NUMERICAL MODELING OF BUOYANT PLUMES IN A TURBULENT, STRATIFIED ATMOSPHERE

by
Ralph G. Bennett
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<td>The name of Pasquill is in common usage today for plume modeling. The bivariate Gaussian plume description was originated by O. G. Sutton (<em>Proc. Roy. Soc. A.</em> 135, pp. 143-165).</td>
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NUMERICAL MODELING OF BUOYANT PLUMES IN A TURBULENT, STRATIFIED ATMOSPHERE

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ABSTRACT

A widely applicable computational model of buoyant, bent-over plumes in realistic atmospheres is constructed. To do this, the two-dimensional, time-dependent fluid mechanics equations are numerically integrated, while a number of important physical approximations serve to keep the approach at a tractable level. A three-dimensional picture of a steady state plume is constructed from a sequence of time-dependent, two-dimensional plume cross sections—each cross section of the sequence is spaced progressively further downwind as it is advected for a progressively longer time by the prevailing wind. The dynamics of the plume simulations are quite general. The buoyancy sources in the plume include the sensible heat in the plume, the latent heat absorbed or released in plume moisture processes, and the heating of the plume by a radioactive pollutant in the plume. The atmospheric state in the simulations is also quite general. Atmospheric variables are allowed to be functions of height, and the ambient atmospheric turbulence (also a function of height) is included in the simulations.

A demonstration of the ability of the model to reproduce the solutions to problems that are known is undertaken. Comparisons to buoyant line-thermal laboratory experiments show that the model calculates the dynamics of the fluid motions to an acceptable accuracy. Comparisons to atmospheric plume rise and dispersion experiments show that the model can simulate individual plumes more accurately than existing correlations because it calculates the effect of the atmospheric turbulence and stratification from first-principles. The comparisons also show that improvements to the model are likely to be made by more accurately describing the anisotropic nature of atmospheric turbulence, and the production of turbulence by the sources of buoyancy.
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1. PROBLEM DESCRIPTION AND SOLUTION

1.1 Introduction

With the rapidly increasing burden of air pollution over recent decades, the engineer's ability to analyze the behavior of an ever-widening assortment of effluents has not kept up with the importance of the consequences of the releases. The reason for this is that the "predictive" models of plume behavior that are currently available universally suffer from a lack of extendability. That is, they need to observe the behavior of an ensemble of the releases that they wish to model before they can form an accurate picture of the release. The models are useful only to the extent that an appropriate ensemble of plumes can be created for study, either as full-scale atmospheric releases, or as scaled-down laboratory experiments. Inasmuch as the important turbulent and thermal characteristics of the atmosphere cannot be simulated in the laboratory, and since an ensemble of plumes with catastrophic consequences (e.g., radioactive plumes from nuclear reactor accidents) may be impractical to produce, plume modeling has needed to take a more universal approach.

The purpose of this work is to construct a widely applicable model of plume behavior in realistic atmospheres. To do this, a "first principles" approach is adopted. A
numerical integration of the fluid mechanics equation is undertaken, while a number of important physical approximations to the problem serve to keep the approach at a tractable level. The advantage of the model presented here is the ability to tackle problems outside of the scope of existing models without greatly increasing the resources spent on the analysis.

1.2 Background and Problem Description

1.2.1 Historical Background

Man has produced and observed bent-over buoyant plumes since the discovery of fire. However, the bent-over plume did not have any great impact on society until the advent of large industrial sources near population centers during the industrial revolution. The number of large industrial sources has increased steadily with the industrialization of many countries. In the recent past, the variety of releases from large industrial sources has increased greatly, and now includes the potentially more harmful effluents from chemical refining and combustion processes, nuclear power plants, and large cooling towers. Also, the steady growth of population centers almost always dictates that these new sources will be located in at least moderately populated areas.

Historically, the ability to analyze the effects of large releases and hence to develop technologies for their
mitigation has not kept pace with the consequences of the releases. To date, the advances have been quite modest: early observations during the industrial revolution suggested the use of tall stacks for lessening the effects of large releases. The strong influence of the synoptic-scale weather on releases (first investigated in order to increase the effectiveness of chemical warfare agents) has largely motivated the Pasquill-type correlations of plume behavior. The hope of simply reducing the consequences by reducing the amount of effluents has stimulated an abundance of filtering, scrubbing, and effluent control technologies. However, increasingly important releases are certain to occur. A brief review here of the existing approaches to plume modeling can indicate the most promising avenue for study.

1.2.2 Characteristics of Bent-Over Buoyant Plumes

The character of the bent-over buoyant plume is central to all of the available plume models. When an effluent stream with a given upward momentum and initial buoyancy is released from a stack into a windy atmosphere, the plume is deflected downwind. This occurs partly because of pressure forces that develop around the plume, and partly because the plume entrains the ambient air, which mixes a lot of downwind momentum into the plume. The deflection quickly causes the plume to bend over (usually within about one stack height) and then to be
carried downstream. The buoyancy of the plume is converted into kinetic energy, and the plume rises under this action for a considerable distance downwind. About 20 years ago it was noted\(^1\) that the motion of the plume in cross section during this rise was essentially that of a two-dimensional turbulent vortex pair. Initially the vortex pair rises and grows without being too dependent upon atmospheric turbulence (although atmospheric stratification is always important). After the kinetic energy of the cross-sectional motions has essentially died out, the plume continues to disperse solely by atmospheric motions. It will be found in the review of plume models that only the detailed numerical plume models provide a method that can easily bridge between the regimes where plume turbulence dominates and where atmospheric turbulence dominates.

1.2.3 Overview of Plume Models

With regard to the detailed three-dimensional nature of plume motions, existing models of plume behavior are found to possess a wide variety of sophistication. The Pasquill-type models, the entrainment models, and the numerical models are considered here.

The Pasquill-type models develop a highly idealized picture of the fluid motions in and around the plume. Pollutants in the plume cross section are assumed to fit Gaussian
distributions of height and width. In essence, the model parameters (standard deviations of the Gaussian distributions) are simply an ad-hoc replica of the experimental results; as such, the models are unable to predict in cases for which experiments have not been performed. The wealth of non-passive effluents and the rich variations in the meteorological state of the atmosphere serve to guarantee that cases outside of the Pasquill-type models will always exist.

The entrainment models develop a much less idealized, and much more physical picture of the fluid motions in the plume. In general, the models make use of the very elegant non-dimensional formulations and similarity relationships that are central to the theory of homogeneous isotropic turbulence. Typically the models are successful at analyzing the initial plume behavior, where the self-generated plume turbulence dominates over the atmospheric turbulence. The entrainment models are generally able to analyze plumes only in fairly simple atmospheres when analytical solutions are sought. But this is not the primary limitation of entrainment models, since in some cases their solutions are found on computers. The limitations of the entrainment models are the condition that the plume self-generated turbulence is dominant over the atmospheric turbulence, (which eventually breaks down for all plumes, commonly at
downwind distances for which the solution is still needed) and the basic entrainment velocity assumption, which cannot be obtained from fundamental constants and scales in a straightforward way.

Numerical plume models are capable of developing the most detailed picture of the fluid motions in the plume. In general, the models seek to integrate a closed set of Reynolds-averaged fluid mechanics equations, either in two or three dimensions. Turbulence leads to a fundamental closure problem in writing this set of equations, so that each model will have a collection of closure assumptions that together form a turbulence model, aside from other assumptions that are made concerning the plume behavior. Numerical plume models are becoming capable of analyzing the most detailed cases, yet they are often limited by the large computing costs. Aside from the computer costs, the tasks of initializing and validating the problem with fully two- or three-dimensional data can also quickly become intractable. Until computer costs are reduced greatly, the most useful numerical plume models will likely have to be two-dimensional. The greatest benefit that comes from such models is the wider range of application of the models, and the ease of extending them to new cases.
1.2.4 Scope of the Work

This work constructs a three-dimensional solution of a steady state plume from a sequence of time-dependent two-dimensional plume cross sections; each plume cross section of the sequence being spaced progressively further downwind as it is advected for a progressively longer time by the prevailing wind. The two-dimensional cross sections are simulated with a time-dependent turbulent fluid mechanics code which integrates the time-averaged equations of continuity, momentum, energy, moisture, and pollutant. The behavior of an individual plume is modeled in this way until the height or radius of the plume reaches several hundred meters, which roughly corresponds to the plume cross section being tens of kilometers downwind of the source.

The dynamics of the plume simulations are quite general. The buoyancy sources in the plume encompass the sensible heat in the plume, the latent heat absorbed or released in plume moisture processes, and the radioactive decay heating of the plume by a radioactive pollutant species in the plume. Buoyancy from chemical reactions could be easily included. The atmospheric state in the simulations accepts atmospheric wind, temperature, water vapor, liquid water, background pollutant, turbulent eddy viscosity, and turbulent kinetic energy as functions of height. The turbulence is treated
with the sophisticated second-order closure model of Stuhmiller\textsuperscript{2}, which allows the turbulent recirculation and entrainment of the plume cross section to be treated in a very natural way.

The model is validated against the Pasquill model\textsuperscript{3} and the entrainment model of Richards\textsuperscript{4} for idealized cases in which these models apply, and for several cases from the LAPPES\textsuperscript{5} field data for actual large power plant stacks. Simulations are obtained for cases outside of the Pasquill and entrainment models, and while no specific field data for these cases exists, the behavior of the simulation agrees with the physical changes imposed on the problems.
2. LITERATURE REVIEW

The literature review in this work undertakes a broad survey of plume modeling. In the first section, existing numerical plume models are discussed, along with the experimental data base that is available for the validation of these detailed plume models. The first section also includes the research that has been done on computational and experimental modeling of two-dimensional line vortex pairs. It is important to include them since the results of such work are very easily interpreted in the context of air pollution problems. In the second section, existing numerical models of the planetary boundary layer are discussed. Again, these models are very easily extended to air pollution problems (with the inclusion of a pollutant transport equation and pollutant source), so it is important to include them in the review.

2.1 Numerical Plume Models

A large number of plume models have been developed that are available as computer programs. Several recent reviews have reported dozens of such models, and it is important to make a distinction regarding them. A majority of the models employ the Gaussian plume assumption; as such, the computer
is simply being used to look up and present the standard handbook calculations, with minor modifications in some cases. These are not "numerical plume models" in the sense that the primitive equations are not being integrated to show the plume development, although computers are being used. Such models are not considered further here. The remaining models in the reviews are truly numerical plume models, and they will be considered next, along with several models that were reported elsewhere.

2.1.1 Three-Dimensional Models

The most sophisticated numerical plume models to date have not yet attempted a second-order turbulence closure to the fully three-dimensional flow field for non-passive pollutants. Some of these features are found in each of the models discussed here, but not all of them. The notes of Rao⁹ and Nappo¹⁰ discuss the desirable features of three-dimensional numerical plume models, and provide a good introduction to future work that may be undertaken.

Donaldson's modeling¹¹ has concentrated on a second-order turbulence closure for a three-dimensional planetary boundary layer simulation with a passive pollutant. Because the pollutant is passive, and hence does not affect the flow field or its turbulence, the turbulence closure only addresses PBL
turbulence, and is independent of the behavior of buoyant plumes. This is in contrast to the method in this work, where the second-order closure is "tuned" to the development of turbulent buoyant plumes, and is largely independent of PBL turbulence development. Lewellen's modeling\textsuperscript{12} begins with a second-order closure to the passive pollutant transport equation, and then adopts the PBL flow field and turbulence from Donaldson's model.\textsuperscript{11} Only integrations of the pollutant transport equation are needed in Lewellen's model because of the adoption of a complete PBL solution. Patankar's model\textsuperscript{13} of a deflected turbulent jet in three-dimensions also uses a second-order closure model, but does not allow for buoyancy and stratification, although it does allow for non-isotropic turbulent transports in the vertical and horizontal directions. A fundamentally different approach to three-dimensional modeling is found in the Atmospheric Release Advisory Capability (ARAC) system.\textsuperscript{15-22} A mass-consistent three-dimensional wind field is interpolated from a small set of local tower wind measurements and used to predict the advection of a passive pollutant. Turbulent diffusion is modeled with a zero equation model, although many other important features such as rainout, wet and dry deposition, and surface terrain have been added.
2.1.2 Two-Dimensional Models

Two two-dimensional numerical plume models have been found in the literature. Henninger's model\textsuperscript{23} solves continuity, momentum, energy, and moisture with a less-sophisticated zero-equation turbulence closure, and with a more sophisticated treatment of moisture. For plumes in a wind, the model chooses the mesh alignment shown in Fig. 3.3.2.1b of Sec. 3.3.2, which is felt to be a less satisfactory choice than that of the present work. Taft's model\textsuperscript{24} is much closer to the model in this work, since it adopts the same mesh alignment (see Fig. 3.3.2.1c in Sec. 3.3.2). The principal differences are that Taft's model employs a one-equation turbulence model, uses a more complex moisture model, and does not make any attempt to describe ambient atmospheric turbulence.

A number of two-dimensional numerical buoyant thermal models have evolved in the literature of meteorology, usually in support of efforts to parameterize the growth of rain clouds. The models have not been applied to air pollution directly, but could be easily converted. Lilly's model\textsuperscript{25} seeks a self-preserving solution for the (dry) buoyant line thermal, and as such, would only be applicable for the early plume behavior when plume self-turbulence is dominating. Johnson's model\textsuperscript{26} is used to study fog clearing on runways.
with helicopter downwash; while the moisture equations are more complex than that in this work, the eddy viscosity is assumed to be constant. Ogura's model\textsuperscript{27} of rain cloud development also assumes a constant eddy viscosity, while Arnason's model\textsuperscript{28} ignores eddy transports altogether. Liu's model\textsuperscript{29} employs a stratification of atmospheric turbulence into two constant eddy viscosity layers. While the treatment of turbulence in these models is very simple, it should be emphasized that these models are focused on precipitation modeling, and they are likely to be helpful in the improvement of the moisture model in this work. A recent review of precipitation modeling is found in Cotton\textsuperscript{30}.

2.1.3 Experimental Studies

The field study that the model in this work is validated against is the Large Power Plant Effluent Study (LAPPES).\textsuperscript{5} Complete field data for stack plumes from three mine-mouth coal-fired plants are found in the four volumes of the study: wind, temperature, and humidity profiles, plant operating characteristics, and plume $SO_2$ concentration cross sections are of the most interest in this work. The Chalk Point Cooling Tower Project (CPCTP)\textsuperscript{31} is also of interest to this work since it provides cooling tower plume cross sections, but plant operating data\textsuperscript{32} was not available during this work.
The experimental laboratory studies that this work is validated against are the papers of Tsang\textsuperscript{33} and Richards.\textsuperscript{4} The experiments study the behavior of two-dimensional line thermals released in a water tank. The ambient receiving fluid in the tank is both laminar and unstratified, and the thermals are fully turbulent.

2.2 Numerical Planetary Boundary Layer Modeling

A three-dimensional numerical model of the planetary boundary layer has been reported by Deardorff\textsuperscript{34-36} that could easily be adapted to local air pollution studies, although the expense is likely to be prohibitive. The model solves the complete set of primitive equations (with an eighteen-equation model of turbulence) in a box that ranges 5 km on a side and 2 km deep. The numerical experiments to date have compared very favorably with several well-documented planetary boundary layer field studies.

To apply the model to a single source of pollutant, a single mesh cell could be initialized with sources of momentum, heat, moisture, pollutant, and turbulence. To accommodate this, a pollutant transport equation would have to be added, and an additional three-equation model of turbulent pollutant fluxes would need to be developed. Time-dependent or steady-state releases could be modeled in great detail in this way.
However, the model currently requires 15 seconds of CPU on a CDC-7600 to simulate 1 second of flow in the atmosphere. Also, the specification of boundary conditions on a three-dimensional mesh with accurate time-dependent micrometeorological data would require a very elaborate reporting network. Nonetheless, the model represents a more sophisticated and potentially more accurate approach than the model in this work.
3. HYDRODYNAMIC MODEL DEVELOPMENT

3.1 Introduction

In order to model buoyant plumes in the atmosphere, the equation set contained in the VARR-II computer code is reinterpreted and expanded. A reinterpretation of the hydrodynamic variables is necessary in order to satisfactorily account for the compressible nature of an atmosphere that is at rest. The equations are expanded in Sec. 3.2.1 to include the transport of a pollutant and radioactive decay heating by the pollutant, and in Sec. 3.2.2, where the transport of water vapor, cloud liquid water, and the energy released or absorbed during the phase changes of water substance are considered. Since so many fundamental changes are made here in reinterpreting the VARR-II equation set, this discussion of the model development undertakes a derivation of the equations; for completeness it reiterates the important assumptions contained in the VARR-II code which were developed outside of this work.

3.2 Hydrodynamic Model Equation Sets

3.2.1 Equations for Dry Atmospheres

The equations for a dry atmosphere are derived in this
section. When the potential temperature is simply reinterpreted as the virtual potential temperature, these equations are applicable to moist plumes in moist atmospheres if none of the moisture undergoes a change of phase, and if the turbulent diffusion coefficients of heat and moisture are equal. A further discussion of virtual potential temperature is found in Sec. 3.2.2.1.

3.2.1.1 Reference State Decomposition

As a starting point for the model development, consider the three-dimensional compressible fluid mechanics equations, where the six primitive variables $\bar{p}$, $\bar{\rho}$, $\bar{T}$, and $\bar{u}_i$ are physically measurable values of the fluctuating pressure, density, temperature, and velocity, respectively:

Continuity Eq:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j) = 0 \quad (3.1)$$

Momentum Eq:

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_i \bar{u}_j) = - \frac{\partial \bar{p}}{\partial x_i} - \bar{\rho} \bar{g}_i + \mu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} \quad (3.2)$$

Energy Eq:

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{T}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{u}_j \bar{T}) = \bar{u}_j \frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \frac{\partial \bar{T}}{\partial x_j} \right) + \frac{1}{c_p} \frac{\partial \bar{\rho}}{\partial t} \quad (3.3)$$
Equation of State:

\[ \tilde{p} = \tilde{\rho} R_d \tilde{T} \]  

(3.4)

These equations have property values \( \mu, c_p, \) and \( k, \) which may depend upon temperature in general. The energy equation has neglected the kinetic energy in the fluid motions, and the equation of state is that for an ideal dry gas.

The variations of temperature, pressure, and density in a static atmosphere are usually "subtracted out" of these equations in meteorological analyses by a reference state decomposition. That is, equations of motion for perturbations about an adiabatic atmosphere are sought by decomposing the primitive variables as

\[
\begin{align*}
\text{the value of a primitive variable} & = \{ \text{its value in an adiabatic atmosphere (function of height only)} \} + \{ \text{a departure from the state at rest} \} \\
\end{align*}
\]

(3.5)

or, in terms of the notation in this work

\[
\begin{align*}
\tilde{p} & \rightarrow P_0 + P \\
\tilde{\rho} & \rightarrow \rho_0 + \rho \\
\tilde{T} & \rightarrow T_0 + T \\
\tilde{u}_i & \rightarrow 0 + u_i
\end{align*}
\]

(3.6)  (3.7)  (3.8)  (3.9)

The state of the dry, adiabatic atmosphere is found by
making the substitutions Eq. 3.6-Eq. 3.9 into Eq. 3.1-Eq. 3.4, and setting the time derivatives and the perturbations $p$, $\rho$, $T$, and $u_i$ to zero. The continuity and energy equations become trivial under this substitution. The momentum equation becomes the hydrostatic equation:

$$\frac{dp_0}{dz} = -\rho_0 g$$  \hspace{1cm} (3.10)

The equation of state is simply

$$P_0 = \rho_0 R_o T_0$$  \hspace{1cm} (3.11)

The First Law of Thermodynamics for an adiabatic process is

$$dQ = 0 = c_p dT_0 - \frac{dp_0}{\rho_0}$$  \hspace{1cm} (3.12)

Dividing by a displacement $dz$ gives

$$\frac{dp_0}{dz} = \rho_0 c_p \frac{dT_0}{dz}$$  \hspace{1cm} (3.13)

and substitution of Eq. 3.13 into Eq. 3.10 gives $\Gamma_d$, the lapse rate of the dry adiabatic atmosphere:

$$\Gamma_d \Xi - \frac{dT_0}{dz} = \frac{g}{c_p} = 9.76^\circ C/km$$  \hspace{1cm} (3.14)

To this point the solution of the adiabatic atmosphere has been presented. Substituting the reference state decomposition, Eq. 3.6-Eq. 3.9 into the equations of motion,
Eq. 3.1-Eq. 3.4, and using the results of the adiabatic atmosphere, Eq. 3.10 and Eq. 3.14, gives the equations of motion for the perturbations:

**Continuity Equation**

\[
\frac{\partial u_j}{\partial x_j} = -\frac{u_j}{\rho_0} \frac{\partial \rho_0}{\partial x_j} + \frac{R_d}{c_p} \frac{k}{\rho_0} \frac{\partial^2 T}{\partial x_j^2} \approx 0 \tag{3.15}
\]

**Momentum Equation:**

\[
\rho_0 \frac{\partial u_i}{\partial t} + \rho_0 u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} - \rho g_i + \mu_0 \frac{\partial^2 u_i}{\partial x_j^2} \tag{3.16}
\]

**Energy Equation:**

\[
\rho_0 \frac{\partial T}{\partial t} + \rho_0 u_j \frac{\partial T}{\partial x_j} = \frac{R_d}{c_p} \frac{\partial^2 T}{\partial x_j^2} \tag{3.17}
\]

**Equation of State:**

\[
\frac{p}{p_0} = \frac{T}{T_0} + \frac{\rho}{\rho_0} + \frac{\rho T}{\rho_0 T_0} \tag{3.18}
\]

The fluid perturbations will generally be assumed to be incompressible in the Boussinesq sense. That is, changes in fluid density are assumed to be produced only by temperature changes, and not by pressure fluctuations. Neglecting the pressure fluctuations in the equation of state, and noting that generally \(\rho T \ll \rho_0 T_0\), the equation of state becomes

\[
\frac{\rho}{\rho_0} \approx -\frac{T}{T_0} \tag{3.19}
\]
which is the familiar Boussinesq equation of state. This equation allows the buoyancy term \((-\rho g_i/\rho_o)\) in the momentum equation (Eq. 3.16) to be similarly approximated. The continuity equation (Eq. 3.15) becomes that of an incompressible fluid, assuming that the fluid motions do not rapidly mix deep layers of the fluid, e.g., comparing length scales of velocity and density:

\[
\left( \frac{1}{|u_j|} \frac{\partial u_j}{\partial x_j} \right)^{-1} \ll \left( \frac{1}{\rho_o} \frac{\partial \rho_o}{\partial x_j} \right)^{-1} \tag{3.20}
\]

and that the heat conduction term in Eq. 3.1 is a small contribution to the divergence. Making these approximations, the equations for the perturbations may be written as

Continuity Eq.:

\[
\frac{\partial u_j}{\partial x_j} = 0 \tag{3.21}
\]

Momentum Eq.:

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_o} \frac{\partial p}{\partial x_i} - \frac{\rho}{\rho_o} g_i + \frac{u_o}{\rho_o} \frac{\partial^2 u_i}{\partial x_j^2} \tag{3.22}
\]

Energy Eq.:

\[
\frac{\partial T}{\partial t} + u_j \frac{\partial T}{\partial x_j} = \frac{p}{\rho_o} \frac{\partial \left( \frac{1}{\rho_o} \frac{\partial T}{\partial x_j} \right)}{\partial x_j^2} \tag{3.23}
\]
Define the potential temperature, $\theta$, as

$$\theta = T \left( \frac{1000\text{mb}}{p} \right) \frac{R}{c_p} \quad (3.24)$$

Differentiating with respect to height finds that the adiabatic atmosphere has a lapse rate of potential temperature of zero,

$$\frac{d\theta}{dz} = 0 \quad (3.25)$$

or that the potential temperature is a constant in an adiabatic atmosphere. Errors introduced by evaluating density with $\theta$ instead of $T$ are assumed to be small (this is investigated in Sec. 3.3.4). Neglecting the perturbation $p$ with respect to $p_0$ in Eq. 3.24, and approximating $\rho_0$ as $\rho(\theta_0)$ in Eq. 3.22, the use of $\theta$ instead of $T$ in the primitive equations (Eq. 3.21-Eq. 3.23) gives

Continuity Eq:

$$\frac{\partial u_j}{\partial x_j} = 0 \quad (3.26)$$

Momentum Eq:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_j}{\partial x_j} = - \frac{1}{\rho(\theta_0)} \frac{\partial p}{\partial x_i} - \frac{\rho(\theta) - \rho(\theta_0)}{\rho(\theta_0)} g_i + \nu \frac{\partial^2 u_i}{\partial x_j^2} \quad (3.27)$$

Energy Eq:

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = - \nu \frac{\partial}{\partial x_j} \frac{\partial^2 \theta}{\partial x_j^2} \quad (3.28)$$
The utility of the potential temperature formulation is that strong variations of pressure and density with height in the hydrostatic approximation of Eq. 3.10 are no longer present in the primitive equations. Initialization errors to the hydrostatic state, if included in the primitive equations, lead to strong transient fluid motions. The transients are neatly avoided by this formulation.

