTERP', X1
PAUSE 'BELOW RANGE IN INTERP'
INTERP = 0.0
ELSEIF( J .EQ. N ) THEN
PAUSE 'ABOVE RANGE IN INTERP'
INTERP = .00000000001
ELSE
IF( J .EQ. 1 ) THEN
JJ = 1
N1 = 3
ELSEIF( J .EQ. N-1 ) THEN
JJ = J-1
N1 = 3
ELSEIF( J .EQ. N ) THEN
JJ = J-2
N1 = 3
ELSE
JJ = J - 1
N1 = 3
ENDIF
CALL POLINT(X(JJ),Y(JJ),N1,X1,Y1,DY)
INTERP = Y1
ENDIF
RETURN
END

C=====================================================================
DOUBLE PRECISION FUNCTION F(U, FRM)
DOUBLE PRECISION U, AA,BB,M, N, LIM

275
591 COMMON /EXPON/ AA, BB, M, N
592 CHARACTER*1 FRM
593
594 IF(FRM .EQ. 'G') THEN
595 F = EXP(-U**2)
596 ELSEIF(FRM .EQ. 'P') THEN
597 IF(U .LT. -1 .OR. U .GT. 1) THEN
598 F = 0.0
599 ELSE
600 F = 1-U**2
601 ENDIF
602 ELSEIF(FRM .EQ. 'R') THEN
603 IF(U .LT. -1 .OR. U .GT. 1) THEN
604 F = 0.0
605 ELSE
606 F = 1.0
607 ENDIF
608 ELSEIF(FRM .EQ. 'A') THEN
609 LIM = SQRT(2*M/(N-M+1))
610 IF(U .LT. -LIM .OR. U .GT. LIM) THEN
611 F = 0.0
612 ELSE
613 F = (1-(N-M+1)/(2*M)*U**2)**(M/(N-M+1))
614 ENDIF
615 ELSE
616 PRINT *, 'INVALID FORM', FRM
617 STOP
618 ENDIF
619 RETURN
620 END
621
622 C ********** ROUTINES FROM NUMERICAL RECIPES **********
623
624 C =------------------------------------------------------------------------
625
626 C Numerical Recipes, p. 90, 1987
627 C Given an array xx of length N, and given a value X, returns
628 C a value J such that X is between XX(J) and XX(J+1).
629 C J = 0 or J = N is returned to indicate that X is out of
630 C range.
631
632 SUBROUTINE LOCATE(XX,N,X,J)
633 DOUBLE PRECISION XX(N),X
634
635 JL = 0
636 JU = N+1
637 10 IF(JU-JL.GT.1) THEN
638 JM = (JU+JL)/2
639 IF((XX(JM).GT.XX(1)).EQV.(X.GT.XX(JM))) THEN
640 JL = JM
641 ELSE
642 JU = JM
643 ENDIF
644 GO TO 10
645 ENDIF
646 J = JL
647 RETURN
648 END
WIDTH3.FOR

09/25/98

C === POLCOE

C Given arrays X and Y of length N containing a tabulated function
C Yi = f(Xi), this routine returns an array of coefficients COF,
C also of length N, such that Yi = sum(COFj * Xi**(j-1))

SUBROUTINE POLCOE(X,Y,N,COF)
DOUBLE PRECISION X(N), Y(N), COF(N), S(15), PHI, FF, B

C PARAMETER (NMAX =15)

DO 11 I=1,N
   PRINT *, X(I), Y(I)
   S(I) = 0.
   COF(I) = 0.

11 CONTINUE
S(N) = -X(1)
DO 13 I=2,N
   DO 12 J = N+1-I, N-1
       S(J) = S(J) - X(I) * S(J+1)

12 CONTINUE
S(N) = S(N) - X(I)

13 CONTINUE
DO 16 J = 1,N
   PHI = N
   DO 15 K = N-1,1,-1
       PHI = K*S(K+1)+X(J)*PHI

14 CONTINUE
FF = Y(J) / PHI
B = 1.
DO 15 K=N,1,-1
   COF(K) = COF(K) + B * FF
   B = S(K) + X(J) * B

15 CONTINUE
RETURN
END

C ===== DDPOLY

C Given the NC coefficients of a polynomial of degree NC-1 as
C an array C with C(1) being the constant term, and given a
C value X, and given a value ND>1, this routine returns the
C polynomial evaluated at X as PD(1) and ND-1 derivatives as
C PD(2), ... PD(ND)