To this point the fully three-dimensional fluid mechanics equations have been decomposed into an adiabatic reference state, and a flow field of perturbations about this state. A number of approximations have simplified the equations for the perturbations to those of a Boussinesq incompressible flow. The equations need to be ensemble-averaged and a turbulence closure formulated, and then the set must be finite-differenced for computer solution.

3.2.1.2 Reynolds Decomposition and Closure

To model the effects of turbulence on the mean flow, each primitive variable in the equation set is decomposed into its time-averaged and fluctuating parts as

\[
\begin{align*}
\text{the value of the perturbation of a primitive variable} & = \text{its ensemble-averaged value} + \text{any fluctuations about its ensemble-average value} \\
\end{align*}
\]

\( (3.29) \)
which is represented here by the decompositions

\[ p = p' + p'' \]  \hspace{1cm} (3.30)
\[ \theta = \theta' + \theta'' \]  \hspace{1cm} (3.31)
\[ \rho = \rho' + \rho'' \]  \hspace{1cm} (3.32)
\[ u_i = u_i' + u_i'' \]  \hspace{1cm} (3.33)

Under this transformation, by selectively ensemble-averaging and subtracting the equations, and by making use of the continuity equation, the primitive equations become

**Continuity Equations**

\[ \frac{\partial \bar{u}_j}{\partial x_j} = 0 \]  \hspace{1cm} (3.34)
\[ \frac{\partial u_j'}{\partial x_j} = 0 \]  \hspace{1cm} (3.35)

**Momentum Equations:**

\[ \frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho(\theta_0)} \frac{\partial \bar{p}}{\partial x_i} + \frac{\rho(\bar{\theta}) - \rho(\theta_0)}{\rho(\theta_0)} g_i \]
\[ + v \frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial}{\partial x_j} (\bar{u}_i u_j') \]  \hspace{1cm} (3.36)

\[ \frac{\partial u_i'}{\partial t} + \bar{u}_j \frac{\partial u_i'}{\partial x_j} + u_j \frac{\partial \bar{u}_i}{\partial x_j} + u_j' \frac{\partial u_i'}{\partial x_j} - \frac{\partial}{\partial x_j} (u_i' u_j') = \]
\[ -\frac{1}{\rho(\theta_0)} \frac{\partial p'}{\partial x_i} + \frac{\rho(\bar{\theta}') - \rho(\theta_0)}{\rho(\theta_0)} g_i + \frac{\partial^2 u_i'}{\partial x_j^2} \]  \hspace{1cm} (3.37)
Energy Equations:

\[
\begin{align*}
\frac{\partial \overline{\theta}}{\partial t} + \overline{u}_j \frac{\partial \overline{\theta}}{\partial x_j} &= \nu Pr^{-1} \frac{\partial^2 \overline{\theta}}{\partial x_j^2} - \frac{\partial}{\partial x_j} \left( \overline{u}_j \overline{\theta}' \right) \tag{3.38} \\
\frac{\partial \theta'}{\partial t} + \overline{u}_j \frac{\partial \theta'}{\partial x_j} + u_j^e \frac{\partial \theta}{\partial x_j} + u_j^e \frac{\partial \theta'}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \overline{u}_j \theta' \right) &= \nu Pr^{-1} \frac{\partial^2 \theta'}{\partial x_j^2} \tag{3.39}
\end{align*}
\]

The set of ensemble-averaged equations (i.e., Eq. 3.34, Eq. 3.36, and Eq. 3.38) suffer from the well-known closure problem due to the generation of the \( \overline{u}_j u'_i \) and \( \overline{u}_j \theta' \) terms by the non-linear advection terms in Eq. 3.27 and Eq. 3.28. Equations 3.37 and 3.39 may be manipulated to produce transport equations for these two new variables:

\[
\frac{D}{Dt} \left( \overline{u}_i u'_j \right) = - \overline{u}_i u'_j \frac{\partial \overline{u}_i}{\partial x_i} - \overline{u}_i u'_j \frac{\partial \overline{u}_i}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \overline{u}_i u'_j u'_i \right) + \frac{1}{\rho_o} \frac{\partial}{\partial x_i} \left( \overline{p} u'_i \right) - \frac{1}{\rho_o} \frac{\partial}{\partial x_i} \left( \overline{p} u'_i \right) + \frac{1}{\rho_o} \overline{p'} \left( \frac{\partial \overline{u}_i}{\partial x_i} + \frac{\partial \overline{u}_i}{\partial x_i} \right)
\]
\[ + \frac{1}{\theta_0} \left( g_i \frac{\partial \theta^r}{\partial x_i} + g_j \frac{\partial \theta^r}{\partial x_j} \right) \]

buoyant production terms

molecular diffusion terms

\[ + \nu \frac{\partial^2 (u_i u_j^r)}{\partial x_k^2} \]

dissipation term

(3.40)

\[ \frac{D}{Dt} \left( \frac{\partial u_i}{\partial x_j} \right) = -\frac{\partial u_i}{\partial x_j} \frac{\partial \theta^r}{\partial x_j} - \frac{\partial u_i}{\partial x_j} \frac{\partial \theta^r}{\partial x_k} \]

production terms

\[ - \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} \theta^r \right) \]

turbulent transport term

\[ - \frac{1}{\rho_0} \frac{\partial}{\partial x_i} \left( \frac{\partial p'}{\partial x_i} \right) \]

pressure diffusion term

\[ + \frac{1}{\rho_0} \frac{\partial}{\partial x_i} \left( \frac{\partial \theta^r}{\partial x_i} \right) \]

tendency toward isotropy term

\[ + \frac{1}{\theta_0} g_i \frac{\partial \theta^r}{\partial x_i} \]

buoyant production term

\[ + \nu \frac{\partial^2 (u_i \theta^r)}{\partial x_j^2} \]

molecular diffusion term
A discussion of the individual terms noted in Eq. 3.40 and Eq. 3.41 can be found elsewhere. These equations were closed by Stuhmiller and the results are listed here for completeness. In Eq. 3.40, the tendency toward isotropy term is neglected, because the turbulence is assumed to be homogeneous, and the molecular diffusion term is neglected because the flow is expected to be highly turbulent. The buoyant production term is also neglected, mainly in order to see how well the turbulence model can do without it, since it was neglected in Stuhmiller's turbulence model. It is found that the incorporation of this term would probably aid the model in reproducing the buoyant line-thermal results (see Sec. 5.2.2).

By further making the assumption that the average flow is two-dimensional in the y-z axes of Fig. 3.1, the following closure is made for the trace of Eq. 3.40, which is the turbulence kinetic energy, $q$, $q \equiv u'_i u'_i$,

$$
\frac{Dq}{Dt} = 2\sigma \left( \frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial z} \right)^2 - 4\alpha q^2 \sigma^{-1}
$$

$$
+ \Gamma \left( \frac{\partial q}{\partial y} \frac{\partial q}{\partial y} + \frac{\partial q}{\partial z} \frac{\partial q}{\partial z} \right)
$$

(3.42)
The flow field of Eqs. 3.42-3.47 is time-dependent and two-dimensional in the \( y-z \) axes. The relationship of the time-dependence to the (downwind) \( x \)-axis is discussed in Sec. 3.3.3.
The off-diagonal terms of the Reynolds stress tensor are related to a scalar eddy viscosity, $\sigma$, where $\overline{u_i' u_j'} = \frac{\sigma}{\partial x_j} \frac{\partial \overline{u_i'}}{\partial x_i}$, and $\sigma$ has the following transport equation:

$$\frac{D\sigma}{Dt} = \frac{\sigma^2}{q} \left( \left( \frac{\partial \overline{v}}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial \overline{v}}{\partial z} + \frac{\partial \overline{w}}{\partial z} \right)^2 \right) - aq$$

$$+ \frac{\gamma}{q} \left( \frac{\partial \overline{v}}{\partial y} \frac{\partial \overline{w}}{\partial z} + \frac{\partial \overline{w}}{\partial z} \frac{\partial \overline{v}}{\partial z} \right) - \Gamma_1 \left( \frac{\sigma^2}{q} \left( \frac{\partial \overline{v}}{\partial y} \frac{\partial \overline{v}}{\partial z} \right) - \frac{\partial \overline{w}}{\partial z} \frac{\partial \overline{w}}{\partial z} \right)$$

(3.43)

Finally, the turbulent fluxes of heat in Eq. 3.41 are related to the turbulent momentum fluxes through a reciprocal turbulent Prandtl number, $\gamma_T$, which is specified along with the three other turbulence constants $\alpha$, $\Gamma$, and $\Gamma_1$. With this turbulence closure, the continuity, momentum, and energy equations become, in a two-dimensional flow

$$\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(3.44)

$$\frac{\partial v}{\partial t} + \frac{1}{\rho(\theta_0)} \frac{\partial}{\partial y} \left( \frac{\partial \overline{v}}{\partial y} \left( \frac{\partial \overline{v}}{\partial y} + \frac{\partial \overline{w}}{\partial z} \right) \right) = -$$

$$- \frac{1}{\rho(\theta_0)} \left( \frac{\partial \overline{v}}{\partial y} \frac{\partial \overline{v}}{\partial z} \right) + \frac{\partial}{\partial z} \left( \sigma \frac{\partial \overline{w}}{\partial z} \right)$$

(3.45)

$$\frac{\partial w}{\partial t} + \frac{1}{\rho(\theta_0)} \left( \frac{\partial \overline{w}}{\partial y} \frac{\partial \overline{w}}{\partial z} \right) + \frac{\partial}{\partial z} \left( \sigma \frac{\partial \overline{w}}{\partial z} \right) =$$

$$- \frac{(1 - \gamma)}{\rho(\theta_0)} \frac{\partial \overline{v}}{\partial z} \overline{w}$$

(3.46)
With an internal energy variable, I, defined as $I = c_p \bar{\rho}$, equations 3.42-3.47 are solved by the VARR-II code. Additional pollutant and moisture transport equations are discussed in the next two sections, and possible modifications to these equations are discussed in section 6.2.

### 3.2.1.2 Pollutant Species Transport Equation

A transport equation for a pollutant species density, $\chi$ is added to the set of Eqs. 3.42-3.47. The pollutant is assumed to be a neutrally buoyant, passive species, although it may be contained in a buoyant stream of effluent. The assumption that the species is neutrally buoyant could be relaxed, but the model is felt to be useful in modeling most dilute pollutants in its present form. The turbulent diffusion of the pollutant is related to the eddy viscosity of momentum by a reciprocal turbulent Schmidt number, $S_\chi$. The transport equation may be written down as:

$$ \frac{\partial \chi}{\partial t} + \frac{\partial}{\partial y} (\bar{\omega} \chi) + \frac{\partial}{\partial z} (\bar{v} \chi) = \frac{\partial}{\partial y} (\nu T \frac{\partial \chi}{\partial y}) + \frac{\partial}{\partial z} (\nu T \frac{\partial \chi}{\partial z}) $$

(3.47)
which is represented here as

\[
\frac{\partial X}{\partial t} + \nabla \cdot (D \nabla X) + \frac{\partial x}{\partial z} = \frac{\partial}{\partial y} \left( \chi \frac{\partial X}{\partial y} \right) + \frac{\partial}{\partial z} \left( \chi \frac{\partial X}{\partial z} \right) - \sum_{i=1}^{N} \lambda^{(i)} \chi
\]  (3.49)

in the notation of Fig. 3.1.

The destruction of \( \chi \) is assumed to be by radioactive decay into any of \( N \) decay channels, so that the rate of destruction of \( \chi \) is the product of \( \chi \) and the sum of its radioactive decay constants \( \lambda^{(i)} \chi \), in Eq. 3.49. This formulation makes no account of sources of the pollutant species through decay of radioactive precursors. It also ignores chemical reactions which could alter the pollutant concentration. However, the extension of the model to include these effects is straightforward.

3.2.1.4 Radioactive Decay Heating

The thermal energy released by radioactive decay of the pollutant is added to the specific internal energy of the fluid. Pollutants may decay by any one of \( N \) different decay channels with decay constant \( \lambda^{(i)} \chi \) and energy \( E^{(i)} \chi \). A fraction \( F^{(i)} \chi \) of the energy is deposited within the plume, yielding an energy release rate of...
\[
\left( c_p \frac{\partial \theta}{\partial t} \right)_{\text{radioactive}} = \frac{4.151 \times 10^{10} \text{ BTU-atoms}}{\text{MeV-lb}_m^-\text{mole}} \sum_{i=1}^{N} F_x^{(i)} E_x^{(i)} \lambda_x^{(i)}
\]

(3.50)

where \( W_{\text{mol}X} \) is the molecular weight of \( X \) in \( \text{lb}_m^-\text{mole} \).

Daughter radiations have been ignored in this formulation, but could be included with their own transport equation. Similarly, alterations of the energy balance caused by chemical reactions has not been treated in this work, but would be easy to address in extensions of this work.

3.2.2 Moist Equations

The inclusion of moisture is considered in this section with the purpose of pointing out the assumptions that allow the equations to be formulated with the concept of virtual potential temperature, in addition to two other moisture variables. The assumptions that are made in this section are important—the moisture model is not meant to be perfectly general; it is expected to do poorly when these assumptions are not valid.
3.2.2.1 Reference State Decomposition

Atmospheric moisture is assumed to be in either the liquid or vapor phases. The amount of vapor is described by the vapor density moisture variable, $\tilde{\rho}_{\text{vap}}$, and the amount of cloud liquid water is described by the liquid density moisture variable, $\tilde{\rho}_{\text{liq}}$. Transport equations for these two variables are written that take note of the turbulent transports of vapor and liquid, and the processes of evaporation and condensation that cause the interchange of vapor and liquid. First, however, the effect of moisture on the buoyancy of a parcel of air is developed and applied to the description of a hydrostatic reference state.

The density of a parcel of moist air is the sum of the dry air, vapor, and liquid densities:

$$\tilde{\rho} = \tilde{\rho}_{\text{dry}} + \tilde{\rho}_{\text{vap}} + \tilde{\rho}_{\text{liq}}$$  \hspace{1cm} (3.51)

In this work the contribution to the density of the typically small amount of cloud liquid water is ignored, (there is usually no liquid water present in the simulations, and when it is present, it is typically less than 1% of the mass of the fluid), so that the concept of virtual potential temperature can be explored. Dropping the $\tilde{\rho}_{\text{liq}}$ term and applying the perfect gas law to $\tilde{\rho}_{\text{dry}}$ and $\tilde{\rho}_{\text{vap}}$ yields:

$$\tilde{\rho} = \frac{\tilde{\rho}_{\text{dry}}}{R_d T} + \frac{\tilde{\rho}_{\text{vap}}}{R_v T} = \frac{(\tilde{\rho}_{\text{dry}} + \tilde{\rho}_{\text{vap}})}{R_d T} = \frac{\tilde{\rho}_{\text{dry}}}{R_d T} + \frac{\tilde{\rho}_{\text{vap}}}{R_v T} = \frac{\tilde{\rho}_{\text{dry}}}{R_d T} + \frac{\tilde{\rho}_{\text{vap}}}{R_v T}$$  \hspace{1cm} (3.52)
where \( \tilde{p} \) is the total pressure, \( m_{\text{vap}} \) and \( m_{\text{dry}} \) are molecular weights and the virtual temperature, \( \tilde{T}_v \), is

\[
\tilde{T}_v = \frac{T}{1 + \frac{\tilde{\rho}_{\text{vap}}/\tilde{\rho}_{\text{dry}}}{m_{\text{vap}}/m_{\text{vap}}}}
\]  

(3.53)

It is very important to note in Eq. 3.52 that the virtual temperature is a fictitious temperature that is used in the dry gas equation of state to give the density of moist air. Generally the virtual temperature is no more than a few degrees higher than the thermodynamic temperature for typical atmospheric conditions.

Following the development in Sec. 3.2.1.1, the variations of virtual temperature, pressure, and density of a static atmosphere are "subtracted out" by making a reference state decomposition:

\[
\begin{align*}
\text{the value of a primitive variable} &= \text{its value in a uniformly moist adiabatic atmosphere (function of height only)} + \text{a departure from the state at rest} \\
\end{align*}
\]  

(3.54)

Or, in the notation of this work:

\[
\begin{align*}
\tilde{p} &+ p_o + p \\
\tilde{\rho} &+ \rho_o + \rho \\
\tilde{T}_v &+ T_{vo} + T_v \\
\tilde{u}_i &+ 0 + u_i
\end{align*}
\]  

(3.55)  

(3.56)  

(3.57)  

(3.58)
the only difference here to the reference state decomposition of Eqs. 3.6-3.9 is in the use of the (fictitious) virtual temperature in order to allow the use of an equation of state that is analogous to Eq. 3.4:

\[ \tilde{\rho} = \frac{\tilde{p}}{R_d \tilde{T}_v} \] (3.59)

Substituting Eqs. 3.55-3.58 into the primitive equation set (Eqs. 3.1-3.3 and Eq. 3.59), and setting the time derivatives and perturbations to zero yields the state of the moist adiabatic atmosphere. The continuity and energy equations are trivial (as before), and the momentum equation becomes the moist hydrostatic equation:

\[ \frac{d\rho_o}{dz} = -\rho_o g \] (3.60)

The equation of state is simply

\[ P_o = \rho_o R_d T_{vo} \] (3.61)

The first Law of Thermodynamics for an unsaturated adiabatic process in this atmosphere is

\[ dQ = 0 = c_p^{\text{moist}} dT_{vo} - dP_o/\rho_o \] (3.62)

Approximating the heat capacity for a moist gas, \( c_p^{\text{moist}} \), as that of a dry gas, \( c_p \), dividing by \( dz \) and substituting Eq. 3.62 into 3.60 yields an approximate lapse rate for a moist, unsaturated atmosphere which is the same as that for a dry adiabatic atmosphere:
To this point the resting state of a moist adiabatic atmosphere has been presented. The neglect of the effect of the liquid water on the total density has allowed the treatment of moisture to duplicate the dry atmosphere equations after the transformation of temperature to virtual temperature. The equations for the perturbations are identical to those of the dry atmosphere developed in Sec. 3.2.1.1, except that temperature is replaced by virtual temperature, and a latent heat release term is included:

**Continuity Eq.**
\[
\frac{\partial u_i}{\partial x_j} = 0 \tag{3.64}
\]

**Momentum Eq.**
\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \frac{T_v}{T_{vo}} g_i + \frac{\mu_0}{\rho_0} \frac{\partial^2 u_i}{\partial x_j^2} \tag{3.65}
\]

**Energy Eq.**
\[
\frac{\partial T_v}{\partial t} + u_j \frac{\partial T_v}{\partial x_j} = \nu Pr^{-1} \frac{\partial^2 T_v}{\partial x_j^2} - \frac{L}{\rho c_p} \left( \frac{\partial \rho_{vap}}{\partial t} \right)_{\text{phase}} \tag{3.66}
\]

The latent heat release term is considered in Sec. 3.2.2.4.

Define the virtual potential temperature, \( \theta_v \), as
Again assume that \( c_{\text{moist}} \) is essentially equal to \( c_p \). Differentiating with respect to height finds that the moist unsaturated adiabatic atmosphere has a lapse of virtual potential temperature that vanishes:

\[
\frac{d\theta_{vo}}{dz} = 0 \quad (3.68)
\]

The result here is that the virtual potential temperature is a constant in the reference state.

Neglecting the perturbation pressure, \( p \), with respect to \( p_0 \) in Eq. 3.56, the use of \( \theta_v \) instead of \( T_v \) in the primitive equations (Eq. 3.64-Eq. 366) gives

**Continuity Eq:**

\[
\frac{\partial u_i}{\partial x_j} = 0 \quad (3.69)
\]

**Momentum Eq:**

\[
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = \frac{-1}{\rho(\theta_{vo})} \frac{\partial p}{\partial x_i} - \frac{\rho(\theta_v) - \rho(\theta_{vo})}{\rho(\theta_{vo})} g_i + \nu \frac{\partial^2 u_i}{\partial x_j^2} \quad (3.70)
\]

**Energy Eq:**

\[
\frac{\partial \theta_v}{\partial t} + u_j \frac{\partial \theta_v}{\partial x_j} = \nu P_r \frac{\partial^2 \theta_v}{\partial x_j^2} - \frac{\theta_v}{\rho_c} \left( \frac{D p_{\text{vap}}}{Dt} \right) \text{phase} \quad (3.71)
\]
The result here is the same as in Sec. 3.2.1.1: the strong variation of pressure with height is no longer present in the primitive equations. This formulation is common (although in slightly different forms) among papers in meteorology.

Transport equations may be written down for the water vapor and liquid water densities according to the conservation scheme:

\[
\begin{align*}
\text{Eulerian time rate of change of vapor or liquid} &= \text{Diffusion of vapor or liquid} + \text{Gain or loss of vapor or liquid due to phase changes} \\
&= \frac{\partial \rho_{\text{vap}}}{\partial t} + u_j \frac{\partial \rho_{\text{vap}}}{\partial x_j} = \nu \text{Sc}_{\text{vap}} \frac{\partial^2 \rho_{\text{vap}}}{\partial x_j^2} + \left( \frac{D \rho_{\text{vap}}}{Dt} \right)_{\text{phase}} \\
&= \frac{\partial \rho_{\text{liq}}}{\partial t} + u_j \frac{\partial \rho_{\text{liq}}}{\partial x_j} = \nu \text{Sc}_{\text{liq}} \frac{\partial^2 \rho_{\text{liq}}}{\partial x_j^2} - \left( \frac{D \rho_{\text{vap}}}{Dt} \right)_{\text{phase}}
\end{align*}
\]

where the gain or loss of vapor due to phase changes, \(\left( \frac{D \rho_{\text{vap}}}{Dt} \right)_{\text{phase}}\), identically shows up as a loss or gain of liquid, and Schmidt numbers that describe the molecular diffusion of vapor and liquid are introduced, respectively. The terminal fall velocities of the liquid water droplets are ignored. The \(\left( \frac{D \rho_{\text{vap}}}{Dt} \right)_{\text{phase}}\) term is discussed in Sec. 3.2.2.3.
Note that any constant background (ambient atmospheric) value of \( \rho_{\text{vap}} \) and \( \rho_{\text{liq}} \) trivially satisfied these equations, so that no new information would be brought into the specification of the reference state by decomposing the variables in these transport equations. That is, \( \rho_{\text{vap}} \) and \( \rho_{\text{liq}} \) do not have a reference state "subtracted away" from them, unlike the other primitive variables \( \bar{p}, \bar{\theta}_v, \) and \( \bar{\rho}. \)

### 3.2.2.2 Reynolds Decomposition and Closure

A Reynolds decomposition of the primitive equations is made as in Sec. 3.2.1.2. Each primitive variable in the equation set is decomposed into its ensemble-averaged and fluctuating parts:

\[
\begin{align*}
\rho & = \bar{\rho} + \rho' \\
\theta & = \bar{\theta} + \theta' \\
\rho_{\text{vap}} & = \bar{\rho}_{\text{vap}} + \rho'_{\text{vap}} \\
\rho_{\text{liq}} & = \bar{\rho}_{\text{liq}} + \rho'_{\text{liq}}
\end{align*}
\]

(3.75)  
(3.76)  
(3.77)  
(3.78)  
(3.79)  
(3.80)

By selectively ensemble-averaging and subtracting the equations, and by making use of the continuity equation, the primitive equations yield the following relationships:

**Continuity Eq:**

\[
\frac{\partial \bar{u}_j}{\partial x_j} = 0
\]

(3.81)
Momentum Eq:
\[
\begin{align*}
\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} &= -\frac{1}{\rho(\theta_{vo})} \frac{\partial P}{\partial x_i} - \frac{\rho(\theta_v) - \rho(\theta_{vo})}{\rho(\theta_{vo})} g_i + \frac{\partial^2 u_i}{\partial x_j^2} \\
&- \frac{\partial}{\partial x_j} (u_i u_j)
\end{align*}
\]  
(3.82)

Energy Eq:
\[
\begin{align*}
\frac{\partial \theta_v}{\partial t} + u_j \frac{\partial \theta_v}{\partial x_j} &= \nu Pr \frac{\partial^2 \theta_v}{\partial x_j^2} - \frac{\partial}{\partial x_j} (u_j \theta_v') - \frac{L}{\rho(\theta_v) c_p} \left( \frac{D\rho_{vap}}{D\tau} \right)_{\text{phase}} \\
& \quad \text{(3.83)}
\end{align*}
\]

and the transport equations for moisture, Eq. 3.73 and Eq. 3.74 yield

Vapor Eq:
\[
\begin{align*}
\frac{\partial \bar{\rho}_{vap}}{\partial t} + u_j \frac{\partial \bar{\rho}_{vap}}{\partial x_j} &= \nu Sc \frac{\partial^2 \bar{\rho}_{vap}}{\partial x_j^2} - \frac{\partial}{\partial x_j} (\bar{\rho}_{vap} u_j') + \left( \frac{D\bar{\rho}_{vap}}{D\tau} \right)_{\text{phase}} \\
& \quad \text{(3.84)}
\end{align*}
\]

Liquid Eq:
\[
\begin{align*}
\frac{\partial \bar{\rho}_{liq}}{\partial t} + u_j \frac{\partial \bar{\rho}_{liq}}{\partial x_j} &= \nu Sc \frac{\partial^2 \bar{\rho}_{liq}}{\partial x_j^2} - \frac{\partial}{\partial x_j} (\bar{\rho}_{liq} u_j') - \left( \frac{D\bar{\rho}_{vap}}{D\tau} \right)_{\text{phase}} \\
& \quad \text{(3.85)}
\end{align*}
\]

Rather than providing the full equations for the correlated fluctuations \(u_i' u_j', u_j' \theta_v', u_j' \bar{\rho}_{vap}', \text{ and } u_j' \bar{\rho}_{liq}'\), the turbulence closure is simply extended from that developed in Sec. 3.2.1.2. The closed set of equations in two-dimensions is, in the
notation of Fig. 3.1

Continuity Eq:
\[ \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \]  
(3.86)

Momentum Eqs:
\[ \frac{Dv}{Dt} = \frac{-1}{\rho(\theta_v)} \frac{\partial p}{\partial y} + \frac{\partial}{\partial y} (\sigma \frac{\partial v}{\partial y}) + \frac{\partial}{\partial z} (\sigma \frac{\partial v}{\partial z}) \]
(3.87)

\[ \frac{Dw}{Dt} = \frac{-1}{\rho(\theta_v)} \frac{\partial p}{\partial z} - \frac{\rho(\theta_v) - \rho(\theta_{vo})}{\rho(\theta_{vo})} g_z + \frac{\partial}{\partial y} (\sigma \frac{\partial w}{\partial y}) + \frac{\partial}{\partial z} (\sigma \frac{\partial w}{\partial z}) \]

Energy Eq:
\[ \frac{D}{Dt} (c_p \theta_v) = \frac{\partial}{\partial y} \left( \gamma_T \frac{\partial c_p \theta_v}{\partial y} \right) + \frac{\partial}{\partial z} \left( \gamma_T \frac{\partial c_p \theta_v}{\partial z} \right) - \frac{L}{\rho(\theta_v)} \frac{D\rho_{vap}}{D_t} \text{\ phase} \]
(3.88)

Vapor Eq:
\[ \frac{D}{Dt} \rho_{vap} = \frac{\partial}{\partial y} \left( \gamma_v \frac{\partial \rho_{vap}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \gamma_v \frac{\partial \rho_{vap}}{\partial z} \right) + \left( \frac{D\rho_{vap}}{D_t} \right) \text{\ phase} \]
(3.89)

Liquid Eq:
\[ \frac{D}{Dt} \rho_{liq} = \frac{\partial}{\partial y} \left( \gamma_{liq} \frac{\partial \rho_{liq}}{\partial y} \right) + \frac{\partial}{\partial z} \left( \gamma_{liq} \frac{\partial \rho_{liq}}{\partial z} \right) - \left( \frac{D\rho_{vap}}{D_t} \right) \text{\ phase} \]
(3.90)

Eddy Viscosity Eq:
\[ \frac{D\sigma}{Dt} = \frac{\sigma^2}{\alpha} \left( \frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial w}{\partial y} \right)^2 + \frac{\partial w}{\partial z} - \left( \frac{\partial w}{\partial z} \right)^2 \]
\[ \alpha q + \]
\[ + \frac{\partial}{\partial q} \left( \frac{\partial q}{\partial x} \sigma \frac{\partial q}{\partial y} \right) \left( \frac{\partial q}{\partial z} \sigma \frac{\partial q}{\partial z} \right) \] 

\[ - \Gamma \left( \frac{\partial q}{\partial x} \right) \frac{\partial q}{\partial y} \] 

\[ + \frac{\partial}{\partial q} \left( \frac{\partial q}{\partial x} \sigma \frac{\partial q}{\partial y} + \frac{\partial q}{\partial z} \sigma \frac{\partial q}{\partial z} \right) \] 

(3.91)

**Turbulence Kinetic Energy Eq:**

\[ \frac{Dq}{Dt} = 2\sigma \left( \frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} + \frac{\partial w}{\partial z} \right)^2 - 4\sigma q - 1 \]

\[ + \Gamma \left( \frac{\partial q}{\partial x} \sigma \frac{\partial q}{\partial y} + \frac{\partial q}{\partial z} \sigma \frac{\partial q}{\partial z} \right) \] 

(3.92)

**Pollutant Eq:**

\[ \frac{Dx}{Dt} = \frac{3}{\partial y} \left( \gamma \frac{\partial x}{\partial y} \right) + \frac{\partial}{\partial z} \left( \gamma \frac{\partial x}{\partial z} \right) - \sum_{i=1}^{N} \lambda_{i}^{(x)} \] 

(3.93)

where reciprocal turbulent Prandtl and Schmidt numbers have been introduced, and are assumed to be constants.

### 3.2.2.3 Equilibrium Cloud Microphysics Model

The cloud microphysics model simply assumes that water vapor and liquid are always in equilibrium. Further, the surface tension of the liquid droplets is ignored. That is, phase equilibrium over a flat surface of water is assumed to exist. A phase diagram that illustrates this equilibrium is
sketched in Fig. 3.2.2.3.1. The liquid-vapor equilibrium curve above 273°K is the locus of points that the saturation vapor pressure, $e_{\text{sat}}(T)$, may take. The vapor density, $\rho_{\text{vap}}$, in the presence of liquid water would be $e_{\text{sat}}(T)/R_{\text{vap}}T$. If there is no liquid available to evaporate, then the vapor density may be less than this saturation value. Below 273°K the subcooled liquid-vapor equilibrium (dashed line) is obeyed. No ice formation is allowed. The entire liquid-vapor equilibrium curve is given by Magnus' formula:\[39
\]

$$\log_{10}e_{\text{sat}} = -\frac{2937.4}{T} - 4.9283 \log_{10}T + 23.5518$$ \hspace{1cm} (3.94)

The $\left( \frac{D\rho_{\text{vap}}}{Dt} \right)$ phase term of Eq. 3.89 and Eq. 3.90 is simply adjusted to make the liquid and vapor coexist. The logic of the moisture model is illustrated in Fig. 3.2.2.3.2. Liquid and vapor are advected and diffused in an initial calculation for each computer cell. This generally results in a non-equilibrium moisture state in the cell, so the cell is allowed to evaporate or condense water in order to restore the equilibrium. The amount of evaporation or condensation in each cell is noted in order to provide the latent heat release term in the energy equation.

3.2.2.4 *Latent Heat Source Term*

The latent heat source term is calculated in each cell
Fig. 3.2.2.3.1 Phase Diagram for Water Substance
Fig. 3.2.2.3.2 Logic Diagram for the Equilibrium Moisture Calculation in a Single Cell during a Single Timestep

- transport vapor and liquid using updated velocities
- calculate $e_{\text{sat}}$ from $T$
- calculate $\rho_{\text{sat}}$ from $e_{\text{sat}}, T$

- $\rho_{\text{vap}} < \rho_{\text{sat}}$
  - $\rho_{\text{vap}} = \rho_{\text{sat}}$
  - $\rho_{\text{vap}} > \rho_{\text{sat}}$

- $\rho_{\text{hy}} > \rho_{\text{sat}} - \rho_{\text{vap}}$
  - $0 < \rho_{\text{hy}} < \rho_{\text{sat}} - \rho_{\text{vap}}$
  - $\rho_{\text{hy}} = 0$

- liquid evaporates
  - $\frac{\rho_{\text{vap}}}{\rho_{\text{sat}} - \rho_{\text{vap}}}$
  - $\frac{\rho_{\text{sat}} - \rho_{\text{vap}}}{\rho_{\text{sat}}}$

- liquid evaporates completely
  - $\frac{\rho_{\text{sat}} - \rho_{\text{vap}}}{\rho_{\text{sat}}}$

- vapor condenses
  - $\frac{\rho_{\text{sat}} - \rho_{\text{vap}}}{\rho_{\text{sat}}}$

- proceed to energy equation
at every step depending on whether evaporation or condensation takes place. The latent heat release term is calculated as

\[
\text{Latent Heat Release} \left[ \frac{\text{BTU}}{\text{lb}_m \text{ sec}} \right] = - \frac{L}{\rho(\theta_v)} \left( \frac{D\rho_{vap}}{Dt} \right)_{\text{phase}}
\]

(3.95)

where the latent heat of vaporization, \( L \), is assumed to be a constant, 1075 BTU/lb\(_m\). The \( \left( \frac{D\rho_{vap}}{Dt} \right)_{\text{phase}} \) is found in the logic diagram of Fig. 3.2.2.3.2.

### 3.3 Model Solution Methodology

#### 3.3.1 The VARR-II Fluid Mechanics Algorithm

The VARR-II computer code\(^{40}\) is the starting point for the model development methodology in this work. In its original form, the VARR-II code solves the two-dimensional time-dependent turbulent fluid mechanics equations of continuity, momentum, and energy for a Boussinesq fluid. (The Boussinesq approximation to the momentum equation is considered in Sec. 3.2.1.1.) Two closure variables, the eddy viscosity, \( \sigma \), and the turbulence kinetic energy, \( q \), are also calculated from their own transport equations. The original VARR-II computer code is quite flexible in the choice of boundary conditions, allowing no-slip, free-slip, continutive inflow/outflow, or prescribed inflow/outflow boundaries.
The VARR-II fluid mechanics algorithm is the Simplified Marker and Cell (SMAC) method. The computer mesh for this method is Eulerian in either Cartesian or cylindrical geometry, and the primitive variables are solved directly, with no transformation to vorticity-stream function variables. The algorithm divides naturally into two sections during each time step: In the first section the velocity field is updated using the previous velocity and pressure fields with mixed central and donor-cell differencing of the equations. These velocities generally do not satisfy the continuity equation, so in a second section a pressure iteration adjusts these velocities until they satisfy continuity. Once the divergence-free updated velocity field is known, the energy and turbulence transport equations are updated, completing the calculational cycle of the time step.

The basic SMAC fluid mechanics algorithm has not been modified in this work. Pollutant and moisture transport equations have been added to the equation set, and they are updated in the same manner as the energy and turbulence variables, using the divergence-free updated velocity field. The stability of the method for problems of an atmospheric scale is considered in Sec. 5.2.1.

3.3.2 Orientation of the Computer Mesh

The optimal orientation of the two-dimensional computer
solution mesh is discussed here. Consider the representative three-dimensional plume in Fig. 3.3.2.1a. The plume has bent over in the imposed (one-dimensional) wind field, and the plume boundaries monotonically expand as the plume proceeds downwind. The most natural possibilities of orienting a two-dimensional solution mesh on this flow are: (1) to align the mesh parallel to the wind and through the center of the plume, as in Fig. 3.3.2.1b, or (2) to align the mesh perpendicular to the flow, as in Fig. 3.3.2.1c.

The advantages of the "crosswind" alignment of Fig. 3.3.2.1c over the "downwind" alignment of Fig. 3.3.2.1b are immediately apparent. In the crosswind alignment a three-dimensional simulation results since in the downwind Lagrangian translation of the computational mesh the time variable becomes a surrogate for the downwind position \( x \), where

\[
x = \int_0^t u(z(t)) \, dt.
\]

The downwind alignment is appropriate only for cases of line-source plumes—in which internal recirculation and entrainment will be of secondary importance to buoyant plume rise and atmospheric turbulent entrainment. Further, the crosswind alignment can take advantage of the centerline symmetry of the turbulent vortex pair to reduce the total mesh area by a factor of two, while the downwind
Fig. 3.3.2.1a Bent-Over Buoyant Plume with Ambient Thermal Stratification.
Fig. 3.3.2.1b

Mesh Alignment Appropriate for a Line Source Release

Fig. 3.3.2.1c

Mesh Alignment Appropriate for a Point Source Release
alignment scheme needs an extraordinarily long x-axis to model the same plume. Overall, the crosswind alignment scheme is about five times smaller than the downwind scheme. The velocity field in the crosswind alignment is that of a two-dimensional turbulent vortex, which typically exhibits strong shearing and entrainment of fluid. The velocity field in the downwind alignment is that of a two-dimensional turbulent deflected jet, which over most of the flow field exhibits a much smaller amount of shearing and entrainment. Clearly, the crosswind alignment scheme is expected to simulate the more important features of the flow.

The singular disadvantage of the crosswind alignment scheme is that it cannot explicitly calculate the shear-produced turbulence of the mean wind field, since the mean wind has no component in the y-z plane. The resolution of this problem is discussed in Sec. 4.3.3.

3.3.3 Downwind Advection of the Mesh

From the discussion in Sec. 3.3.2, the computer solution mesh is aligned perpendicular to the wind. The time evolution of the flow field of the plume cross section is drawn in Fig. 3.3.3.1. The choice of an appropriate downwind advection velocity of the computer mesh is needed in order to reconstruct
Fig. 3.3.3.1 Reconstruction of the Three-dimensional Plume. Wind vectors as a function of height are shown.
the full steady state plume, i.e., the time of the computer simulation must be related to a downwind distance. The choice is difficult because the wind profile dictates that fluid elements at different heights will advect downwind at different rates. A simple approximation is that the advection velocity should be equal to the "pollutant averaged" wind speed:

$$\Delta x \over \Delta t = \frac{\int_{0}^{\infty} \int_{0}^{\infty} u(z) \chi(y,z)dydz}{\int_{0}^{\infty} \int_{0}^{\infty} \chi(y,z)dydz}$$

The finite difference form of Eq. 3.96 is written in Fig. 3.3.3.1. The calculation of this quantity is performed in the "statistics package" of Sec. 3.3.7. A further refinement of the solution scheme is discussed in Sec. 6.2.1.

In practice, for plumes that are released from tall stacks, the amount of wind shear that the plume encounters is ordinarily moderate and does not greatly alter the plume behavior.

### 3.3.4 Property Data

The original VARR-II computer code allows for quadratic fitting of air property data versus temperature. In view of the fact that potential temperature is substituted for
temperature in moist simulations, the scheme of fitting property data to temperature must be examined. The air property data to be fitted includes density, specific internal energy, dynamic viscosity, thermal conductivity, and heat capacity at constant pressure. The coefficients of the quadratic fits for dry air data are listed in Table 3.3.4.1, along with the quadratic form that they are used in. The effect on the property value of the substitution of θ or θ_v for T is considered next.

The use of T or T_v in the perfect gas law yields, by definition, the correct density of a dry or moist parcel of air, respectively. A quadratic fit of the perfect gas law over a small temperature range of interest would yield essentially exact results for the density as well. The calculation of densities with θ or θ_v substituted into the formula for T is also appropriate because θ or θ_v vary from T by very little compared to the absolute temperature. Recall that θ or θ_v is used in the problem formulation to eliminate the compressible nature of the hydrostatic atmosphere. The relevant density variations in the momentum equation are the relative density variations, and the criteria for the use of, say θ_v for T is that

\[
\frac{\rho(T) - \rho(T_o)}{\rho(T_o)} = \frac{\rho(\theta_v) - \rho(\theta_{vo})}{\rho(\theta_{vo})}
\]

(3.97)
### Table 3.3.4.1 Property Values of Air

<table>
<thead>
<tr>
<th>i</th>
<th>symbol</th>
<th>property</th>
<th>units</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$c_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\rho$</td>
<td>density</td>
<td>$\text{lb}_m/\text{ft}^3$</td>
<td>$2.0 \times 10^{-7}$</td>
<td>$-1.78 \times 10^{-4}$</td>
<td>$0.086394$</td>
</tr>
<tr>
<td>2</td>
<td>$I$</td>
<td>internal energy</td>
<td>$\text{BTU}/\text{lb}_m$</td>
<td>$4.3 \times 10^{-6}$</td>
<td>$1.71 \times 10^{-1}$</td>
<td>$78.357$</td>
</tr>
<tr>
<td>3</td>
<td>$\nu$</td>
<td>dynamic viscosity</td>
<td>$\text{lb}_m/\text{ft} \cdot \text{sec}$</td>
<td>$-1.0 \times 10^{-6}$</td>
<td>$1.92 \times 10^{-3}$</td>
<td>$1.0932$</td>
</tr>
<tr>
<td>4</td>
<td>$K$</td>
<td>thermal conductivity</td>
<td>$\text{BTU}/\text{ft} \ \text{sec}^{0_R}$</td>
<td>$0$</td>
<td>$2.59 \times 10^{-5}$</td>
<td>$0.01313$</td>
</tr>
<tr>
<td>5</td>
<td>$C_p$</td>
<td>heat capacity at constant pressure</td>
<td>$\text{BTU}/\text{lb}_m \ \text{O}_R$</td>
<td>$0$</td>
<td>$-2.00 \times 10^{-6}$</td>
<td>$0.24008$</td>
</tr>
</tbody>
</table>

The property $i$ can be expressed as:

$$i = a_i (T-460^{0_R})^2 + b_i (T-460^{0_R}) + c_i$$

Where $T$ is in $^{0_R}$.
with a similar condition for $\theta$ in dry simulations. This relation holds with about four percent accuracy for the most extreme cases encountered in this work.

The specific internal energy is originally fitted versus T. Again, the fact that $\theta$ or $\theta_v$ is close to T compared to the absolute temperature allows them to be interchanged without significant error. The specific internal energy is accurate to about 4 percent under this substitution.

The values of dynamic viscosity and thermal conductivity are important only if the flow becomes laminar. None of the simulations in this work are expected to encounter regions of laminar flow, so the fitted values of molecular viscosity and thermal conductivity are unimportant.

The specific heat varies slowly with temperature, and the substitution of $\theta$ or $\theta_v$ for T results in only a 0.02 percent error for typical cases.

The necessary property data for equilibrium conditions of water vapor and cloud liquid water are included in Secs. 3.2.2.3 and 3.2.2.4. The inclusion of water in the simulations is assumed to have a negligible effect on the property data of the air-water mixture, except for the density, which is corrected through the use of the virtual temperature.
3.3.5 Mesh Initialization and Boundary Conditions

3.3.5.1 Input Profiles

Seven vertical profiles are required for a simulation. Five of the profiles serve to specify the boundary conditions on the computer mesh, one profile (the mean wind speed) is needed by the statistics package, and one profile (the hydrostatic pressure) is needed by the equilibrium moisture thermodynamics model. The required profiles are listed in Table 3.3.5.1. Each vertical profile consists of a set of values that are representative of the cell-centered temperature, wind speed, etc. The number of values is obviously equal to the number of fluid cells in the z-direction. The extension of the model to time-dependent vertical profiles is considered in Sec. 6.2.2.

3.3.5.2 Boundary Conditions

Boundary conditions must be specified for each of eight variables on the four walls of the computer mesh. The walls of the computer mesh are numbered in Fig. 3.3.5.1. Wall #1 is in the plume centerline with the real computer simulation to its left. For this purpose, wall #1 is a free-slip solid wall. Wall #4 always represents the earth, and is specified to be a no-slip wall. The earth is assumed to be a perfect
Table 3.3.5.1
Required Input Profiles

<table>
<thead>
<tr>
<th>Atmospheric Profile</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>virtual potential temperature</td>
<td>°F</td>
</tr>
<tr>
<td>water vapor density</td>
<td>lbm/ft³</td>
</tr>
<tr>
<td>cloud liquid water density</td>
<td>lbm/ft³</td>
</tr>
<tr>
<td>eddy viscosity</td>
<td>ft²/sec</td>
</tr>
<tr>
<td>turbulence kinetic energy</td>
<td>ft²/sec²</td>
</tr>
<tr>
<td>mean wind speed(^A)</td>
<td>ft/sec</td>
</tr>
<tr>
<td>hydrostatic pressure(^B)</td>
<td>millibars</td>
</tr>
</tbody>
</table>

A. The mean wind speed is required by the statistics package of Sec. 3.3.7.

B. The hydrostatic pressure is required by the equilibrium moisture thermodynamics model of Sec. 3.2.2.3.
Fig. 3.3.5.1 Wall Numbering Scheme
reflector of pollutant and humidity in this work. This assumption could be easily modified to account for deposition of pollutant, sources of humidity, etc., for any case of specific interest. Walls #2 and #3 are chosen to be sufficiently far away from the plume so that negligible error is introduced in making them solid and free-slip. In practice, the plumes rise toward wall #3 and begin to deflect when their 10% boundary intersects the wall. This serves as a rough criterion on when to stop the computer simulation.