SUBROUTINE DDPOLY(C, NC, X, PD, ND)
DOUBLE PRECISION C(NC), PD(ND), CONST, X

PD(1) = C(NC)
DO 11 J = 2,ND
   PD(J) = 0.0

11 CONTINUE
DO 13 I = NC-1,1,-1
   NND = MIN(ND, NC+1-I)
   DO 12 J = NND,2,-1
       PD(J) = PD(J) * X + PD(J-1)

12 CONTINUE
WIDTH3.FOR

09/25/98

1 PD(I) = PD(I) * X + C(I)

13 CONTINUE

14 CONST = 2.

15 DO 14 I=3,ND

16 PD(I) = CONST * PD(I)

17 CONST = CONST * I

18 CONTINUE

19 RETURN

20 END

C ===== POLINT ======================================

C Given arrays XA and YA, each of length N, and given a value X,
C this routine returns a value Y, and an error estimate DY. If
C P(x) is the polynomial of degree N-1 such that P(XAi) = YAi,i=1..n
C then the returned value Y = P(X)

SUBROUTINE POLINT(XA,YA,N,X,Y,DY)

PARAMETER (NMAX = 10)

DOUBLE PRECISION XA(N), YA(N), C(NMAX), D(NMAX)

DOUBLE PRECISION X, Y, DY

NS = 1

DIF = ABS(X-XA(1))

DO 11 I=1,N

DIFT = ABS(X-XA(I))

IF(DIFT.LT.DIF) THEN

NS = I

DIF = DIFT

ENDIF

C(I) = YA(I)

D(I) = YA(I)

CONTINUE

Y = YA(NS)

NS = NS - 1

DO 13 M = 1,N-1

DO 12 I=1,N-M

HO = XA(I) - X

HP = XA(I+M) - X

W = C(I+1) - D(I)

DEN = HO - HP

IF(DEN.EQ.0.) PAUSE

DEN = W/DEN

D(I) = HP * DEN

C(I) = HO * DEN

CONTINUE

IF(2 * NS .LT. N-M) THEN

DY = C(NS+1)

ELSE

DY = D(NS)

NS = NS - 1

ENDIF

Y = Y + DY

CONTINUE

RETURN

END

C == RK4

278
SUBROUTINE RK4(Y, DYDX, N, X, H, YOUT)

PARAMETER (NMAX = 10)

DOUBLE PRECISION Y(N), DYDX(N), YOUT(N), YTEMP(NMAX),

* 

DYT(NMAX), DYM(NMAX)

DOUBLE PRECISION HH, H, XH, X, H6

HH = H * 0.5

H6 = H / 6.

XH = X + HH

DO 11 I=1,N

11 YT(I) = Y(I) + HH * DYDX(I)

CALL DERIVS(XH, YT, DYT)

DO 12 I=1,N

12 YT(I) = Y(I) + HH * DYT(I)

CALL DERIVS(XH, YT, DYM)

DO 13 I = 1,N

13 YT(I) = Y(I) + H * DYM(I)

DYM(I) = DYT(I) + DYM(I)

CALL DERIVS(X+H, YT, DYT)

DO 14 I = 1,N

14 YOUT(I) = Y(I) + H6*(DYDX(I) + DYT(I) + 2. * DYM(I))

C

PRINT *, 'rk4 ', h6, y, dydx, n, x, yout

RETURN

END

C ============== RKQC ===============

SUBROUTINE RKQC(Y, DYDX, N, X, HTRY, EPS, YSCAL, HDID, HNEXT)

PARAMETER (NMAX=10, PGROW=-.20, PSHRNK=-.25, FCOR=1. / 15.,

* 

ONE=1.0, SAFETY=0.9, ERRCON=6.E-4)

DIMENSION YSCAL(N)

DOUBLE PRECISION Y(N), DYDX(N), YTEMP(NMAX),

* 

YSAV(NMAX), DYSAV(NMAX)