A summary of the boundary conditions is found in Table 3.5.5.2. The solid-wall, no-slip and free-slip conditions are found in the specification of the two velocity components, \( v \) and \( w \). The reflective conditions are due to the "perfect reflecting walls" assumption; they are foregone at wall #2 for the five variables that are known as functions of height.

3.3.5.3 Mesh Initialization

The entire computer mesh in Fig. 3.3.5.2 is first initialized with the known atmospheric profiles of virtual potential temperature, eddy viscosity, turbulence kinetic energy, water vapor density, and cloud liquid water content. The entire mesh is initialized with a single background value of pollutant, and the velocity field is initialized to be at rest. The plume cells in the figure are then initialized by volume-averaging
Table 3.3.5.2
Boundary Conditions

<table>
<thead>
<tr>
<th>Variable</th>
<th>Wall #1</th>
<th>Wall #2</th>
<th>Wall #3</th>
<th>Wall #4</th>
</tr>
</thead>
<tbody>
<tr>
<td>y-velocity, v</td>
<td>S</td>
<td>S</td>
<td>F</td>
<td>N</td>
</tr>
<tr>
<td>z-velocity, w</td>
<td>F</td>
<td>F</td>
<td>S</td>
<td>S</td>
</tr>
<tr>
<td>virtual potential temperature</td>
<td>R</td>
<td>*</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>eddy viscosity</td>
<td>R</td>
<td>*</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>turbulence kinetic energy</td>
<td>R</td>
<td>*</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>pollutant</td>
<td>R</td>
<td>R</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>water vapor density</td>
<td>R</td>
<td>*</td>
<td>R</td>
<td>R</td>
</tr>
<tr>
<td>liquid water density</td>
<td>R</td>
<td>*</td>
<td>R</td>
<td>R</td>
</tr>
</tbody>
</table>

S--solid wall (normal velocity = 0)
N--no-slip (tangent velocity = 0)
F--free-slip (normal derivative of tangent velocity = 0)
R--reflective (normal derivative = 0)
*--specified as profiles of height (z)
the plume sources of energy, pollutant, and moisture over those cells, using mean wind speed at that height to define the depth of the cells swept out in one second. The initial eddy viscosity and turbulence kinetic energy in the plume cells are set to about 100 times that of the surrounding atmosphere—in practice, the plume turbulence values very quickly relax into values that are consistent with the flow field. No initial volume-averaged momentum is given to the plume cells. Instead of this, an effective stack height increment due to momentum is added to the actual stack height in specifying the location of the center of the plume cells.

3.3.6 Mesh Coarsening Capability

Model programming has been undertaken to allow the mesh spacing to be doubled periodically during the simulations, while keeping the same number of fluid cells on the whole computer mesh. The motivation for this is the desire to keep the growing plume cross section away from the unphysical (solid wall) top and right mesh boundaries. When the simulation is "coarsened," the mesh spacing doubles, which reduces the plume cross section by a factor of four. The calculation is restarted, and the simulation proceeds on a mesh that has four times the area of the old mesh, but the same number of fluid cells.

The coarsening procedure is outlined in Fig. 3.3.6.1. In
(a) Step One - Four Cell Averaging

(b) Step Two - Initialization of New Cells

Figure 3.3.6.1 Mesh Coarsening Procedure Steps
a first step (a) the entire mesh is swept over, four cells at a time. Note that the number of cells vertically or horizontally must be even in order to do this. The fluid variables in these four cells are averaged in the following way: the cell specific internal energy, momenta, and turbulence kinetic energy are mass-averaged over the four cells, since these variables are defined on a per unit mass of air basis. The cell pollutant, eddy viscosity, and moisture variables are simply averaged over the four cells, since these variables are not defined on a per unit mass of air basis. The cell pressure is set to zero, which conforms with the usual starting guess procedures in running VARR-II. The average cell made up from these four cells is now stored in its proper place on the larger mesh, which is half of the distance to the origin vertically and horizontally. When the entire mesh has been swept, four cells at a time, the old mesh has now been relocated in the lower left corner, and is one-fourth of its old size.

In a second step (b) the remaining three-quarters of the mesh needs to be initialized. This "new" area is swept row-by-row in ascending order. The velocity field is assumed to be initially at rest, and the pressure field is initially set to zero. The remaining atmospheric state variables are all specified from a master library of profiles. When the "new" area has been initialized, the calculation is restarted with the
vertical and horizontal mesh spacings doubled.

The computer mesh may be coarsened up to five times during a simulation—this would result in a final mesh that is \(2^5 \times 2^5 = 1024\) times as large as the original mesh. The five times are user specified, and need not take place at regular intervals.

3.3.7 **Plume Statistics Package**

At regular intervals specified by the user, the program calls on a statistics package to calculate a number of important plume statistics without printing out the data of the entire computer mesh. The quantities that are reported by the statistics package are listed in Table 3.3.7.1. The average plume advection velocity is the feature discussed in Sec. 3.3.3, and is defined in Eq. 3.96.
Table 3.3.7.1

Data Reported by the Plume Statistics Package

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
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<tr>
<td>Current Number of Pressure Iterations</td>
<td>(none)</td>
</tr>
<tr>
<td>Current Time Step Size</td>
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</tr>
<tr>
<td>Center Height of Pollutant Field</td>
<td>ft</td>
</tr>
<tr>
<td>Total Specific Internal Energy on Mesh</td>
<td>BTU</td>
</tr>
<tr>
<td>Average Downwind Advection Velocity</td>
<td>ft/sec</td>
</tr>
<tr>
<td>Plume Downwind Distance</td>
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</table>
4. DESCRIPTION OF ATMOSPHERIC TURBULENCE

4.1 Introduction

This chapter describes in detail how atmospheric turbulence is represented in the model. The description begins with the knowledge (e.g., from a set of measurements) of the common atmospheric variables as functions of height: the set includes the wind speed and direction, virtual potential temperature, water vapor density, and cloud liquid water density. The important processes that are responsible for the characteristic shapes of these profiles are outlined, and the concept of layers in the atmosphere arises naturally in the explanation of the interdependencies of the profiles. With a working knowledge of the dominant phenomena in the atmospheric layers, the problem of prescribing the atmospheric turbulence is undertaken. For the model in this work, the atmospheric turbulence is specified with profiles of eddy viscosity and turbulence kinetic energy. The relation of these two variables to the other profiles, and their inclusion into the model occupies most of this chapter.

4.2 Atmospheric Profiles of Wind, Temperature, and Humidity

The vertical atmospheric profiles considered in this work
are assumed to have been measured with some appropriate meteorological instruments over a flat terrain. For instance, a tower with a series of instruments at various heights would produce essentially pointwise values of the variables, which could then be linearly interpolated between the measurement heights to produce the full profiles. It is assumed that the measurements were time-averaged for at least 20 minutes so that there is very little time-dependence in the profiles. Alternatively, a radiosonde (balloon) ascent is commonly used for measuring vertical profiles, although the measurement averaging times are not long enough to completely average over the larger atmospheric eddies.

The measured atmospheric wind profiles have several common features. First, the atmospheric wind vanishes at the ground. This is in accord with the no-slip velocity boundary condition of real fluids. Second, the time-averaged (i.e., averaged over about 20 minutes) vertical velocity is very small at any height. This is because the very low frequency (of the order of 1 per day) vertical velocities are due to the synoptic scale subsiding or lifting motions associated with fronts; these velocities are usually only about 10 cm/sec. Because the average vertical velocities are small, the wind at any height is assumed to be parallel to the ground. Generally, the wind speed increases with height and commonly exhibits some turning with height--
especially in the first several hundred feet of elevation, where pressure gradient, Coriolis, and frictional forces are all important.

The fact that the wind vector may very roughly approximate a logarithmic profile,\textsuperscript{44} an Ekman spiral,\textsuperscript{45} or a thermal wind relation,\textsuperscript{46} is only of minor interest here since the actual wind profile determines the behavior of an individual plume. In this work, the turning of the wind with height is not represented in the hydrodynamic simulations, although the prospect of including it is considered among the extensions of the model outlined in Sec. 6.2. Also, the difficulty of defining an average wind direction when there are only light, variable winds at a station dictates that the computer simulations are not expected to be accurate for winds of less than about 5 knots.

The temperature and humidity profiles directly provide the information about the local stability of vertical atmospheric and plume motions. No approximations to the temperature or humidity profiles are needed to incorporate them into the simulations. The temperature and humidity profiles are used to evaluate the virtual potential temperature profile: Note that in defining equations for virtual potential temperature (Eq. 3.53 and Eq. 3.67) the temperature, humidity, and pressure are required at any height. To this end the pressure profile could have been measured by itself, or calculated with any of
a number of approximations (dry hydrostatic, moist hydrostatic, various interpolations between points, etc.) Whatever assumptions are made, the pressure profile consistent with these assumptions must be input to the simulation where it is used to recalculate the correct temperature from the virtual potential temperature and humidity for the equilibrium moisture thermodynamics model.

4.3 Turbulence in the Planetary Boundary Layer

4.3.1 Introduction

The planetary boundary layer (PBL) is a boundary layer in a rotating, stratified, multi-component fluid whose moisture component can undergo changes of phase. Further, the boundary conditions on fluxes of momentum, sensible and latent heats, and radiant energy can vary greatly over large and small distances (i.e., distances that are large or small in comparison to the depth of the boundary layer), and are typically strongly coupled to the flow. Although a number of excellent reviews have been written at many levels of detail, the basic notions of turbulence in the planetary boundary layer are developed here with the aim of pointing out the limitations of the description of the PBL turbulence embodied in the computer simulations.
4.3.2 Layers in the PBL and Important Processes

Without much loss in generality, it is assumed in this work that all of the energy in turbulent atmospheric motions ultimately comes from the sun. Although it is possible to conceive of special situations where this is not quite true (for example, the turbulence near a busy expressway, much of which is caused by mechanical stirring and buoyant exhausts), the atmospheres which are encountered in this work are free of man-made turbulence, except for the buoyant plumes themselves! For the purposes of illustration, the solar energy which produces atmospheric turbulence may be divided into two streams: (1) that part of the solar energy that produces the large synoptic-scale pressure patterns on the earth, which in turn drives the wind and produces turbulence in regions of the atmosphere of sufficiently large wind shear, and (2) that part of the solar energy that produces the local thermal stratification of the atmosphere, which in turn produces turbulence in regions of sufficiently unstable stratification. The turbulence that is produced by the first stream is called "mechanically produced turbulence," and that produced by the second stream is called "buoyancy produced turbulence." The thermal stratification that is produced by the second stream is usually formulated in terms of virtual potential temperature, so that
moisture and latent heat effects are naturally included in the
"buoyancy produced turbulence." There are two mechanisms that
destroy atmospheric turbulence: (1) viscous dissipation, which
is always at work in a turbulent flow, and (2) buoyant destruc-
tion, which is present in regions of stable thermal stratifi-
cation.

From the preceding discussion it is expected that in a
region in steady state the mechanisms of turbulence production
and destruction will be balanced, and that the turbulence
kinetic energy will maintain a value that is commensurate with
the destruction rate. Very commonly in micrometeorological
studies, the regions that these processes are studied in are
simplified to layers, so that the description of atmospheric
turbulence becomes one-dimensional—the single dimension is then
height. The situation is illustrated in Fig. 4.3.2.1. In the
uppermost layer of laminar flow, the strong geostrophic winds
usually have very small wind shears with height, and are usu-
ally associated with stably stratified air, so that there is
little or no turbulence. The next layer down usually is a
region of buoyancy produced turbulence with only small wind
shear—the buoyancy is typically from solar heating at the
ground and latent heat release in cloud formation (clouds ob-
viously affect the amount of solar heating at the ground, so
that these effects are strongly coupled). The layer nearest
Fig. 4.3.2.1 The Concept of Layers in the Planetary Boundary Layer. Atmospheric turbulence is assumed to be variable in one-dimension only in this figure. The turbulence is steady-state.
to the ground typically exhibits a lot of wind shear due to the no-slip condition at the ground, so that mechanically produced turbulence is present in addition to buoyant production, and turbulence kinetic energy is usually a maximum somewhere in this layer.

The particular illustration of atmospheric layers in Fig. 4.3.2.1 is certainly not unique. Many investigators have coined names for layers to illustrate different refinements on the processes in the PBL. Such terms as the surface layer, Ekman layer, subcloud layer, cloud layer, inner layer, outer layer, tower layer, convection layer, inversion layer, super-adiabatic layer, and viscous sublayer are common, but they do not represent anything more sophisticated than treating the atmosphere as one-dimensional.

The prospect of treating the atmospheric state as two-dimensional—now including its downwind development as well as its profile with height—is considered in Sec. 5.4.1 in conjunction with the modeling of a fumigation episode.

4.3.3 Prescription of the Eddy Viscosity

The prescription of the eddy viscosity in the two-dimensional mesh of the crosswind alignment scheme of Fig. 3.3.2.1c is considered in this section. It was mentioned in Sec. 3.3.2...
that the absence of any mean wind component (by definition) in the crosswind direction means that, away from the plume, and as far as the computer simulation is concerned, there is no explicit mechanical production of turbulence in the atmosphere. In fact, what takes place in the atmosphere is that the turbulence kinetic energy component, $u'^2$, and the Reynolds stress, $u'w'$, of the downwind $x$-$z$ plane are feeding into the crosswind $y$-$z$ plane turbulence kinetic energy component, $v'^2$, and Reynolds stress, $v'w'$, through the return to isotropy term in Eq. 3.40. For this work, the assumption is made that the return to isotropy term is very strong, so that the turbulence is isotropic. Experiments on atmospheric return to isotropy indicate that this assumption is reasonably good. It is seen in the discussion of the results in Chapter Five that this is probably the most limiting assumption in the work with regard to being able to model real atmospheres. The eddy viscosity as a function of height in the downwind $x$-$z$ plane is estimated from a number of prescriptions for eddy viscosity that are correlated from mean wind and temperature profiles, then the eddy viscosity in the crosswind $y$-$z$ plane is assumed to be the same as in the $x$-$z$ plane under the assumption of isotropy.

The incorporation of an ambient eddy viscosity profile on the simulation mesh finds two problems. First, any
arbitrary eddy viscosity imposed on the mesh cells at the start of the simulation will, in the absence of sufficient mechanical and buoyant production, rapidly decay down to the molecular kinematic viscosity. Second, the turbulence field inside the plume must be allowed to develop on its own. The method of incorporating the ambient eddy viscosity profile in light of these problems is as follows: to start the simulation, the cells outside of the initial plume cells are initialized with the eddy viscosity profile, depending on their height in the mesh. After each time step, each cell on the mesh is tested to see if it has fallen below the prescribed eddy viscosity profile at its height. If it has, its eddy viscosity is simply reset to the ambient value. If it has not fallen below the ambient value, presumably because either the plume-induced turbulence or the turbulently diffused turbulence from neighboring cells is dominating, then the cell eddy viscosity value is left alone. In this way, the far field always maintains the ambient atmospheric turbulence values, and the plume turbulence, if greater than the ambient turbulence, is left to develop on its own. Overall, this method has the effect of adding a non-uniform source term to the eddy viscosity equation—the term always adjusts itself to yield the original eddy viscosity in the far field, and to "turn itself off" if the plume turbulence is dominating. Mathematically, the
inequality
\[ \sigma(y,z,t) \geq \sigma_{\text{library}}(z) \] (4.1)

has been added to the equation set, where \( \sigma_{\text{library}}(z) \) is the prescribed eddy viscosity profile as a function of height.

Before discussing the available prescriptions of eddy viscosity, it should be noted that the potentially most accurate method of prescribing the eddy viscosity for an individual release would be to actually measure it in the field—perhaps simply by estimating it from bivane wind fluctuation data. The effort in this work to arrive at workable prescriptions from the micrometeorological literature is motivated by the total absence of these measurements in existing plume field data. The particular prescriptions that are recommended here are used only because they offer a simple way to estimate the eddy viscosity profile.

A number of prescriptions for the eddy viscosity in the outer boundary layer of the atmosphere as a function of height have been reviewed. A summary of the various prescriptions is presented in Table 4.3.3.1, where they are separated into two major groups—those that require wind speed and direction profiles, and those that do not. Those which do not require wind profiles as input are easier to use because the wind profiles need not be measured (e.g., with instrumented towers or
Table 4.3.3.1 Comparison of Eddy Viscosity Prescriptions

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<th>Author(s)</th>
<th>Neutral</th>
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<th>Unstable</th>
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<td></td>
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<tr>
<td>Blackadar\textsuperscript{59}</td>
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<td>no</td>
<td>no</td>
</tr>
<tr>
<td>Blackadar and Ching\textsuperscript{60}</td>
<td>no</td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td>Yamamoto and Shimanuki\textsuperscript{61}</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
<tr>
<td>Nieuwstadt\textsuperscript{64}</td>
<td>yes</td>
<td>yes</td>
<td>yes</td>
</tr>
</tbody>
</table>

**Prescriptions that do not require wind profiles:**

<p>| | | | |</p>
<table>
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<th></th>
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</tr>
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<tr>
<td>O'Brien\textsuperscript{62}</td>
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<td>yes</td>
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<tr>
<td>Bornstein\textsuperscript{63}</td>
<td>yes</td>
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</tbody>
</table>
balloons). However, they are not expected to be as accurate, since the wind profile has taken an ideal shape. All of the models in Table 4.3.3.1 are searched for applicability to neutral, stable, and unstable atmospheres.

It is recommended that if the wind speed and direction profiles have been measured, the prescriptions of Blackadar,\textsuperscript{59,60} and Yamamoto and Shimanuki\textsuperscript{61} should be used. If the wind speed and direction profiles have not been measured, the prescriptions of Bornstein\textsuperscript{63} or O'Brien\textsuperscript{62} should be used. The prescription of Nieuwstadt\textsuperscript{64} requires a substantial numerical analysis of the profiles and has not been tested.

Any of these prescriptions must be used with caution since all of them are only capable of providing an estimate to the eddy viscosity. The greatest difficulty in using these prescriptions is that they typically require values for quantities that were not measured, such as the heat flux at the ground, the roughness height, geostrophic velocity, etc.

4.3.4 Prescription of the Turbulence Kinetic Energy

The prescription of the turbulence kinetic energy (TKE) in the two-dimensional mesh of the crosswind alignment scheme of Fig. 3.3.2.1c is considered in this section. The turbulence kinetic energy suffers from exactly the same problem as the eddy viscosity in Sec. 4.3.3.: in the absence of explicit
buoyant and mechanical production of turbulence on the two-dimensional mesh, the turbulence kinetic energy would gradually decay away entirely. To satisfactorily avoid this problem, the concept of the turbulent "return to isotropy" is again invoked to allow the turbulent kinetic energy produced by the mean flow shearing and buoyancy to be fed into the crosswind motions. A turbulence kinetic energy profile is needed, so that it may maintain the turbulence for mesh cells that lack the sufficient turbulence production in exactly the same way that an eddy viscosity profile maintains the eddy viscosity for the mesh.

Ideally, the TKE profile should be measured or deduced from other profiles for an actual atmosphere. In fact, however, prescriptions for the turbulence kinetic energy from mean wind and temperature profiles are not generally available in the literature. The actual prescription of the turbulence kinetic energy profile in this work has had to come from the following, very approximate analysis of the transport equations.

Consider the TKE transport equation in a region away from the plume. The vertical and horizontal velocities, \( v \) and \( w \), are zero, and the eddy viscosity, \( \sigma \), and TKE, \( q \), are functions of height, \( z \), only; with the resulting expression being
\[
\frac{\partial q}{\partial t} = \frac{-4aq^2}{\sigma} + \Gamma \frac{\partial}{\partial z} (\sigma \frac{\partial q}{\partial z}) \quad (4.2)
\]

For a properly time-independent TKE, there must be a balance of dissipation and diffusion in Eq. 4.2; or

\[
\frac{4aq^2}{\sigma} = \Gamma \frac{\partial}{\partial z} (\sigma \frac{\partial q}{\partial z}) \quad (4.3)
\]

Performing a scale analysis of the terms, noting that \( \Gamma / 4a \approx 10 \) and that the depth of the planetary boundary layer is taken equal to \( L_{\text{eddy}} \), one obtains the result

\[
q \sim 10 \frac{a^2}{L_{\text{eddy}}^2} \quad (4.4)
\]

For typical values in the atmosphere, \( \sigma \sim 100 \text{ ft}^2/\text{sec} \) and \( L_{\text{eddy}} \sim 10^3 \text{ ft} \), giving the value

\[
q \sim 10^{-3} \text{ sec}^{-1} \quad (4.5)
\]

Note that for a highly idealized picture of turbulence, with eddies of a single size, \( L_{\text{eddy}} \), and velocity, \( u_{\text{eddy}} \),

\[
q \sim u_{\text{eddy}}^2 \quad (4.6)
\]

\[
\sigma \sim u_{\text{eddy}} L_{\text{eddy}} \quad (4.7)
\]

and therefore

\[
q \sim \frac{u_{\text{eddy}}}{L_{\text{eddy}}} \quad \text{[sec}^{-1}] \quad (4.8)
\]
This states that \( q/\sigma \) is simply the inverse of the eddy turnover time. The scale analysis (Eq. 4.5) of the \( q \) transport equation shows that the choice \( q = 10^{-3} \text{sec}^{-1} \sigma \) should roughly allow \( q \) to have a constant value. The fact that this choice of \( q \) agrees with the eddy turnover time of roughly the most diffusive atmospheric eddies \( 10^3 \) seconds, or about 15 minutes) lends support to the idea that \( \sigma \) and \( q \) have been chosen consistently in this scheme.

The crude specification of \( q_{\text{library}}(z) \) has been found to be satisfactory in this work primarily because the turbulence kinetic energy only indirectly influences the eddy viscosity, so that errors in estimating TKE are tolerated much more than the errors in estimating the eddy viscosity. The preceding analysis, since it is a scale analysis, only provides a very approximate estimate of the turbulence kinetic energy profile. Mathematically, the inequality

\[
q(y,z,t) > q_{\text{library}}(z) = 10^{-3} \text{sec}^{-1}\sigma_{\text{library}}(z)
\]  

(4.9)

has been added to the equation set, where \( q_{\text{library}}(z) \) is the prescribed turbulence kinetic energy profile as a function of height.
5. **RESULTS**

5.1 **Introduction**

The discussion of the results of the computer plume simulations is very naturally divided into two sections corresponding to the two regimes of plume behavior outlined in Sec. 1.2.2. To illustrate the two regimes, typical values of effluent temperature, velocity, and pollutant are shown in Fig. 5.1.1 for several stations downwind of a large combustion source. At the stack exit, the plume rushes upward at 20\(\text{m/sec}\), is about 100\(\text{C}\) above the ambient air temperature, and has an \(\text{SO}_2\) concentration of about 100 000 pphm (parts per hundred million). At the second station the plume has become diluted about 200 times. Without a detailed picture of its cross section, it may be stated generally that its average temperature excess is now only about 0.5\(\text{C}\) and its turbulent velocity fluctuations (disregarding those induced by its buoyancy) are about 10 cm/sec—and these are just about on the level of observed atmospheric fluctuations. However, the plume \(\text{SO}_2\) concentration is still many times higher than the background \(\text{SO}_2\) level, so that the plume is recognizable by its \(\text{SO}_2\) concentration field, but not by its temperature or velocity fields. Throughout this first regime the plume
Fig. 5.1.1 Plume Regimes. The plume behavior is divided at the point at which the plume temperature and velocity fluctuations are reduced to levels that are indistinguishable from atmospheric fluctuations.
velocity and temperature fluctuations have been stronger than the atmospheric fluctuations, so that in a large part the plume motions have been dominated by the plume properties. Throughout the second regime the atmospheric motions are responsible for the plume dilution to the point where the pollutant becomes indistinguishable from the background level, and the plume disappears.

The selection of these regimes is very natural in the discussion of the results. The results that are applicable in the plume dominated stage will address the question of how adequately the dynamics of a buoyant, deflected plume are simulated. Such results are found in Sec. 5.2. The results that are applicable in the atmospheric dominated stage will address the question of how adequately the atmospheric turbulence is being simulated. Such results are found in Sec. 5.3. The results in Sec. 5.4 are essentially model extensions that are applicable in the atmospheric dominated regime for Sec. 5.4.1, and the plume dominated regime for Sec. 5.4.2, but which do not have a body of experimental results to be compared with.

The plume simulations that are presented in this chapter have been included for several different reasons. The general simulation in Sec. 5.2.1 is included to acquaint the reader with the general features of the buoyant line-vortex. The
detailed comparison of simulations like the one in Sec. 5.2.1 with experimental results is made in Sec. 5.2.2. The effect of thermal stratification on the buoyant line vortex is then developed in the simulation of Sec. 5.2.3. The simulations for comparison with actual field studies again considers the neutral atmosphere case in Sec. 5.3.1. The effect of thermal stratification is then developed in the simulation of Sec. 5.3.2, where a large stack plume in a low-level inversion is studied. Simulations that demonstrate the model extensions are found in Sec. 5.4.

5.2 Comparisons to Analytical Models

5.2.1 General Nature of the Solutions

The general nature of all the computer solutions in this work is discussed in this section. All of the simulations are performed on a 20 cell by 20 cell mesh, although the cell height and width vary between different simulations. The time step size is selected by the program at each time step, and is usually from one-tenth of a second to several seconds. The selection of a time step size is performed by the code, where it always chooses the smallest step size from a choice of
a diffusion condition,

\[ DT = \frac{TSTEP}{\max(\sigma) \left( \frac{1}{Dy^2} + \frac{1}{Dz^2} \right)} \quad (5.1) \]

a Courant condition,

\[ DT = \frac{TSTEP \min(Dx,Dz)}{\max(v,w)} \quad (5.2) \]

or a simple rate of change condition,

\[ DT = \frac{0.2 \max(v,w)}{(\max(v,w) - \max(v_{\text{old}},w_{\text{old}}) + 10^{-6})} \quad (5.3) \]

where TSTEP usually has a value of 0.01. As a practical matter, it is found that the time steps have to be reduced beyond these conditions by about a factor of 25 for the mesh cell sizes encountered in this work. This allows the code to conserve energy in the computer mesh cells within an acceptable tolerance. The non-conservation of energy arises from the first order accuracy of the differencing scheme for the advection terms. Full donor cell differencing of the advection terms is found to give the best answers in the simulations—less than full donor cell differencing produces noticeable nonlinear instabilities in the flow.

A simple plume development is found in Figures 5.2.1.1 to 5.2.1.6. Figure 5.2.1.1 interprets the mesh cell quantities found in the following figures. In Fig. 5.2.1.2, the
ordered-pair notation for locating cells
e.g., 3rd cell from left, 2nd from bottom

X X X X 0.0 X X X
X X X (3, 2) X
X X 49.999 F X
X X X X X
X 1 0.0

DZ X TNU = 1.000E+00 X
X TKE = 1.000E-03 X
X CHI = 1.000E-05 X
X VAP = 1.000E-07 X
X LIQ = 1.000E-07 X
X X X X X X X X X X X X

w velocity, ft/sec
v velocity, ft/sec

TNU is eddy viscosity in ft²/sec
TKE is turbulence kinetic energy in ft²/sec²
CHI is pollutant concentration in lbm/ft³
VAP is water vapor density in lbm H₂O/ft³
LIQ is liquid water density in lbm H₂O/ft³

Fig. 5.2.1.1 Key to Cellwise Quantities for Figs. 5.2.1.2, 5.2.1.3, 5.2.1.4, 5.2.1.6, and 5.3.2.1.
Fig. 5.2.1.2 Initialized Plume Cross Section at 0 sec.

DY = 100 ft, DZ = 200 ft.
Disregard moisture values.
entire 400 mesh cells are initialized at rest and at 50°F, except for one warm cell (2,4) centered 500 ft high (and on the left boundary) which is at rest and at 68°F. Each mesh cell is 200 ft high and 100 ft wide. The ambient turbulence is set uniformly to 1 ft²/sec in eddy viscosity and $10^{-3}$ ft²/sec² in turbulence kinetic energy, which are essentially laminar values compared to the values that develop inside the plume cell.

After 20 seconds of development (see Fig. 5.2.1.3) a vortex circulation has formed in the vicinity of the warm fluid, and mixing has brought the warmest fluid cell (2,4) from 68°F to 61.24°F. The strongest updraft (6.57 ft/sec) occurs in the warmest cell, and the downdrafts tend to be weaker, since they are spread over a larger area.

After 80 seconds of development (see Fig. 5.2.1.4) the plume has risen 379 ft. Considerable mixing has reduced the warmest cell temperature to 52.9°F from 68°F, and the updraft has now increased to 10.8 ft/sec. Again, the vortex circulation is very easy to identify and it occupies a progressively larger area as the plume cross section grows. The turbulence kinetic energy field at this point in time is illustrated in Fig. 5.2.1.5, where the maximum TKE occurs in the updraft region and is about 1600 times that of the ambient field.

After 200 seconds of development (see Fig. 5.2.1.6), the
Fig. 5.2.1.3 Plume Cross Section at 20 sec.

DY = 100 ft, DZ = 200 ft.

Disregard moisture values.
Fig. 5.2.1.4 Plume Cross Section at 80 sec.

DY = 100 ft, DZ = 200 ft.

Disregard moisture values.
Fig. 5.2.1.5 Turbulence Kinetic Energy Profile at 80 sec. Contours of TKE in ft²/sec². The maximum TKE is 1.82 ft²/sec², and the minimum TKE is 0.001 ft²/sec² (throughout the far field).
Fig. 5.2.1.6 Plume Cross Section at 200 sec.

DY = 100 ft, DZ = 200 ft.

Disregard moisture values.
plume has risen 1003 feet. The warmest cell in the plume is barely 1°F warmer than the surroundings, and the updraft velocity has remained constant. The plume cross section has grown considerably, and the maximum TKE has dropped by a factor of two from its value at 80 seconds.

The effect of adding an initial internal circulation to the plume cross section is developed in Figures 5.2.1.7 and 5.2.1.8. In Fig. 5.2.1.7, the initial circulation is shown. The mesh cells are not 50 ft by 50 ft, although the same size plume is initialized as in the earlier discussion. The uniform 3 ft/sec circulation pattern is simply a rough guess at the actual circulation. Simulations to 40 seconds with and without the circulation are found in Fig. 5.2.1.8. The presence of an initial circulation makes only a small difference between the runs, as seen in the selected velocity and temperature values. The initialization of all of the subsequent simulations with no initial circulation is presumed to introduce little error into the results, i.e., the dynamics are strongly affected by the buoyancy, and not by the initial circulation.

The effect of ambient atmospheric turbulence is developed in Figures 5.2.1.9 and 5.2.1.10. The initialization is the same as in Fig. 5.2.1.7 without the initial circulation, but with 50 ft square cells. In Figure 5.2.1.9, the ambient
Fig. 5.2.1.7 Initialized Plume Cross Section with Internal Circulation.
Fig. 5.2.1.8 Plume comparison at 40 sec of simulation showing the small effect of an initial circulation on the plume development.
Fig. 5.2.1.9 Plume development in a moderately turbulent atmosphere. Mean flow field velocity vectors are shown.
Fig. 5.2.1.10 Plume development in a very turbulent atmosphere. Mean flow field velocity vectors are shown.
eddy viscosity is maintained at a uniform 15 ft$^2$/sec. The resultant plume cross section at 40 seconds has developed the usual circulation, and its warmest cell is found to be 6.05°F above ambient. In strong contrast to this is the plume cross section of Fig. 5.2.1.10 which has a much stronger ambient turbulence field below 850 ft, and a much weaker turbulence field above 850 ft. The fictitious eddy viscosity profile quoted in Fig. 5.2.1.10 reflects a very turbulent boundary layer whose depth is about 850 ft. The resultant plume cross section at 40 sec is markedly different. The strong atmospheric dispersion has resulted in a much more diffuse plume whose maximum cell temperature is about one-third that of the previous run, although the plume rise is quite similar. This agrees with the notion that plume rise is dominated by the thermal stratification of the atmosphere (which is neutral in both cases here), and to a much lesser extent by other factors. Plume dispersion, which is very different in the two cases here, is affected strongly by the turbulent state of the atmosphere (which in turn is strongly affected by the thermal stratification of the atmosphere, among other factors).

The effects of using continuative outflow$^{68}$ versus free-slip solid walls for the top and right boundaries was studied. The alternative assumptions produce little difference
between runs. The solid free-slip walls give more satisfactory results, although they are somewhat unrealistic physically, as are the continuative walls. Further refinement of the boundary conditions is expected to have little influence on the solutions.

5.2.2 Turbulent, Buoyant Line-Vortex Results

The results of the plume simulations in the plume dominated regime (see Fig. 5.1.1) are discussed here. To obtain these results, the ambient turbulence level should be less than one-tenth of the plume turbulence, so that the ambient turbulence will have only a small effect on the results. Plume simulations are compared to the experimental results of Richards\(^4\) and Tsang.\(^{33}\) Tsang's results are generally more accurate since his experimental technique is more sophisticated, but Richards was first to set down the basic similarity arguments.

Similarity and dimensional analyses by Richards and Tsang have revealed the formula for the plume top height, \(Z\), versus the plume radius, \(R\), and the formula for \(Z\) versus time, \(T\). The concept of a virtual origin of \(Z\) and \(T\) simplifies the results in their analyses. Briefly, the virtual origin \((T_*, Z_*)\) is the limit where the plume radius vanishes, much as if the plume had emanated from a single point at time \(T_*\).
This is shown in Fig. 5.2.2.1, where the two formulas are quoted. Two universal constants, N and C, are found in the formulas. Tsang found that N = 3.0 and C = 1.9 provided a very good fit to dense salt water line thermals released in a tank of still, fresh water. The flow inside the line thermals is turbulent.

Tsang's results are simulated with the computer and presented in Fig. 5.2.2.2. Essentially, the virtual origin \((T_*, Z_*)\) is free to be chosen to provide the best agreement between experimental and calculational results. The plume center height (not top height) is to be compared—the formula quoted in the figure is readily derived from the formulas in Fig. 5.2.2.1. The calculated values are represented by the points, and the experimental results (with an optimal \(T_*\) and \(Z_*\)) are represented by the solid line. Since ambient atmospheric turbulence is not important, the comparison serves to test the turbulence model by making sure that it can reproduce the self-similar plume development. The results are acceptably accurate through several hundred seconds of development. The calculated plume is found to rise a little too fast, so that a more "diffusive" turbulence model would be more accurate. The VARR turbulence constants, \(\alpha\), \(\Gamma\), and \(\Gamma_1\), were varied in an effort to accomplish this. The dissipation constant, \(\alpha\), was decreased tenfold to allow
\[ Z - Z_0 = NR, \quad (Z - Z_0)^{3/2} = C\left[\frac{A_0 \Delta \rho g}{\rho}\right]^{1/2}(T - T_*) \]

Fig. 5.2.2.1 Geometry for plume analyses.
Fig. 5.2.2.2 Comparison of Computational and Experimental Results for Plume Rise versus Elapsed Time for Buoyant Line-Thermals.
the turbulence to persist with less dissipation. The turbulent transport constants, $r$ and $r_1$, were increased tenfold to enhance turbulent diffusion. Alone or in any combination these variations produced little more than a 20 ft decrease of plume rise at 200 sec. Thus, these line-thermal results are largely independent of the model constants. The only term not associated with these constants (see Eq. 3.43) is the production term. It is suggested here that the production term is probably too small because it neglects buoyant production in favor of mechanical production alone. This hypothesis was not tested further in this work, however.

5.2.3 Brunt-Vaisala Period of a Turbulent, Buoyant Parcel

As a test of the hydrodynamic model, the Brunt-Vaisala period of a buoyant parcel in a stably stratified atmosphere is calculated. Briefly, the Brunt-Vaisala period is the period of the oscillation of a parcel of fluid that is perturbed from its equilibrium level in a stably stratified fluid. A consideration of the restoring force on the parcel yields the formula

$$\text{Brunt-Vaisala period} = \sqrt{\frac{g}{\frac{\partial \theta}{\partial z}T}} \quad [\text{sec}]$$

(5.4)
For typical atmospheric values of $T$ and $d\theta/dz$, the period is hundreds of seconds. Computer simulation to hundreds of seconds is too costly, so the stratification, $d\theta/dz$, is increased to $0.1^\circ F/ft$—about a twentyfold increase over typical atmospheric values—which decreases the predicted period to 81 sec and allows much more inexpensive simulations.

The entire computer mesh, $10^3$ ft by $10^3$ ft, was initialized to this stable stratification, and a warm parcel was placed at an elevation of 300 ft. The results of two different runs are shown in Fig. 5.2.3.1. In a first run, the parcel had a small buoyancy parameter:

$$\frac{F}{U} \equiv \frac{gQ_h}{\rho_s c_p T_s U} = 4.6 \times 10^3 \text{ ft}^3/\text{sec}^2$$

which resulted in the lower curve. The curve exhibits a Brunt-Vaisala period of 92 seconds, and a fair amount of "jitteriness"—which is not surprising since the total parcel motion is much less than one cell spacing, so that the motion is not very well resolved on the mesh. In a second run, the parcel had a larger buoyancy parameter:

$$\frac{F}{U} = 4.6 \times 10^4 \text{ ft}^3/\text{sec}^2$$

which resulted in the upper curve. The curve exhibits a Brunt-Vaisala period of 102 seconds, and a much smoother motion since several mesh cells have been traversed, and thus
Fig. 5.2.3.1 Demonstration of the Brunt-Vaisala period. Parameters for these runs are discussed in the text.
the motion is better resolved on the mesh in this run.

Overall the agreement between calculated and observed values is good, considering that the classic Brunt-Vaisala problem allows no turbulent mixing, while the simulations in this work allow it. Generally, the action of turbulent mixing is to rapidly diffuse the temperature field and to slow the period of oscillation.

For comparison to these results, the parcel motion in a neutral atmosphere for the stronger \((F/U = 4.6 \times 10^4 \text{ ft}^3/\text{sec}^2)\) run has been included in Fig. 5.2.3.1. The stratification thus has a very strong effect on the motion.

5.3 Comparisons to Field Studies

5.3.1 Pasquill Dispersion and Briggs Plume Rise in Neutral Atmospheres

A comparison of plume simulation and experiments both in the plume and atmospheric dominated regimes (see Fig. 5.1.1) are discussed here for neutral atmospheres. To obtain these results, the ambient atmospheric turbulence is estimated from the discussion in Chapter Four. The plume simulations are started in the plume dominated regime and the simulations are run out to times where the plume excess temperature is very small, and the plumes are followed with the pollutant species concentration. The atmospheres in this section all have dry
adiabatic lapse rates of temperature.

A comparison to Briggs'\textsuperscript{70} plume rise for neutral atmospheres is made in Fig. 5.3.1.1. Briggs' work found that the plume rise and downwind distance, when nondimensionalized with a length $L$, 

$$L \equiv \frac{F}{U^3} = \frac{g Q_h}{c_p \rho_0 T_0^4} \left[ \frac{\text{ft}^4}{\text{sec}^3} \right]$$ \hspace{1cm} (5.5)

yields a $2/3$ power law relation between the plotted values for a wealth of field data. To interpret the data from the simulations, the plume rise is taken as the plume center height minus the virtual origin height (i.e., the rise from the virtual origin), and the downwind distance is then the product of the downwind velocity and the elapsed time from the virtual origin (see Fig. 5.2.2.1). For the run in Fig. 5.3.1.1, the distance, $L$, for a 1000 MWt release in a 30 mph wind is 11.3 ft when calculated with Eq. 5.5. The agreement is generally good between calculation and experiment; the errors of estimation of $Z$, and $T$, and the uncertainty in the ambient turbulence level all contribute to the discrepancy. Also, the data point at $X/L = 78$ is taken from the initialized plume cross section at time $t = 0$ which is not a physically accurate picture of the plume. The good agreement between calculation and experiment at this point is felt to be simply a cancellation of opposing errors.
Fig. 5.3.1.1 Briggs' Comparison of Plume Rise in Neutral Atmospheres Compared with a Computer Simulation of a 1000 MWt Release in a 30 mph Wind. From the analysis in the text, $L = 11$ ft, $\Delta h$ is interpreted as $Z - Z_*$, and $x$ is interpreted as $U(T - T_*)$. 
A comparison to Pasquill's plume dispersion in neutral atmospheres (exactly the Pasquill D class) is made in Fig. 5.3.1.2. The Pasquill dispersion curves are taken from Turner's workbook, whose values are corrected from older sources of dispersion data. The calculated plume dispersion is taken from plume cross section printouts at four different times during the simulations. The calculated plume dispersion follows the Class D dispersion fairly well, but with a trend toward overpredicting the dispersion at points closer than the point 1/2 km downwind. This overprediction is again related to the finite plume size at time \( t = 0 \) in the initialization scheme. This error affects the earlier solution greatly, but has a decreasing effect on the solution at longer times. The error bars in the figure represent the error associated with increasing or decreasing the plume cross sectional area by one mesh cell. This gives a rough notion of the errors expected when the mesh cells are interpreted as being either entirely inside or outside of the plume. Note that these one-cell error bars decrease as the total number of cells in the plume increases with downwind distance. The trend to underpredict the dispersion at large distances reflects probable errors in the estimation of the ambient turbulence. Also note that since the turbulence is assumed to be isotropic, the calculated horizontal and vertical
Fig. 5.3.1.2 Turner's Horizontal Dispersion versus Distance Downwind Compared to a Computer Simulation of a 1000 MWt Release in a 30 mph Wind.
dispersion will not differ greatly; therefore, Pasquill dispersion cases that have significantly different \( \sigma_y \)'s, and \( \sigma_z \)'s (e.g., extreme stability) will be difficult for this model to duplicate.

5.3.2 LAPPES SO\(_2\) Dispersion Studies

A number of comparisons to a well-studied plume from the LAPPES field experiments are made in this section. The plume emanating from stack No. 1 of the Keystone coal-fired generating station at about 8 a.m. on October 20, 1967 is modeled with a computer simulation. Information about the ambient weather and plant operating characteristics are provided in the LAPPES study. Experimental helicopter SO\(_2\) plume cross sections and SO\(_2\) bubbler data are available for comparison.

The computer simulation is initialized in Fig. 5.3.2.1 in the following way: The stack is releasing heat at 28.6 \( \times \) 10\(^6\) cal/sec. Half of this is to be arbitrarily put into three mesh cells that are 164 ft (50 m) high and 492 ft (150 m) wide. The other half of the heat resides in the mirror image of these cells. Using a Briggs plume rise correlation for the rise induced by the initial momentum of the effluent (20 m/sec exit velocity) yields a rise of about 100 ft. The three cells are then to be centered at the
stack height (800 ft) plus the momentum rise height (100 ft), or 900 ft. If the cells are all 164 ft high, then the center of cell (2,7) is at 902 ft—thus cells (2,6), (2,7), and (2,8), are to be initialized with half of the heat release. Checking the prevailing winds for cells (2,6), (2,7), and (2,8) finds that they sweep out 7.3 million cubic feet in one second. Releasing $14.3 \times 10^6$ cal into $7.3 \times 10^6 \text{ ft}^3$ gives a temperature rise of $0.47^\circ\text{F}$, and this is added to the ambient air temperature in these cells in Fig. 5.3.2.1, which shows the computer initialization in the vicinity of the plume cells. This whole initialization process is admittedly crude, particularly in the treatment of momentum, but it gives very satisfactory answers.

The experimental results for this plume are found in Figs. 5.3.2.2 and 5.3.2.3. The former figure shows the prevailing wind speed, direction and potential temperature. The weather was clear on that morning, and a sizeable low-level inversion had formed during the night to about 250 m depth. The flow above 250 m was essentially neutrally stratified and flowed from the west. The turning of the wind with height is ignored in the computer simulation, but the wind speed and potential temperature values are input directly onto the computer mesh. The ambient humidity was fairly low due to a wide subsidence inversion over most of the computer mesh,
Fig. 5.3.2 Weather for 20 October 1967 at the Keystone Plant.
Fig. 5.3.2.3 Comparison of Computational and Helicopter Results at 4.8 km Downwind.
so humidity is neglected in this simulation. Turbulence values are calculated for a neutral atmosphere from Blackadar, and the turbulence in the inversion layer is suppressed by a factor of 100 in the absence of any better information about the turbulence in the stably stratified region. The eddy viscosity is of the order of 100 ft$^2$/sec in the neutral region, and about 1 ft$^2$/sec in the stable region.

The helicopter plume cross section at 4.8 km downwind is drawn in Fig. 5.3.2.3 as the jagged outline. The outline connects the measured SO$_2$ horizontal traverses, and represents essentially a 1 percent boundary of SO$_2$. A mass balance of SO$_2$ in the plume cross section finds only 55 percent of the SO$_2$ that was emitted at the stack. It is suggested that much of the remaining 45 percent of the SO$_2$ could be found below 200 m, since the helicopters flew no lower than this (for safety) yet were still finding SO$_2$ at this level. The computer simulation at 600 sec is superposed on the experimental plume outline. Again, the computer trace represents about a 1 percent boundary of SO$_2$. Except for the two large "wings" of SO$_2$, the agreement is fairly good. The "wings" are likely produced by low frequency horizontal turbulent eddies generated in the region of the turning of the wind—but since the turbulence on the computer is assumed to be isotropic, this cannot be corrected in these runs in any simple way.
To put the computer and experimental results into perspective, a handbook calculation of the plume \( \text{SO}_2 \) is undertaken here. The trouble with the analysis of the plume of October 20 is to decide whether the stable or neutral conditions have the greatest effect on the behavior, since only one stratification can be used in handbook estimates. The plume rise and dispersion in an F class (stable inversion) is presented in Fig. 5.3.2.4. Note that the plume rise fits the data well, but the dispersion is too small (the dispersion is the 3\( \sigma \), or 1 percent level value). The plume rise and dispersion in a D class (neutral layer) is presented in Fig. 5.3.2.5. Note that the plume rise is too large, while the dispersion is fairly close to the actual, but is also not able to reproduce the "wings" of \( \text{SO}_2 \). It is seen that either single choice of stability does not agree as well as the computer simulation (which was able to follow the plume through both regions of stability). This generality in the computer simulations appears to be a major source of improvement over the handbook estimates.

The comparison of experimental and computational plume cross sections is continued in Fig. 5.3.2.6 for the plume at 10.0 km. The helicopter results have the jagged outline in Fig. 5.3.2.6. A mass balance of \( \text{SO}_2 \) yields only 29 percent of the emitted \( \text{SO}_2 \), which brings the experimental
Fig. 5.3.2.4 Comparison of Handbook Calculations and Helicopter Results at 4.8 km Downwind. Pasquill Stability Class F.
Fig. 5.3.2.5 Comparison of Handbook Calculations and Helicopter Results at 4.8 km Downwind. Pasquill stability class D.
Fig. 5.3.2.6 Comparison of computational and experimental results at 10.0 km downwind for the 20 Oct 67 Keystone #1 plume.
results into question. The computer simulation is superposed, but not much emphasis should be placed on the comparison since the helicopter results appear to be inaccurate on the basis of the low mass balance.