DOUBLE PRECISION XSAV, X, H, HH

C

PRINT *, 'rkqc ', y, dydx, n, x, htry

XSAV = X

DO 11 I=1,N

11 YSAV(I) = Y(I)

DYSAV(I) = DYDX(I)

CONTINUE

H = HTRY

1 HH = 0.5 * H

CALL RK4(YSAV, DYSAV, N, XSAV, HH, YTEMP)

X = XSAV + HH

CALL DERIVS(X, YTEMP, DYDX)

CALL RK4(YTEMP, DYM, X, HH, Y)

X = XSAV + H

IF(X.EQ.XSAV) PAUSE 'STEP SIZE NOT SIGNIFICANT IN RKQC.'

CALL RK4(YSAV, DYSAV, N, XSAV, H, YTEMP)

ERRMAX = 0.0

DO 12 I=1,N

YTEMP(I) = Y(I) - YTEMP(I)

R = YTEMP(I) / YSCAL(I)
ERRMAX = MAX(ERRMAX, ABS(R))
12 CONTINUE
ERRMAX = ERRMAX / EPS
IF (ERRMAX.GT.ONE) THEN
   H = SAFETY * H * (ERRMAX**PSHRNK)
GO TO 1
ELSE
HDID = H
IF (ERRMAX.GT.ERRCON) THEN
   HNEXT = SAFETY * H * (ERRMAX**PGROW)
ELSE
   HNEXT = 4. * H
END IF
DO 13 I = 1,N
   Y(I) = Y(I) + YTEMP(I) * FCOR
13 CONTINUE
RETURN
END

C -----------------------------------------------

SUBROUTINE GEN_OUTPUT(Z, W, DWDX)
CHARACTER*1 T_
DOUBLE PRECISION Z, W, DWDX
DOUBLE PRECISION KZ, DKZ, GETKZ, GETDKZ, GETDKDP, DPDZ, MOMENTTO

CHARACTER*1 FRM, DOMAIN
DOUBLE PRECISION A, QT, KSX
DOUBLE PRECISION PC(100), KAPX(100), KAPZ(100), THO(100),
   & SPC(100), STHO(100), W0, KAPZ0,
   * INTERP, P, TO, STO, M2, MEXP, NEXP, AA, BB

DOUBLE PRECISION A1, A2, W_ANAL
DOUBLE PRECISION DELRHO, G
COMM /PARAMS/, W0, KAPX, KAPZ, PC, SPC, THO, STHO, KAPZ0, A,
   & QT, KSX, N2, N, FRM, DOMAIN
COMM /EXPON/, AA, BB, MEXP, NEXP
COMM /DENSE/, DELRHO, G

T_ = CHAR(9)
KZ = GETKZ(W)
DKZ = GETDKZ(W, DWDX, KZ)
DPDZ = DKZ/GETDKDP(KZ)

IF (FRM.EQ. 'A') THEN
   c evaluate analytical solution
   A1 = W0**((MEXP+NEXP+1)/MEXP)
   A2 = A* (MEXP+NEXP+1) * AA * BB**(- (NEXP+1)/MEXP)
   * (W0*KAPZ0)**((NEXP-MEXP+1)/MEXP)**2 / (DELRHO*G*MEXP**2)
   W_ANAL = (A1 - A2)**(MEXP/(NEXP+1+MEXP))
   P = (KZ/BB)**(1/MEXP)
   TO = -999.
   STO = -999.
   SP = -999.
   M2 = -999.
   WRITE (2, ' (8(F15.7, A1)) ')
   & 2, T_, W, T_, W_ANAL, T_,
WIDTH3.FOR

* KZ, T_, DKZ,T_,
* P,T_, DPDZ,T_,
* Z
WRITE(6,'(8(G15.7,1X))')
& Z,W,W_ANAL,DWDX,DPDZ
ELSE
P = INTERP(KAPZ,PC,KZ,N)
TO = INTERP(KAPZ,THO,KZ,N)
STO = INTERP(KAPZ,STHO,KZ,N)
SP = INTERP(KAPZ,SPC,KZ,N)
M2 = MOMENTTO(W,KZ)
WRITE(2,'((11(F15.7,A1))')
& Z,T_, W,T_,
M2,T_,
KZ, T_, DKZ,T_,
P,T_, SP,T_, DPDZ,T_,
TO,T_, STO,T_,
Z
WRITE(6,'(8(G15.7,1X))')
& Z,W,DWDX,DPDZ
ENDIF
RETURN
END