Two other tests of the model with the October 20 plume are found in Figs. 5.3.2.7 and 5.3.2.8. Four SO$_2$ bubblers were placed on a small hill at 65 m elevation above the stack base, at 6.5 km downwind. The bubbler 1/2 hour averages were all averaged together to yield a 12 pphm ground-level SO$_2$ concentration. The central region of the simulated plume cross section is copied in Fig. 5.3.2.7. Each SO$_2$ concentration represents the value in a single computer mesh cell. The dashed line is drawn through the plume at the 65 m elevation, where the 12 pphm experimental value compares very well with the predicted values inside the plume.

The entire simulation was carried to 12 km downwind. The maximum ground level SO$_2$ concentration is plotted at 2 km intervals in Fig. 5.3.2.8. Even at 12 km the SO$_2$ has not yet reached a maximum. However, the maximum SO$_2$ in the plume (calculated at 12 km) is 33 pphm, while the ground level is already 17 pphm—so the maximum calculated value will have to be between 17 and 33 pphm. A handbook estimate of the maximum ground level concentration (taken from Eq. 3.146 of Slade) yields 47 pphm at 17 km downwind in neutral D class
Fig. 5.3.2.7 Comparison of the computer simulation of the 20 Oct 67 Keystone #1 plume cross section with the half-hour average SO$_2$ concentration at 65 m. The values in the boxes are the mesh cell [SO$_2$] in pphm predicted by the code at 6.5 km downwind. An average [SO$_2$] of 12 pphm was recorded in four SO$_2$ bubblers at 65 m elevation and 6.5 km downwind. The dashed line at 65 m represents the bubbler elevation on the computer mesh.
Fig. 5.3.2.8 Maximum ground-level SO₂ concentrations predicted in the computer simulation of the 20 Oct 67 Keystone #1 plume.
stability (which is roughly an upper bound for this value) and 22 pphm at 90 km downwind in stable E-class stability (which is roughly a lower bound for this value). The calculated value must therefore fall somewhere between these handbook estimates which lends credence to the results, even though the actual maximum ground level $SO_2$ value was not calculated.

5.4 Results of Model Extension

5.4.1 Fumigation Episode

A computer simulation that approximates a fumigation episode is presented in this section. No particular episode is intended to be represented by this run, but several of the general features of a fumigation episode near a shoreline site in the Great Lakes area are included. These episodes are commonly characterized by a wind off of a large cool lake on a sunny spring day. The air that has traveled over the lake has developed a deep stable layer because of sensible heat exchange with the cool lake water. As this deep stable layer streams inland, the strong solar heating at the ground causes a deepening unstable thermal boundary layer to develop. This layer is characterized by strong mixing as vigorous turbulent thermal convection sets in. Plumes released in the stable air exhibit small plume rise and dispersion until they encounter the growing boundary layer
from below. Quite rapidly they have their pollutants spread to the ground, in a sense "fumigating" a relatively small area with high pollutant concentration.

A rough calculation was performed to demonstrate this. The plume in a stable inversion from Sec. 5.3.2 was released over a deepening turbulent layer coming up from the ground. The situation is shown in Fig. 5.4.1.1. At 0, 20, 50, 100, and 200 seconds the turbulent layer (eddy viscosity = 1000 ft$^2$/sec) is deepened by an increment of 100 meters--this is represented by the staircase in Fig. 5.4.1. The plume that is released at 0 km is about half engulfed in the turbulent layer at 1 km, and almost entirely engulfed at 2 km. The strong turbulent mixing has produced ground level concentrations a factor of 4 and 8 times higher at these stations than the results of Sec. 5.3.2. This agrees qualitatively with actual fumigation episode results, and serves to demonstrate the ability of the model to extend into these important cases. A more refined calculation of the boundary layer, and actual weather and plume data from a shoreline site would be needed to more carefully test this type of simulation.

5.4.2 Plumes with Change of Phase

Model validation has not been carried out for plumes
Fig. 5.4.1.1 Fumigation Episode at a Shoreline Site.
Cross sections are plume SO$_2$. Ground-level [SO$_2$] discussed in text.
with change of phase. The available Chalk Point data were incomplete during this work and could not be used. The balloon data from several mechanical draft towers at the Commanche plant\textsuperscript{74} suffers from a lot of scatter from a variety of sources, and data were only obtained very close to the towers, which casts doubt on the ability of the simulations to handle this case.

From preliminary work with saturated parcels of air on the computer mesh, the model is found to suffer from oscillations that are due to the explicit nature of the moisture equilibrium calculation. The oscillations can be brought under control by reducing the timestep size, but a more fundamental solution to this problem is recommended in Sec. 6.2.3.
6. CONCLUSIONS AND RECOMMENDATIONS

6.1 Model Validation

A widely applicable calculational model of buoyant bent over plumes has been developed. The advantage of the model is its ability to treat problems outside the scope of existing plume models without greatly increasing the resources required for the analyses. The acceptance of the model, however, must begin with a demonstration of its ability to reproduce the solutions to problems that are known to be solvable. This demonstration has proceeded along two lines in this work—problems in which the plume properties dominate the flow, and problems in which the atmospheric turbulent mixing dominates the flow. Some overlap between these simple regimes occurs, but overall this organization serves to highlight the causes of the particular successes and discrepancies in the model validation work.

The results of Sec. 5.2 deal mainly with the plume dominated motions. Generally it is found that very good agreement with laboratory experiments is obtained. In particular, the buoyant line-vortex motions and the Brunt-Vaisala period of a buoyant cylinder of fluid are studied, and they compare very favorably with the predictions. However, the
unsuccessful attempts to "tune" the turbulence model coefficients point out the rather limiting assumptions contained in the present turbulence model, particularly with regard to buoyant production of TKE. To the model's credit, it has been noted\(^7\) that wall-free turbulent flows are the most difficult to "tune," and that the model does a credible job in its current form.

The results of Sec. 5.3 deal mainly with the atmospheric dominated motions. There is a large amount of overlap into the plume-dominated motions in the Briggs plume rise and Pasquill dispersion results, but these cases both represent experiments that were actually performed in the atmosphere, and they exhibit a fair amount of scatter in their data because of this. Again, the agreement between calculation and experiment is good. The results of the LAPPES individual plume study provides the best indication of where the calculational model is expected to benefit the modelers of plumes. In the limited number of calculations contained in that section, it is found that the calculational model agrees with the experimental results more closely than the current handbook estimates simply because it has made a more fundamental calculation, taking into account the actual micrometeorological profiles. Furthermore, the model provides a relatively accurate starting point for the detailed description of other
important processes in a plume: chemical reactions, visibility, radiation dose rates, etc.

6.2 Recommendations

6.2.1 Calculational Scheme to Include Wind Shear Effects

A brief overview of a plausible calculational scheme that would address one of the important effects of wind shear on the plume dynamics is discussed here. The effect is that of the dilution of the plume properties as the plume rises into progressively stronger winds. The process is sketched in Fig. 6.2.1.1, and is well-known to plume modelers. A constant release of pollutant (illustrated in Fig. 6.2.1.1), momentum, sensible heat, moisture, etc., diluted into air that moves with a velocity $u(Z_0)$ will have a density proportional to the inverse of the velocity. A plume property that is released into a stronger wind, $u(Z)$, will be correspondingly more dilute. This effect is important in buoyant plumes when the plume updrafts and downdrafts in the presence of a wind shear cause parcels of the plume to change their downwind advection rate. Clearly, the problem is fully three-dimensional (though it can be in steady state), but a very restrictive assumption may afford a useful recasting of the two-dimensional problem. This assumption is discussed next.
$\chi(z) \sim R/u(z)$

$\chi(z_0) \sim R/u(z_0)$

$\chi(z_0) > \chi(z)$ for $u(z) > u(z_0)$

Fig. 6.2.1.1 Dilution of a Steady Release of Pollutant.
Consider the advection and turbulent diffusion of a pollutant in three dimensions (the results extend directly to momentum, sensible heat, etc.):

\[ \frac{\partial \chi}{\partial t} + u \frac{\partial \chi}{\partial x} + v \frac{\partial \chi}{\partial y} + w \frac{\partial \chi}{\partial z} = \gamma \chi \nabla^2 \chi \]  

(6.1)

Assuming that the system is in steady state, we have

\[ u \frac{\partial \chi}{\partial x} + v \frac{\partial \chi}{\partial y} + w \frac{\partial \chi}{\partial z} = \gamma \chi \nabla^2 \chi \]  

(6.2)

In the presence of a steady uniform wind field, \( u_o \), the first term is commonly interpreted as the time-rate-of-change for an observer moving with the wind, and is written as \( \frac{\partial \chi}{\partial t_o} \),

where \( u_o t_o = \chi \). This contains the important assumption that the plume **always** has the downwind velocity \( u_o \)--implying infinite accelerations at the stack exit, to be sure. In a strong wind field the downwind diffusion is commonly neglected with respect to the downwind advection, so the gradient operator has only \( y \) and \( z \) derivatives. If the wind field is allowed to have shears, then the first term may be represented as

\[ u(z) \frac{\partial \chi}{\partial x} = \frac{u(z)}{u(z_o)} \left( u(z_o) \frac{\partial \chi}{\partial x} \right) = \frac{u(z)}{u(z_o)} \frac{\partial \chi}{\partial t_o} \]  

(6.3)

where \( u_o \) has been arbitrarily chosen to be \( u(z_o) \). This interpretation allows the equation to be formulated as
This equation holds the assumption that any parcel of air in the plume, when advected into a region of stronger wind, immediately takes on the local wind velocity and is correspondingly diluted. Note that it also causes parcels that are decelerated to concentrate their properties, which is physically unrealistic, but hopefully is not too serious an error since plume rise and updrafts are almost always stronger than downdrafts. The important feature that this scheme hopes to address is the dilution (usually by about 10 to 50 percent) of plume buoyancy, momentum, and moisture, which affect the plume dynamics. The procedure could be extended to every transport equation in the equation set—only the effect on the divergence condition in the fluid mechanics algorithm has not been studied. Its satisfaction would still be required as a constraint on the solution.

6.2.2 Calculational Scheme for Time-Dependent Release or Weather

The simulation of "mildly" time-dependent plumes can be made with the model. Essentially, the governing assumption here is that the prevailing weather or effluent properties
will advect downwind, and never affect the flow that precedes or follows it. The situation is developed in Fig. 6.2.2.1, where a stack is assumed to have a set of exit properties, \( \Omega \), that are piecewise-constant in time over periods of 100 sec. To reconstruct the behavior, an initial simulation with the properties at time \( t_0 \), \( \Omega(t_0) \) is made to 300 sec. The plume properties changed at time \( t_0 \) to 100 sec, so a second simulation is made with properties \( \Omega(t_0 + 100) \) to 200 sec. Again the plume properties changed at time \( t_0 + 200 \) sec, so a third simulation is made with properties \( \Omega(t_0 + 200) \) to 100 sec. The actual plume is then "cut and pasted" from the pertinent data in the simulations as shown at the bottom of the figure. The calculation is somewhat wasteful, since 600 sec of simulation produces only 300 sec of results—but the scheme surely saves time and storage over a fully three-dimensional calculation. Eventually, for sufficiently "strong" time-dependence the scheme becomes too laborious with respect to a three-dimensional calculation.

6.2.3 Cloud Microphysics Model

The limited success of the equilibrium moisture thermodynamics model is due to its explicit differencing. In short, the model is ignorant of the latent heat released in a current timestep, and it adjusts the equilibrium conditions without
Fig. 6.2.2.1 Simulation of a Time-Dependent Plume in Steady-State Weather. Scheme is discussed in the text.
this knowledge. The resultant oscillations in the equilibrium conditions are not surprising, nor is the ability to control them with very small timesteps. If the calculation was made implicit--essentially iterating on the coupled latent heat release equation and Magnus' formula for liquid-vapor equilibrium--the timesteps could be relaxed back to their original size.

The prospect of incorporating a non-equilibrium moisture model is not investigated in this work. The limitations of the equilibrium model have not been sufficiently explored to justify the change at this point.
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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<tbody>
<tr>
<td>$A_0$</td>
<td>initial line-vortex area ($ft^2$)</td>
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<tr>
<td>$C$</td>
<td>experimental constant, 1.9</td>
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<tr>
<td>$C_p$</td>
<td>heat capacity at constant pressure (BTU/lb_m °R)</td>
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<td>$c_{moist}$</td>
<td>heat capacity of moist air at constant pressure (BTU/lb_m °R)</td>
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<tr>
<td>$D_T$</td>
<td>timestep size (sec)</td>
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<td>$D_Y$</td>
<td>cell width (ft)</td>
</tr>
<tr>
<td>$D_Z$</td>
<td>cell height (ft)</td>
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<tr>
<td>$e_{sat}(T)$</td>
<td>saturation vapor pressure of water (mb)</td>
</tr>
<tr>
<td>$E(i)$</td>
<td>energy of the $i^{th}$ decay channel from pollutant species $\chi$ (MeV)</td>
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<tr>
<td>$F(i)$</td>
<td>fractional energy deposition for $i^{th}$ radioactive decay channel from pollutant species $\chi$</td>
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<td>$g$</td>
<td>acceleration due to gravity ($ft/sec^2$)</td>
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<td>$I$</td>
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<td>$k$</td>
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<td>$L$</td>
<td>buoyancy parameter (ft)</td>
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<td>$L_{eddy}$</td>
<td>eddy length scale (ft)</td>
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<tr>
<td>$L_{vap}$</td>
<td>latent heat of vaporization of water (BTU/lb_m)</td>
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<td>$N$</td>
<td>experimental constant, 3.0</td>
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<tr>
<td>$\tilde{p}$</td>
<td>physically measurable pressure (millibars)</td>
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<tr>
<td>$P$</td>
<td>pressure perturbation about an adiabatic reference state (mb)</td>
</tr>
<tr>
<td>$P_0$</td>
<td>pressure in a quiet adiabatic atmosphere (mb)</td>
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</table>
\( \bar{p} \) \hspace{2cm} \text{time average pressure perturbation (mb)}

\( p' \) \hspace{2cm} \text{fluctuating pressure perturbation (mb)}

\( Pr \) \hspace{2cm} \text{Prandtl number}

\( q, q(y,z,t) \) \hspace{2cm} \text{turbulence kinetic energy per unit \( lb_m \) (ft}^2/\text{sec}^2)\)

\( q_{\text{library}}^{(z)} \) \hspace{2cm} \text{prescribed turbulence kinetic energy profile (ft}^2/\text{sec}^2)\)

\( Q \) \hspace{2cm} \text{heat (BTU)}

\( Q_H \) \hspace{2cm} \text{heat emitted at stack exit (BTU/sec)}

\( R(T) \) \hspace{2cm} \text{plume radius as a function of time (ft)}

\( R_{\text{dry}}, R_d \) \hspace{2cm} \text{gas constant for dry air (ft}^3 \text{ mb}/\text{lb}_m °\text{R})\)

\( R_{\text{vap}}, R_v \) \hspace{2cm} \text{gas constant for water vapor (ft}^3 \text{ mb}/\text{lb}_m °\text{R})\)

\( Sc_{\text{liq}} \) \hspace{2cm} \text{Schmidt number for liquid water}

\( Sc_{\text{vap}} \) \hspace{2cm} \text{Schmidt number for water vapor}

\( t, T \) \hspace{2cm} \text{time (seconds)}

\( t_0 \) \hspace{2cm} \text{x}/u_0 (sec)

\( T_* \) \hspace{2cm} \text{time coordinate of virtual origin (sec)}

\( T_\infty \) \hspace{2cm} \text{physically measurable temperature (°R)}

\( T \) \hspace{2cm} \text{temperature perturbation about an adiabatic reference state (°R)}

\( T_0 \) \hspace{2cm} \text{temperature in a quiet adiabatic atmosphere (°R)}

\( T_s \) \hspace{2cm} \text{temperature of stack effluent (°R)}

\( T_v \) \hspace{2cm} \text{virtual temperature (°R)}

\( T_{vo} \) \hspace{2cm} \text{virtual temperature in a quiet adiabatic atmosphere (°R)}

\( u \) \hspace{2cm} \text{downwind velocity (ft/sec)}

\( u_o, U \) \hspace{2cm} \text{windspeed, constant with height (ft/sec)}

\( u_{\text{eddy}} \) \hspace{2cm} \text{turbulent velocity scale in an eddy (ft/sec)}

\( \bar{u}, \ddot{u} \) \hspace{2cm} \text{velocity (ft/sec)}

\( u_i, u_j \) \hspace{2cm} \text{velocity (ft/sec)}
\( \bar{u}_i, \bar{u}_j \)  
\( u_i', u_j' \)  
\( \overline{u_i u_j} \)  
\( u_i', \theta' \)  
\( u_i', u_j', u_k' \)

- time average velocity (ft/sec)
- fluctuating velocity (ft/sec)
- Reynolds stress tensor \( (ft^2/sec^2) \)
- correlation of fluctuating velocity and temperature
- triple correlation of fluctuating velocity \( (ft^3/sec^3) \)
- crosswind velocity (ft/sec)
- geostrophic wind (ft/sec)
- vertical velocity (ft/sec)
- molecular weight of the pollutant species \( \text{(lb}_m/\text{lb}_m \text{-mole)} \)
- downwind distance (ft)
- cartesian coordinate (ft)
- crosswind distance (ft)
- height (ft)
- height coordinate of virtual origin (ft)
\( \alpha, \alpha_1 \)  
- turbulence constants

\( \gamma_L \)  
- reciprocal turbulent Schmidt number for liquid water

\( \gamma_T \)  
- reciprocal turbulent Prandtl number for heat

\( \gamma_V \)  
- reciprocal turbulent Schmidt number for water vapor

\( \gamma_X \)  
- reciprocal turbulent Schmidt number for pollutant

\( \Gamma \)  
- turbulence constant

\( \Gamma_1 \)  
- turbulence constant

\( \Gamma_d \)  
- dry adiabatic lapse rate (\(^\circ\)R/ft)

\( \varepsilon_h \)  
- eddy diffusivity of heat (ft\(^2\)/sec)

\( \varepsilon_m \)  
- eddy diffusivity of momentum (ft\(^2\)/sec)

\( \varepsilon_X \)  
- eddy diffusivity of pollutant (ft\(^2\)/sec)

\( \bar{\theta} \)  
- potential temperature (\(^\circ\)R)

\( \bar{\theta} \)  
- potential temperature perturbation about an adiabatic reference state (\(^\circ\)R)

\( \theta_o \)  
- potential temperature in a quiet adiabatic atmosphere (\(^\circ\)R)

\( \bar{\theta} \)  
- time average potential temperature (\(^\circ\)R)

\( \theta' \)  
- fluctuating potential temperature (\(^\circ\)R)

\( \theta_v \)  
- virtual potential temperature (\(^\circ\)R)

\( \theta_{v0} \)  
- virtual potential temperature in a quiet adiabatic atmosphere (\(^\circ\)R)

\( \bar{\theta}_v \)  
- time average virtual potential temperature (\(^\circ\)R)

\( \theta_v' \)  
- fluctuating virtual potential temperature (\(^\circ\)R)

\( \lambda_X \)  
- decay constant for \( i^{th} \) radioactive decay channel from pollutant species \( X \) (sec\(^{-1}\))
\( \mu \)  
dynamic viscosity (lbm/sec. ft)

\( \nu \)  
kinematic viscosity (ft\(^2\)/sec)

\( \rho_{\text{dry}} \)  
density of dry air (lbm/ft\(^3\))

\( \rho_{\text{liq}} \)  
liquid water density (lbm/ft\(^3\))

\( \rho_{\text{liq}} \)  
time average liquid water density (lbm/ft\(^3\))

\( \rho'_{\text{liq}} \)  
fluctuating liquid water density (lbm/ft\(^3\))

\( \rho_s \)  
density of stack effluent (lbm/ft\(^3\))

\( \rho_{\text{sat}} \)  
saturation water vapor density (lbm/ft\(^3\))

\( \rho_{\text{vap}} \)  
water vapor density (lbm/ft\(^3\))

\( \bar{\rho}_{\text{vap}} \)  
time average water vapor density (lbm/ft\(^3\))

\( \rho'_{\text{vap}} \)  
fluctuating water vapor density (lbm/ft\(^3\))

\( \sigma, \sigma(y, z, t) \)  
eddy viscosity (same as \( \epsilon_m \)) (ft\(^2\)/sec)

\( \sigma_{\text{library}}(z) \)  
prescribed eddy viscosity profile (ft\(^2\)/sec)

\( \chi \)  
pollutant density (lbm/ft\(^3\))
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13. S. Patankar, et. al., "Prediction of the Three-Dimensional Velocity Field of a Deflected Turbulent Jet," 


45. **Ibid.**, Chapter 18.7.

46. **Ibid.**, Chapter 12.