C === ODEINT ==================================================================
SUBROUTINE ODEINT(YSTART,NVAR,X1,X2,EPS,H1,HMIN,NOK,
* NBAD)
PARAMETER (MAXSTP=10000, NMAX=1, TWO=2.0, ZERO=0.0, TINY=1.E-30)
COMMON /PATH/ DXSAV
COMMON /PATH2/ KMAX, KOUNT
DOUBLE PRECISION DXSAV, X
DOUBLE PRECISION YSTART(NVAR), Y(NMAX), DYDX(NMAX), YOUT, DYOUT
DIMENSION YSCAL(NMAX)
X = X1
H = SIGN(H1,X2-X1)
NOK = 0
NRAD = 0
KOUNT = 0
DO 11 I=1,NVAR
  Y(I) = YSTART(I)
11 CONTINUE
XSAV = X - DXSAV * TWO
DO 16 NSTP = 1, MAXSTP
CALL DERIVS(X,Y,DYDX)
DO 12 I=1,NVAR
  YSCAL(I) = ABS(Y(I)) + ABS(H*DYDX(I)) + TINY
12 CONTINUE
IF(KMAX.GT.0) THEN
  IF(ABS(X-XSAV) .GT. ABS(DXSAV)) THEN
    IF(KOUNT .LT. KMAX - 1) THEN
      KOUNT = KOUNT + 1
      CALL GEN_OUTPUT(X,Y(I),DYDX(I))
      XSAV = X
      ENDIF
    ENDIF
  ENDIF
END
WIDTH3.FOR

09/25/98

945 ENDIF
946 947 IF((X+H-X2)*(X+H-X1).GT.ZERO) H = X2-X
948 CALL RKQC(Y,DYDX,NVAR,X,H_EPS,YSCAL,HDID,HNEXT)
949 IF(HDID.EQ.H) THEN
950 NOK = NOK + 1
951 ELSE
952 NBAD = NBAD + 1
953 ENDIF
954 IF((X-X2)*(X2-X1).GE.ZERO) THEN
955 DO 14 I=1,NVAR
956 YSTART(I) = Y(I)
957 CONTINUE
958 IF(KMAX.NE.0) THEN
959 KOUNT = KOUNT + 1
960 C
961 XP(KOUNT) = X
962 YOUT = Y(1)
963 DYOUT = DYDX(1)
964 CALL GEN_OUTPUT(X,YOUT,DYOUT)
965 ENDIF
966 RETURN
967 ENDIF
968 IF(ABS(HNEXT).LT.HMIN) PAUSE 'STEPSIZE SMALLER THAN MINIMUM'
969 H = HNEXT
970 CONTINUE
971 PAUSE 'TOO MANY STEPS'
972 RETURN
973 END
974
975 DOUBLE PRECISION FUNCTION GAMMLN(XX)
976 DOUBLE PRECISION XX
977 DOUBLE PRECISION COF(6), STP, HALF, ONE, FFP, X, TMP, SER
978 DATA COF,STP/76.18009173D0, -86.50532033D0, 24.01409822D0,
979 & -1.231739516D0, 0.120858003D-2,
980 & -5.36382D-5, 2.50662827465D0/
981 DATA HALF, ONE, FFP/0.5D0, 1.0D0, 5.5D0/
982 X = XX - ONE
983 TMP = X + FFP
984 TMP = (X+HALF)*LOG(TMP) - TMP
985 SER = ONE
986 DO 11 J=1,6
987 X = X +ONE
988 SER = SER + COF(J)/X
989 CONTINUE
990 GAMMLN = TMP + LOG(STP*SER)
991 RETURN
992 END
993
994 DOUBLE PRECISION FUNCTION BETA(Z,W)
995 DOUBLE PRECISION Z,W,GAMMLN
996 BETA = EXP(GAMMLN(Z) + GAMMLN(W) -GAMMLN(Z+W))
997 RETURN
998 END
999
1000