58. Ibid., Vol. 1, p 280.


68. Ibid., p. 37.


APPENDIX

Computer Code Listing
**** *
TO SET ELEMENTS OF REAL OR INTEGER ARRAYS TO ZERO. A1,A2,... * ERAS0010 0001
* ARE ARRAY NAMES AND N1,N2,... ARE INTEGER VALUES OR * ERAS0020 0002
* EXPRESSIONS GIVING THE ARRAY SIZES. * ERAS0030 0003
** I.E. - CALL ERASE(C,26*31,N,7*31,E,254) ** ERAS0040 0004
* ** ERAS0050 0005
*** ERAS0060 0006
* *** ERAS0070 0007
**** ERAS0080 0008

ERASE START 0
SAVE (14,12),*
BALR 12,0
USING *,12
SR 0,0
SR 2,2  PARAMETER LIST INDEX=0
L 6,=F'4'

E1 L 3,0 (2,1) LOAD 3 WITH ARRAY ADDRESS
L 4,4(2,1) LOAD 4 WITH ADDRESS OF ARRAY LENGTH
L 7,0 (4) LOAD 7 WITH ARRAY LENGTH-1 TIMES 4
SLA 7,2
SR 7,6
SR 5,5

E2 ST 0,0 (5,3) STORE ZERO
BXLE 5,6,E2
LTR 4,4 TEST FOR LAST ARGUMENT IN LIST
BM RETN
A 2,=F'8'
PICK UP NEXT ARGUMENT PAIR
B E1

RETN RETURN (14,12),T
END

INTEGER BUFL,CF,CF1,CFB,CFC,CFI,CFL,CFR,CFS,CFT,CQF,ERP,TD,VMP,
1 VTP
REAL NU,LIQ,LIQO,LIQ1,LOUT
DIMENSION CF (1),CQ (1),QCON (1),P (1),RX (1),RZ (1),TQ (1),TS (1),U (1),
1 W (1),ER (1),FFX3(132),FFX3(102),PBTIN (2),UO (1),WO (1),TQO (1),
2 TSO (1),SIE(1),SIEO (1),CHI (1),CHIO (1)
A,VAP (1),VAPO (1),LIQ(1),LIQO(1)

RGBMN60A 0032
RGBMN60A 0036
RGBMN60A 0031
RGBMN60A 0033
RGBMN60A 0034
RGBMN60A 0035
RGBMN60A 0036

PAGE 1
COMMON/PROP/SIGN
COMMON/EXTRA/NT3, NT4, NT5, T4MT3, T4MT4, T4MT5, T3N, T4N, T5N, COPBD
1COPBE, COPBF, COPTD, COPTE, COPTF, COPRD, COPRF, COPFL, COPLE,
2COPLE, OFOBTD, OFOBTE, OFOBTF, OFOBRE, OFOBRD, OFOBRF, IRESET,
*NCYCLS, TADD, NIV, IOBRAN
COMMON/INDEX/NWPC, K2NCL
COMMON/LARGE/DIFFCO(2400)

EQUIVALENCE (A(1), CF), (A(2), U), (A(3), W), (A(4), P), (A(5), TQ),
1 (A(6), TS), (A(7), ER, CO), (A(8), JO), (A(9), WO), (A(10), TQO),
2 (A(11), TS0), (A(12), SIE), (A(13), SIE0), (A(14), RX), (A(15), RZ),
3 (A(16), IICFR), (A(17), IICFL), (A(18), IICFT), (A(19), IICPB),
A (A(20), CHI), (A(21), CHIO).
B (A(22), VAP), (A(23), VAPO), (A(24), LIQ0), (A(25), LIQ0),
4 (ZERO1(1), ALP), (ZERO2(1), NT3), (ZERO3(1), AI), (ZERO4(1), DROU)

C  NOTF.  END - END OF NON-EXECUTABLE STATEMENTS

C  NOTF. NWPC = NUMBER OF WORDS PER MESH CELL
CALL ERASE (ZERO1(1), 1155, ZERO2(1), 608, ZERO3(1), 16, ZERO4(1), 14000)
NWPC=25 NWPCL=4 IVDI=5 IVDO=6

100 WRITE (IVDO, 1)
READ (IVDI, 2) IBR, KBR, IPRFM, NHCYCLS, TADD, IRESET
ERF=0 IF (IPRFM.GT.0) CALL FLMINI
IF (IBR.EQ.0) GO TO 700 IF (ERF.EQ.1) GO TO 700

400 PRINT 11 CALL VSET WRITE (IVDO, 3)
IF (ERF.EQ.1) GO TO 700 PRINT 12
CALL VM IF (ERF.EQ.1) GO TO 700
GO TO 100
700 IF (IPRPM.GT.0) CALL FLMPFIN
C ****** FORMATS ****** FORMATS ****** FORMATS ******
  1 FORMAT(1H1,22H MAIN PROGRAM CALLED )
  2 FORMAT (2(5X,15),7X,I2,I11,F10.4,5X,I5)
  3 FORMAT (1H ,27H SUBROUTINE VSET FINISHED .)
  11 FORMAT (1H ,25H SUBROUTINE VSET CALLED .)
  12 FORMAT (1H ,23H SUBROUTINE VM CALLED .)
STOP
END

BLOCK DATA
COMMON/LARGE/DIFFCO(2400)
REAL DIFFCO/2400.0*1.0/
END
SUBROUTINE IDLE
INTEGER WFL,CF,CF1,CFB,CFC,CFI,CFL,CFR,CFP,CFS,CFT,CPF,ERF,TD,VNTP,
  WTP
REAL NU,LIQ,LIQO,LIQI,LOUT,
DIMENSION CF(1),CQ(1),OCON(1),P(1),RX(1),RZ(1),TO(1),TS(1),U(1),
  W(1),ER(1),PPX3(102),PPY3(102),PBTIM(2),UO(1),WO(1),TO(1),
  TS(1),SIF(1),SIFC(1),CHI(1),CHIC(1),
  VAP(1),VAPO(1),LIQ(1),LIQO(1), LIQI(1)
!VAP(1),VAPO(1),LIQ(1),LIQO(1), LIQI(1)
 3,TFMP(25),FMP(25),TMYT1(25),T1N(25),TMYT2(25),T2N(25),
 4,COPBA(25),COPBB(25),COPBC(25),COPTA(25),COPTB(25),COPTC(25),
 5,COPRA(25),COPRB(25),COPRC(25),COPFA(25),COPFB(25),COPFC(25),
 6,OFOTSA(25),OFOTBA(25),OFOTBC(25),
 7,OFOTRA(25),OFOTBB(25),OFOTBC(25),TAU(10),USL(32),USLOB(20),
 8,USROB(20),USTOB(20),USBOR(20),
 9,COFD(25),COFE(25),COFTD(25),COFTE(25),COPTE(25),COFTP(25),
*COFBD(25),COFRE(25),COPLD(25),COFLE(25),COFRP(25),
  AOFOTDA(25),OFOTBE(25),OFOTBD(25),OFOTRE(25),
  B OFOTTP(25),OFOTBF(25),
CTMYT3(25),TMYT4(25),TMYT5(25),T3N(25),T4N(25),T5N(25),
* IICFR(1),IICFL(1),IICFPT(1),IICFPR(1)
  * ZERO1(1165),ZERO2(608),ZERO3(16),ZERO4(3)
DIMENSION ZSIE(22),ZTQ(22),ZTS(22),ZVP(22),ZLO(22),ZAP(22),WSP(22)
DIMENSION TRSTRT(5),WZSIP(100),WZTQ(100),WZTS(100)
ENTRY TAPEA
REWIND A
READ (8) A,ZERO1,ZERO2,ZERO4,NWPCL
WRITE (IVDO,50) TD,TIMET,NCYC
IDATIN=1
NCYCB=NCYC
IRSTR=1
C *****FORMATS ***** FORMATS ***** FORMATS ***** FORMATS *****
50 FORMAT(1H,19H TAPE FILE NUMBER =,I4,9H TIMET =,1PE12.4,
1 16H CYCLE NUMBER =,I6)
RETURN
ENTRY TAPWRI
TD=TD+1
ITW=ITAPW
REWIND A
WRITE (8) A,ZERO1,ZERO2,ZERO4,NWPCL
WRITE (IVDO,51) TD,TIMET,NCYC
C *****FORMATS ***** FORMATS ***** FORMATS ***** FORMATS *****
51 FORMAT(1H,19H TAPE FILE NUMBER =,I4,9H TIMET =,1PE12.4,
1 16H CYCLE NUMBER =,I6)
RETURN
ENTRY COARSE
C RESTART ON A COARSER MESH FOR IBR AND KBR EVEN ONLY
IHALF=IBP2/2
KHALF=KBP2/2
C MANAGES ATMOSPHERIC PROFILES DURING RESTARTS ON A COARSER MESH
DO 90 K=2,KHALF
ZTQ (K)=(ZTQ (2*K-2)+ZTQ (2*K-1))/2.0
ZTS (K)=(ZTS (2*K-2)+ZTS (2*K-1))/2.0
ZLQ (K)=(ZLQ (2*K-2)+ZLQ (2*K-1))/2.0
ZVP (K)=(ZVP (2*K-2)+ZVP (2*K-1))/2.0
ZAP (K)=(ZAP (2*K-2)+ZAP (2*K-1))/2.0
WSP (K)=(WSP (2*K-2)+WSP (2*K-1))/2.0
90 ZSIE (K)=(ZSIE (2*K-2)+ZSIE (2*K-1))/2.0
ZSIF (1)=ZSIE (2)
ZTS (1)=ZTS (2)
\[\text{ZTQ}(1) = \text{ZTQ}(2)\]
\[\text{ZLO}(1) = \text{ZLO}(2)\]
\[\text{ZVP}(1) = \text{ZVP}(2)\]
\[\text{ZAP}(1) = \text{ZAP}(2)\]
\[\text{WSP}(1) = \text{WSP}(2)\]
\[\text{KBP1} = \text{KHA LP1} + 1\]
\[\text{DO 95 K = KHP1, KBR1}\]
\[\text{ZTQ}(K) = \text{WZTQ}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZTS}(K) = \text{WZTS}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZLO}(K) = \text{WZLO}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZVP}(K) = \text{WZVP}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZAP}(K) = \text{WZAP}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{WSP}(K) = \text{WASP}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZSIE}(K) = \text{WZSIE}((\text{NRSTR} \times \text{KBR} / 2) + \text{K} - 1)\]
\[\text{ZSIF}(\text{KBP2}) = \text{ZSIF}(\text{KBP1})\]
\[\text{ZTS}(\text{KBP2}) = \text{ZTS}(\text{KBP1})\]
\[\text{ZTQ}(\text{KBP2}) = \text{ZTQ}(\text{KBP1})\]
\[\text{ZLO}(\text{KBP2}) = \text{ZLO}(\text{KBP1})\]
\[\text{ZVP}(\text{KBP2}) = \text{ZVP}(\text{KBP1})\]
\[\text{ZAP}(\text{KBP2}) = \text{ZAP}(\text{KBP1})\]
\[\text{WSP}(\text{KBP2}) = \text{WSP}(\text{KBP1})\]
\[\text{C PRECOMPUTES DATA ASSOCIATED WITH DZ, DX FOR USE IN VM}\]
\[\text{DX} = 2.0 * \text{DX}\]
\[\text{DZ} = 2.0 * \text{DZ}\]
\[\text{RDX} = 1.0 / \text{DX}\]
\[\text{RDZ} = 1.0 / \text{DZ}\]
\[\text{HD} = 0.5 * \text{DX}\]
\[\text{HDZ} = 0.5 * \text{DZ}\]
\[\text{RDZS} = 1.0 / (\text{DZ} * \text{DZ})\]
\[\text{BETA} = 0.5 * \text{R0} / ((\text{RD} * \text{RD} + \text{RDZ} * \text{RDZ})\]
\[\text{EPSB} = 4.0 * \text{NU} / \text{MIN1}((\text{DX}, \text{DZ})\]
\[\text{RDXDZS} = 1.0 / ((\text{RD} * \text{RD} + \text{RDZ} * \text{RD})\]
\[\text{X1} = \text{FLOAT}(\text{IBR}) * \text{DX}\]
\[\text{Z1} = \text{FLOAT}(\text{KBR}) * \text{DZ}\]
\[\text{RLENH} = 1.0 / \text{AMAX1}(\text{X1}, \text{Z1})\]
\[\text{C BEGINS CELL BY CELL AVERAGING}\]
DO 110 I=2,IBP1
DO 100 K=2,KBP1
IK=1+NWPC*(((I-1)*KBP2)+K-1)
IF(I.GT.THALF.OR.K.GT.KHALF) GO TO 200
C COMPUTES INDICES FOR FLUID CELLS
   J=2*(I-1)
   L=2*(K-1)
   IKR=1+NWPC*(((J-1)*KBP2)+L-1)
   J=2*I-1
   IKPR=1+NWPC*(((J-1)*KBP2)+L-1)
   K=2*J-1
   ICPR=1+NWPC*(((J-1)*KBP2)+L-1)
C COMPUTES FLUID CELL DENSITIES FOR CELL MASS AVERAGING
   CIT=CI-SIE(IKR)
   TEMPIL=SI(AI,BI,CIT,-1)
   CIT=CI-SIE(IPKPR)
   TEMPUL=SI(AI,BI,CIT,-1)
   CIT=CI-SIE(IKPR)
   TEMPUR=SI(AI,BI,CIT,-1)
   RHOLL=AR*TEMPL*TEMPL*BR*TEMPL+CR
   RHOLR=AR*TEMPL*TEMPLR*BR*TEMPLR+CR
   RHOLL=AR*TEMPL*TEMPLR*BR*TEMPLUL+CR
   RHOUR=AR*TEMPLR*TEMPLUR*BR*TEMPLUR+CR
   RHOSUM=RHIROL*RHOLR*RHOUl+RHOURL
C MASS AVERAGING OF FLUID CELLS FOR RESTART ON COARSER MESH
   U(IK)=(U(IK)*RHOLL+U(IPKPR)*RHOLR+U(IPKPR)*RHOUl+U(IPKPR))/RHOSUM
   V(IK)=(V(IK)*RHOLL+V(IPKPR)*RHOLR+V(IPKPR)*RHOUl+V(IPKPR))/RHOSUM
   W(IK)=(W(IK)*RHOLL+W(IPKPR)*RHOLR+W(IPKPR)*RHOUl+W(IPKPR))/RHOSUM
   AOSUM=RHIROL+RHIROL+RHOURL+RHOURL
A*RHOUR/RHOSUM  
TS(IK) = (TS(IPKR) + TS(IPKR) + TS(IPKR) + TS(IPKR)) / 4.00  
TSO(IK) = (TSO(IPKR) + TSO(IPKR) + TSO(IPKR) + TSO(IPKR)) / 4.0  
TQ(IK) = (TQ(IPKR) * RHOLL + TQ(IPKR) * RHOLL + TQ(IPKR) * RHOLL + TQ(IPKR) * RHOLL) / 4.00  
A*RHOUR/RHOSUM  
TQO(IK) = (TQO(IPKR) * RHOLL + TQO(IPKR) * RHOLL + TQO(IPKR) * RHOLL + TQO(IPKR) * RHOLL) / 4.0  
A*RHOUR/RHOSUM  
SIE(IK) = (SIE(IPKR) * RHOLL + SIE(IPKR) * RHOLL + SIE(IPKR) * RHOLL + SIE(IPKR) * RHOLL) / 4.00  
A*RHOUR/RHOSUM  
SIEO(IK) = (SIEO(IPKR) * RHOLL + SIEO(IPKR) * RHOLL + SIEO(IPKR) * RHOLL + SIEO(IPKR) * RHOLL) / 4.00  
P(IK) = 0.0  
GO TO 120  

C INITIALIZATION OF CELLS THAT WEREN'T IN THE PREVIOUS RUN  
200 U(IK) = 0.0  
UO(IK) = 0.0  
WO(IK) = 0.0  
SIE(IK) = ZSIE(K)  
SIEO(IK) = ZSIE(K)  
TS(IK) = ZTS(K)  
TSO(IK) = ZTS(K)  
TQ(IK) = ZTQ(K)  
TQO(IK) = ZTQ(K)  
CHI(IK) = BKGND  
CHIO(IK) = BKGND  
LIQ(IK) = ZLQ(K)  
LIQO(IK) = ZLQ(K)  
VAP(IK) = ZVAP(K)  
VAPO(IK) = ZVAP(K)  

RGBD55A  0.289  
RGBD55A  0.290  
RGBD55A  0.291  
RGBD55A  0.292  
RGBD55A  0.293  
RGBD55A  0.294  
RGBD55A  0.295  
RGBD55A  0.296  
RGBD55A  0.297  
RGBD55A  0.298  
RGBD55A  0.299  
RGBD55A  0.300  
RGBD55A  0.301  
RGBD70A  0.302  
RGBD70A  0.303  
RGBD70A  0.304  
RGBD70A  0.305  
RGBD55A  0.306  
RGBD55A  0.307  
RGBD55A  0.308  
RGBD55A  0.309  
RGBD55A  0.310  
RGBD55A  0.311  
RGBD55A  0.312  
RGBD55A  0.313  
RGBD55A  0.314  
RGBD55A  0.315  
RGBD55A  0.316  
RGBD55A  0.317  
RGBD55A  0.318  
RGBVM70A  0.319  
RGBVM70A  0.320  
RGBVM70A  0.321  
RGBVM70A  0.322  
RGBVM70A  0.323  
RGBVM70A  0.324  

PAGE  9
P (IK) = 0.0
100 CONTINUE
RETURN
ENTRY FILMCO
RETURN
ENTRY FLMCAL
RETURN
ENTRY FLMINI
RETURN
ENTRY FLMPIN
RETURN
ENTRY FLMGEN
RETURN
ENTRY WREQ
RETURN
ENTRY VRFLM
RETURN
END
FUNCTION SI (XTBL, YTBL, X, N)
COMMON/PROP/SIGN
DIMENSION XTLB(1), YTBL(1)
IF ( X .LT. 0 ) GO TO 230
IF (X .LT. XTLB(1)) GO TO 16
IF (X .GT. XTLB(N)) GO TO 31
DO 10 I = 1, N
IF (X .EQ. XTLB(I)) GO TO 21
IF (X .LT. XTLB(I)) GO TO 26
10 CONTINUE
16 J1 = 1
J2 = 2
GO TO 50
21 SI = YTBL(I)
GO TO 100
26 J1 = I-1
J2 = I
GO TO 50
31 J1 = N-1
J2 = N
50 SI=YTBL(J1) + (YTBL(J2) - YTBL(J1)) * (X-YTBL(J1)) / (YTBL(J2) - YTBL(J1))
100 RETURN
C NOTE. ROOTS OF QUADRATIC EQUATION - A*X**2 + B*X + C = 0.0
200 A=YTBL(1)
B=YTBL(1)
C=X
IF (A. NE. 0.0) GO TO 205
SI=-1.0*C/B
RETURN
205 CONTINUE
D=B*B - 4.*A*C
IF ( D ) 210,220,220
210 PRINT 211
RETURN
220 DS=SQR(D)
IF (SIGN) 224,224,226
224 SI = -1.0 * (B + DS) / (2.0 * A)
GO TO 230
226 SI = (DS - B) / (2.0 * A)
GO TO 230
230 CONTINUE
RETURN
C ***** FORMATS ***** FORMATS ***** FORMATS *****
211 FORMAT(1H,28H ERROR - ROOTS ARE COMPLEX .)
END
SUBROUTINE VRPT
DIMENSION TPT(50,50)
INTEGER BUFL,CF,CF1,CP,CP1,CPF,CPF,CPF1,CPF1,CFL,CF2,CF21,CF2P,CF2F,CPF2,CPF21,CPF2F
IVTP,CFOUT
REAL MU,LIQ,LIQ0,LIQ1,LOUT
DIMENSION UOUT(7),VOJT(7),IOUT(7),KOUT(7),CFOUT(7),QOUT(7),
1 SOUT(7),TOUT(7),XOUT(7),GOUT(7),LOUT(7)
DIMENSION CF (1),Q (1),QCON (1),P (1),RX (1),RZ (1),TQ (1),TS (1),U (1),
1 W (1),ER (1),FPX3(102),FPY3(102),PBTIM(2),UO (1),WO (1),TQO (1)
COMMON /VRMAT3/ AI, BI, CI, AR, BR, CR, AMU, BMU, CMU, AK, BK, CK, ACP, BCP, CCP

COMMON/PROP/SIGN
COMMON/EXTRA/NT3, NT4, NT5, TYMAT3, TYMAT4, TYMAT5, T3N, T4N, T5N, COPBD,
1COPBE, COPBF, COPTD, COFTD, COPTP, COPFD, COFTP, COPRE, COPFR, COPFLD, COPLE,
2COPLE, COP Те, ТОФБЕ, ТОФВЕ, ТОФЕ, ТОФБП, ТИРЕ, ТИСТ,
*N CYCLS, TADD, HIV, IV, IO BRAN
COMMON/INDEX/NWPCL, K2NCL
COMMON/PLMCON/ DROU, DROU, IPRFM
COMMON/LARGE/DIFPCO(2400)
EQUIVALENCE (A(1), CP), (A(2), U), (A(3), W), (A(4), P), (A(5), TQ),
1 (A(6), T5), (A(7), ER, CQ), (A(8), UO), (A(9), WO), (A(10), TQ0),
2 (A(11), TSO), (A(12), SIE), (A(13), SIEO), (A(14), RX), (A(15), RZ),
3 (A(16), IICFR), (A(17), IICPL), (A(18), IICPT), (A(19), IICFB),
A (A(20), CHI), (A(21), CHIO),
B (A(22), VAP), (A(23), VAPO), (A(24), LIQ), (A(25), LIQ0),
4 (ZERO 1(1), ALP), (ZERO 2(1), NT3), (ZERO 3(1), AI), (ZERO 4(1), DROU)

C NOTE. END - END OF NON-EXECUTABLE STATEMENTS.

C PRODUCES A CELL BY CELL OUTPUT OF STORED VARIABLES (22 X 22 ONLY)

WRITE (IVDO, 5)
96 DO 103 ILOOP=1, 4
I REST=(ILOOP-1)*5
97 DO 102 KLOOP=1, 5
K REST=(KLOOP-1)*5
98 DO 100 KIN=1, 5
K=23-KIN-KREST
IF (K.EQ.0) GO TO 101
DO 99 IPART=1, 7
I=IP ART+1 REST
IK=1+NWPC*(((I-1)*KBP2)+K-1)
OUT (IPART)=U (IK)
V OUT (IPART)=W (IK)
T OUT (IPART)=I
K OUT (IPART)=K
C F OUT (IPART)=C F (IK)
Q OUT (IPART)=TQ (IK)
SOUT(IPART)=TS(IK)
XOUT(IPART)=CHI(IK)
GOUT(IPART)=VAP(IK)
LOUT(IPART)=LIQ(IK)
SIEC=SIE(IK)
CIT=C1-SIEC
TOUT(IPART)=SI(AI,BI,CIT,-1)
IF(CF(IK)<GE.30) TOUT(IPART)=P(IK)
99 CONTINUE
WRITE(IVDO,20) (VOUT(L),L=1,7)
WRITE(IVDO,10)
WRITE(IVDO,30) (IOUT(L),KOUT(L),L=1,7)
WRITE(IVDO,40) (TOUT(L),L=1,7)
WRITE(IVDO,50) (CFOUT(L),UOUT(L),L=1,7)
WRITE(IVDO,70) (SOUT(L),L=1,7)
WRITE(IVDO,60) (QOUT(L),L=1,7)
WRITE(IVDO,80) (XOUT(L),L=1,7)
WRITE(IVDO,90) (GOUT(L),L=1,7)
WRITE(IVDO,90) (LOT(L),L=1,7)
100 CONTINUE
101 WRITE(IVDO,7) TIMET,NCYC,ITER,DT
WRITE(IVDO,5)
102 CONTINUE
103 CONTINUE
RETURN
5 FORMAT('1')
7 FORMAT(1H,5HTIME=,1PE12.4,3H , ,14HCYCLE NUMBER =,15,3H , ,
12H PRESSURE ITERATION NUMBER =,14,3H , ,4HDT =,E12.4)
10 FORMAT('1',7('X',17X))
20 FORMAT('1',7(5HXXXXX,1X,F7.3,1X,4HXXXXX))
30 FORMAT('1',7(1HX,5X,'(',I2,'I2,')',5X))
40 FORMAT('1',7(1HX,3X,F7.3,1X,'',F',4X))
50 FORMAT('1',7(1HX,3X,F7.3,1X,F',4X'))
60 FORMAT('1',7(1HX,2X,TKE=',1PE10.3,1X))
70 FORMAT('1',7(1HX,2X,'TNU=',1PE10.3,1X))
C NOTE. END - END OF NON-EXECUTABLE STATEMENTS.
C
C NOTE. VSMT IS RESPONSIBLE FOR MESH, PARTICLE AND FILM INITIALIZATION.
C
IDATIN=0
IF( IBR.EQ.0 ) CALL TAPRSA
C NOTE. READS, WRITES PRIMARY INPUT DATA.
READ (IVDI, 1) LABEL

PAGE 16
READ (IVDI,2) DT,TPRT,TPLT,TWTD,TFIN,ITAPW,NPRT,IDIAG,LPR,IOBS
1,IDG,KG
WRITE (IVDO,50) IBR,KBR,IPRFM,NCYCLS,TADD,IRESET
WRITE (IVDO,1) LABEL
WRITE (IVDO,51) DT,TPRT,TPLT,TWTD,TFIN,ITAPW,NPRT,IDIAG,LPR,IOBS
1,IDG,KG
RDT=1./DT
IF (IPRFM.LT.1) TPLT=2.*TFIN
TPL=TPLT
TPR=TPRT
TDD=TWTD
IF (IDATIN.LT.1) GO TO 100
TIMET=TIMET+TADD
TWTD=TIMET
TPRT=TWTD
TPLT=TPRT
CALL MESHMK
IF (IPRFM.LT.1) GO TO 500
CALL FILGEN
CALL FILMC0
GO TO 500

C NOTE. INITIALIZES CONSTANTS.
100 TIMET=0.0
IRSTRT=0
TD=0
NCYC=0
NCYCB=0
EM6=1.E-6

C NOTE. INITIALIZES CELL INDEX QUANTITIES.
IBP1=IBR+1
KBP1=KBR+1
IBP2=IBR+2
KBP2=KBR+2
I2K2=IBP2*KBP2*NWPC
KNC=KBR*NWPC
K2NC=KBP2*NWPC
K2NCL = KBP2 * NWPC1
IKP2=IBR*K2NC  VRS12420  0613
IKMK = I2K2 + 2*K2NC  0614
RIKKB=1./FLOAT(IBR*KBR)  0615
C NOTF. GENERATES BOTH MESH AND FILM REGIONS, RESPECTIVELY.
CALL MESHMK
IF( IPRFM.LT.1 ) GO TO 2000
CALL FILMEN
CALL FILMCO
2000 WRITE(IVDO,60)  0618
500 K2NCL=KBP2*NWPC1
WRITE(IVDO,70)  0619
WRITE(IVDO,80)  0620
I1=2
K1=2
I2=IBP1  0621
K2 = KBP1
KBL = 0
KK = 0
DO 510 I=I1, I2
KK = KK + K2NC
KBL = KBL + K2NCL
LWPC = 1
LWPCL = 1
DO 510 K=K1, K2
LWPC = LWPC + NWPC
LWPCL = LWPC + NWPC
IK = KK + LWPC
IKL = KBL + LWPC
IKP = IK + K2NC
IKM = IK - K2NC
IKP = IK + NWPC
IKM = IK - NWPC
CPF = CP(IK)
CPX = CP(IKP)
CPF = CP(IK)
PAGE 18
CFT = CF(IKP)
CPB = CF(IKM)
IF (CFC.NE.1) GO TO 510
IF (CFP.NE.1) DIFPCO(IKL) = 0.0
IF (CFP.NE.1) DIFPCO(IKL+2) = 0.0
IF (CFC.NE.1) DIFPCO(IKL+1) = 0.0
IF (CFP.NE.1) DIFPCO(IKL+3) = 0.0
DCR = DIFPCO(IKL)
DCT = DIFPCO(IKL+1)
DCL = DIFPCO(IKL+2)
DCB = DIFPCO(IKL+3)
WRITE(IVDO,75) I,K,IKL,CFC,CFP,CPL,CPB,DCR,DCT,DCL,DCB
510 CONTINUE
511 CONTINUE
520 RETURN
C ****** FORMATS ****** FORMATS ****** FORMATS ******.
 1 FORMAT(20A4)
 2 FORMAT(5F8.3,5I2,2I3)
50 FORMAT(1H4X,4HIBR=,I5/,5X,4HKB=,I5/,3X,6HIPRF=,I2/,5X,
  8HNCYCLST=,I10/,5X,5HTADD=,E12.5,5X,7HIRES=,I5)
51 FORMAT(1H5X,3HD=,1PE12.5/4X,5HTPR=,E12.5/4X,5HTPL=,E12.5/
  4X,5HTWD=,E12.5/4X,5HTFIN=,E12.5/3X,6HTAPW=,I2/4X,5HNPRT=,I2/
  2X6HIDIA=,I2/5X,4HLPR=,I2/4X,5HIOBS=,I2/5X,4HIDG=,I3/5X,4HKDG=,
  3I3)
52 FORMAT(1H104H ** ERROR 001 - MESH ARRAY A() IS DIMENSIONED TOO
  SMALL FOR MESH PARAMETERS, I.E. IFR AND KBR. ***)
60 FORMAT(1H16,63H NOTE: COMPLETION OF VSET - VARR II SET UP G
  ENEATION .)
70 FORMAT(1H1)
75 FORMAT(1H916,4F6.1)
99 FORMAT(1H5X,1HJ,5X,1HK,4X,2HIK,3X,3HKL,3X,3HFC,3X,3HFCF,3X,
  1 3HCP,3X,3HCL,3X,3HCFB,3X,3HDCR,3X,3HDCT,3X,3HDC,3X,3HDCB)
END
SUBROUTINE MESHMK
INTEGRAL TW PL,CP,CPI,CPB,CF,CPI,CPL,CPF,CFS,CFT,CQF,ERF,TD,VTIP,
  1 VTP
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<th>REAL</th>
<th>LIQ</th>
<th>LIQO</th>
<th>LIQF</th>
<th>LOUT</th>
<th>RGBMN60A</th>
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<td>TIMT4, TISOSE, TPL, TPLT, TRPT, TRPT, TO, TSD, TTD, TWD, U, W,</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>USR (32), USTOB (22), USB (22), USO (10), FXF3, FFY3,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>AN, AW, CW, EPSB, UBLI, UBRi, WBBI, WBTI, WEPS, WOBI, NTPAS, TGAM, CSUBP,</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>T0, SIE, IDG, KDG, TI, MAT, EHOQ, AT, TNU, TK, TMTF, FN, TMT1, TIN, TNYMT2,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T2N, PFRAN, NRESX, NFLOW, NT1, NT2, TSTEP, KDBRC, UDBE, COPBA, COPBB,</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>COFBC, COPTA, COPTB, COPTC, COFRA, COPPB, COPRC, COPLA, COPLB, COPLC</td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
NFLOW = -NFLOW
190 CONTINUE
READ (IVDI, 12) (TMYF(I), FN(I), I=1,NFLOW )
READ (IVD1, 12) (TMT1(I), T1N(I), I=1,MT1 )
READ (IVDI, 12) (TMYT2(I), T2N(I), I=1,NT2 )
IF (NT3.EQ.0) GO TO 195
READ (IVDI, 12) (TMYT3(I), T3N(I), I=1,NT3)
IF (NT4.EQ.0) GO TO 195
READ (IVDI, 12) (TMYT4(I), T4N(I), I=1,NT4)
IF (NT5.EQ.0) GO TO 195
READ (IVDI, 12) (TMYT5(I), T5N(I), I=1,NT5)
195 CONTINUE
IF (NTAU.LT.1) GO TO 200
READ (IVDI, 12) (TAU(I), I=1,NTAU )
C NOTE. READ COEFFICIENTS A, B, AND C FOR THE BOTTOM EXTERIOR BOUNDARY.
200 READ (IVDI, 13) I,COPA,COPB,COPC,COPD,COFE,COFF
IF (I.LT.1) GO TO 210
COPA(I) = COPA
COPB(I) = COPB
COPC(I) = COPC
COPD(I) = COPD
COFE(I) = COFE
COFF(I) = COFF
WRITE (IVDO, 64) I, COPA(I), COPB(I), COPC(I), COPD(I), COFE(I), COFF(I)
1 COFF(I)
GO TO 200
C NOTE. READ COEFFICIENTS A, B, AND C FOR THE TOP EXTERIOR BOUNDARY.
210 READ (IVDI, 13) I,COPA,COPB,COPC,COPD,COFE,COFF
IF (I.LT.1) GO TO 220
COPA(I) = COPA
COPB(I) = COPB
COPC(I) = COPC
COPD(I) = COPD
COFE(I) = COFE
COFF(I) = COFF
WRITE (IVDO, 64) I, COPA(I), COPB(I), COPC(I), COPD(I), COFE(I)
1 COPTF(I)  
GO TO 210
C NOTE. READ COEFFICIENTS A, B, AND C FOR THE RIGHT EXTERIOR BOUNDARY.
220 READ (IVDO, 13) I, COFA, COFB, COFC, COFD, COFE, COFF
IF ( I.LT.1 ) GO TO 230
COFR (I) = COFA
COFRB (I) = COFB
COFRC (I) = COFC
COFRD (I) = COFD
COFRE (I) = COFE
WRITE (IVDO, 64) I, COFA, COFB, COFC, COFD, COFE, COFF
1 COFRF(I)
GO TO 220
C NOTE. READ COEFFICIENTS A, B, AND C FOR THE LEFT EXTERIOR BOUNDARY.
230 READ (IVDO, 13) I, COFA, COFB, COFC, COFD, COFE, COFF
IF ( I.LT.1 ) GO TO 240
COFL (I) = COFA
COFLB (I) = COFB
COF LC (I) = COFC
COFLD (I) = COFD
COFLE (I) = COFE
WRITE (IVDO, 64) I, COFLA (I), COFLB (I), COFLC (I), COFLD (I), COFLE (I).
1 COFLF(I)
GO TO 230
C NOTE. READ COEFFICIENTS A, B, AND C FOR THE TOP INTERIOR OBSTACLE.
240 READ (IVDO, 13) I, COFA, COFB, COFC, COFD, COFE, COFF
IF ( I.LT.1 ) GO TO 250
OFOBTA (I) = COFA
OFOB TB (I) = COFB
OFOBTC (I) = COFC
OFOBD (I) = COFD
OFOBTE (I) = COFE
OFOBT F (I) = COFF
WRITE (IVDO, 64) I, OFOBTA (I), OFOB TB (I), OFOBTC (I), OFOBD (I),
1000 E (I), OPBTF(I)
GO TO 240

C NOTE. READ COEFFICIENTS A, B, AND C FOR THE RIGHT INTERIOR OBSTACLE.

250 READ (IVDO, 13) I, COFA, COFB, COFC, COFD, COFE, COFF
IF (I.LT.1) GO TO 310
OPOBRA(I) = COFA
OPOBRC(I) = COFB
OPOBRD(I) = COFC
OPOBRF(I) = COFD
OPOBRE(I) = COFE
OPOBRI(I) = COFF
WRITE (IVDO, 64) I, OPOBRA(I), OPOBRC(I), OPOBRD(I), OPOBRE(I), OPOBRI(I)
1000 E (I), OPBTF(I)
GO TO 250

310 READ (IVDO, 14) I, K, RXC, RZC
WRITE (IVDO, 65) I, K, RXC, RZC
IF (I.LT.1) GO TO 320
IK = (K-1) * NWPC + (I-1) * K2NC + 1
RX(IK) = RXC
RZ(IK) = RZC
GO TO 310

320 CONTINUE
WRITE (IVDO, 50) DX, DZ, GZ, ALX, ALZ, CYL, B0, EPS, VMIN
WRITE (IVDO, 51) KWR, KWL, KWT, KWB, PSLIP, ALP, GAM, ALP0, GAM1, NU, TQJET
* TSJET
WRITE (IVDO, 59) AAW, BAW, C AW, W E PS, KDER BC, UBR I, UBLI, WBTI, WBBI
WRITE (IVDO, 58) WOBI, UOBI, CSUBPO
WRITE (IVDO, 60) TGAM, TO, TI, TSTEP, MAT, NRESX
WRITE (IVDO, 52) AI, BI, CI, AR, BR, CR, AMU, BMU, CMU
WRITE (IVDO, 53) AK, BK, CK, ACP, BCP, CCP, SIGN
WRITE (IVDO, 61) MPLOW, NT1, NT2, NTAU
WRITE (IVDO, 57) ( TAU(I), I = 1, NTAU )
NMAX = AMAX0( MPLOW, NT1, NT2 )
WRITE (IVDO, 62)
DO 319 I = 1, NMAX
WRITE (IVDO, 63) I, TYPF(I), FN(I), TYMT1(I), T1N(I), TYMT2(I), T2N(I)

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319 CONTINUE
   NMAX=AMAX0(NT3,NT4,NT5)
   DO 321 I=1,NMAX
   WRITE(IVDO,66) TYMT3(I),T3N(I),TYMT4(I),T4N(I),TYMT5(I),T5N(I)
321 CONTINUE
C NOTE. GENERATION OF MESH CELL SIZES
   RDX=1./DX
   RDZ=1./DZ
   HDX=.5*DX
   HDZ=.5*DZ
   RDZS=1./(DZ*DZ)
   BETA=.5*B0/(RDX*RDX + RDZ*RDZ)
   IF( KDERBC.GT.0 ) FSLIP=1.0
   IF( CYL.GT.1.E-6 ) KWL=1
   EPSB=4.*NU/AMIN1( DX, DZ )
   NTPAS=1
   IF( ALX.LT.EM6 .OR. ALZ.LT.EM6 ) NTPAS=2
   RDZDZS=1./(RDX*RDX + RDZ*RDZ)
   X1=FLOAT( IBR )*DX
   Z1=FLOAT( KBR )*DZ
   RLENGTH=1./AMAX1( X1,Z1 )
   EPS0=EPS
   TP=TI + 459.7
C NOTE. CALCULATION OF SPECIFIC MATERIAL FOR SIE INITIAL AND RHOO
   GO TO( 400,420,440,460 )MAT
C NOTE. COMPUTATION FOR SODIUM MATERIAL
900 SIIII=0.38935*TR - 0.553E-4*TR**2 + 0.11378E-7*TR**3 - 29.02
   RHOO=59.566 - 7.9504E-3*TI - .28728E-6*TI**2 + 0.06035E-9*TI**3
   RHOO=59.566 - 7.9504E-3*TI - 0.28728E-6*TI**2 + 0.06035E-9*TI**3
   AT=397.17/TR + 1.0203
   TMU=(10.0**AT/3600.)/TR**0.4925
   NU=TMU/RHOO
   TK=0.015085 - 5.2167E-6*TI + 5.809E-10*TI**2
   CSUBP=0.38935 - 1.106E-4*TI + 0.341E-7*TI**2
   RPRA=TK/( CSUBP*TMU )
   GO TO 500
C NOTE. COMPUTATION FOR WATER MATERIAL.

420 SI=I=1.074*TI - 32.0 13
    RHOI = 62.742 - 0.372E-2*TI - 0.44E-4*TI**2
    RHO  = 62.742 - 0.372E-2*TI - 0.44E-4*TI**2
    BT=44.6*(TI+207.0) - 5.0
    TMU=1.622*10**BT
    NU=TMU/RHOI
    TK=8.369E-5 + 2.368E-7*TI - 5.89E-10*TI**2
    CSUBP=1.0004
    RPRAN=TK/(CSUBP*TMU)
    GO TO 500

440 SI=II=AI*TI*TI + BI*TI + CI
    RHOII=AR*TI*TI + BR*TI + CR
    RHOO = AR*TO*TO + BR*TO + CP
    TMU = AMU*TI*TI + BMU*TI + CMU
    TK  = AK*TI*TI + BK*TI + CK
    CSUBP=ACP*TI*TI + DCP*TI + CCP
    NU=TMU/RHOII
    RPRAN=TK/(CSUBP*TMU)
    GO TO 500

460 CONTINUE
    NU=TMU/RHOII
    RPRAN=TK/(CSUBP*TMU)

C NOTE. NI=NUMBER OF LEFT MOST CELL, NR=NUMBER OF RIGHT MOST CELL,
C NOTE. GENERATION OF INTERIOR MESH CELLS, I.E. FLUID AND OBSTACLE.

500 IF (IDATIN.GT.0. AND. IRESET.EQ.0) GO TO 590
    READ(IVDI,5) NL, NR, NB, NT, ICETY
    WRITE(IVDI,54) NL, NR, NB, NT, ICETY
    TP( NLEQ. ) GO TO 700
    READ(IVDI,6) SI, IQ, TS, UI, W, C, VA, LI
    WRITE(IVDI,55) SI, IQ, TS, UI, W, C, VA, LI
    I1=NL
    I2=NR
    K1=NB
    K2=NT
    KK=1 + (I1-2)*K2NC

RGMK60A
R3GMK60A

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DO 589 I=I1,I2
KK=KK + K2 NC
LWPC=(K1-2)*NWPC
DO 579 K=K1,K2
LWPC=LWPC + NWPC
IK=KK + LWPC
CF(IK) = ICELTY
C NOTE. FOR OBSTACLES WITH TAU FACTORS - SET SIEI = OBSTACLE TEMPERA -
C NOTE. TURE IN F DEGREES .
SIE(IK)=SIEI
IF( ICELTY.GE.30 .AND. NTAU.GT.0 ) P(IK)=SIEI
TQ(IK)=TQI
TS(IK) =TSI
U(IK)=UI
W(IK)=WI
CHI(IK)=CHII
VAP(IK)=VAPI
LIQ(IK)=LIQI
SIEO(IK) =SIE (IK)
TQQ(IK) =TQ(IK)
TSS(IK)=TS (IK)
UO (IK) =U (IK)
WO (IK)=W (IK)
CHIO(IK) =CHI(IK)
VAPO (IK) =VAP(IK)
LIQO (IK) =LIQ(IK)
578 CONTINUE
579 CONTINUE
589 CONTINUE
GO TO 500
590 CONTINUE
C NOTE. GENERATION OF EXTERIOR BOUNDARY MESH CELLS .
700 I1=1
TSMAX=-1.0E+20
TMAX=TSMAX
WMAX=TMAX
UMAX=WMAX
TSMIN=+1.0E+20
TMIN=TSMIN
WMIN=TMIN
UMIN=WMIN
TQMAX=-1.0E+20
I2=IBP2
K1=1
K2=KBP2
KK=1+(I1-2)*K2NC
DO 789 I=I1,I2
KK=KK+K2NC
FWPC=(K1-2)*NWPC
DO 779 K=K1,K2
FWPC=FWPC+NWPC
IK=KK+FWPC
UMAX=AMAX1(UMAX,U(IK))
WMAX=AMAX1(WMAX,W(IK))
UMIN=AMIN1(UMIN,U(IK))
WMIN=AMIN1(WMIN,W(IK))
TSMAX=AMAX1(TSMAX,TS(IK))
TSMIN=AMIN1(TSMIN,TS(IK))
TQMAX=AMAX1(TQMAX,TQ(IK))
CFC=CP(IK)
IF( K.EQ.K1 .AND. CFC.LT.11 ) CF(IK)=10
IF( K.EQ.K2 .AND. CFC.LT.11 ) CF(IK)=10
IF( I.EQ.I1 .AND. CFC.LT.11 ) CF(IK)=10
IF( I.EQ.I2 .AND. CFC.LT.11 ) CF(IK)=10
IF( I.EQ.I1 .AND. K.EQ.K1 ) CF(IK)=2
IF( I.EQ.I1 .AND. K.EQ.K2 ) CF(IK)=2
IF( I.EQ.I2 .AND. K.EQ.K1 ) CF(IK)=2
IF( I.EQ.I2 .AND. K.EQ.K2 ) CF(IK)=2
IF( CFC.LT.20 .OR. I BTS.EQ.0 ) GO TO 770
C NOTF. FLAGS CPLLS SURROUNDING THE OBSTACLE CELL.
CFR=CP(IK+K2NC)
CFL=CP(IK-K2NC)
CFT=CF(IK+NWPC)
CPF=CF(IK-NWPC)
IICPP(IK)=1
IICFL(IK)=1
IICPT(IK)=1
IICPB(IK)=1
IF (CPF NE.1) IICPP(IK)=0
IF (CFL NE.1) IICFL(IK)=0
IF (CPT NE.1) IICPT(IK)=0
IF (CBF NE.1) IICPB(IK)=0
770 CONTINUE
779 CONTINUE
789 CONTINUE
RETURN
C ***** FORMATS ***** FORMATS ***** FORMATS ***** FORMATS *****
1 FORMAT (10F8.3)
2 FORMAT (4I2,4F8.3)
5 FORMAT (4I5,4I2)
6 FORMAT (8F9.3)
7 FORMAT (4F9.3,4I2,4F9.3)
8 FORMAT (3F9.3)
10 FORMAT (4F9.3,2I2)
11 FORMAT (7X,I3,5(5X,I3),7X,I3)
12 FORMAT (AF8.3)
13 FORMAT (3X,I3,2X,4F9.3)
14 FORMAT (2(3X,I3),2(5X,F8.3))
50 FORMAT (1H,5X,3HDX=,1PE12.5/6X,3HDX=,E12.5/6X,3HGZ=,E12.5/6X,3HGX=,E12.5/
1 6X,3HGZ=,E12.5/5X,4HALX=,E12.5/5X,4HALZ=,E12.5/5X,4HCYL=,E12.5/
2 6X,3HBO=,E12.5/5X,41EPS=,E12.5/4X,5HVMIN=,E12.5)
51 FORMAT (1H,4X,4HKX=,I2/5X,4HKX=,I2/5X,4HKW=,I2/5X,4HKW=,I2/
1 3X,6HFL=,1PE12.5/5X,4HALP=,E12.5/5X,4HGA=,E12.5/4X,5HALPO=,
2E12.5/4X,5HGA=,E12.5/6X,5HGY=,E12.5/3X,6HTJQJET=,E12.5/3X,
36HTJET=',E12.5)
52 FORMAT (1H,5X,3HAI=,1PE12.5/6X,3HBI=,E12.5/6X,3HCI=,E12.5/
1 6X,3HAR=,E12.5/6X,3HRB=,E12.5/6X,3HCR=,E12.5/5X,4HNU=,E12.5/
2 5X,4HBMU=,E12.5/5X,4HCUMU=,F12.5)

R3B MK6 OA

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| FORMAT | (IH ,5X,3HAK=,1PE12.5/6X,3HBK=,E12.5/6X,3HCK=,E12.5/5X,  |
|        | 14HACP=,E12.5/5X,4HBCP=,E12.5/5X,4HCCP=,E12.5/5X,5HSIGN=,E12.5)  |
| FORMAT | (IH ,3HNL ,15,3HNR ,15,3HBV ,15,3HNT ,15,8HICETYP ,12) |
| FORMAT | (IH ,3X,5HSEI=,1PE12.5/5X,4HTQI=,E12.5/5X,4HTSI=,E12.5/  |
|        | 16X,3HUT=,E12.5/5X,3HWI=,E12.5/5X,4HCHI=,E12.5/5X,4HVAP=,E12.5/5X,4RGBNM60A  |
|        | 2HLIQ=,E12.5) |
| FORMAT | (IH ,20H TAU FOR OBSTACLES =,7(2X,1PE12.5)  |
| FORMAT | (IH ,3X,5HWOBI=,1PE12.5/4X,5HUBI=,E12.5/1X,8HCSUBPOB=,  |
|        | 1 E12.5) |
| FORMAT | (IH ,5X,3HAW=,1PE12.5/6X,3HBB=,E12.5/6X,3HCC=,E12.5/  |
|        | 1 4X,5HWEPS=,E12.5/2X,7HKDERBC=,I2/4X,5HUBRI=,E12.5/4X,5HUBLI=,  |
|        | 2 E12.5/4X,5HWTBI=,E12.5/4X,5HWTBMI=,E12.5) |
| FORMAT | (IH ,3X,5HTGAM=,1PE12.5/6X,3HTO=,E12.5/6X,3HTI=,E12.5/  |
|        | 1 3X,6HTSTEP=,E12.5/5X,4HMAT=,I2/1X,8HNRSEXP=,I2) |
| FORMAT | (IH ,7H NFLOW ,1I3,5H NT1 ,I3,5H NT2 ,I3,5H NT3 ,I3,5H NT4 ,  |
|        | 1 I3,5H NT5 ,I3,6H NTAU ,I3) |
| FORMAT | (IH ,3X,1HI ,9X,4HTYMP ,12X,2HFN ,11X,5HTYTM1 ,11X,3HT1N ,11X,  |
|        | 1 5HTYTM2 ,11X,3HT2N) |
| FORMAT | (IH ,2X,1I3 ,2X,6(2X,1PE11.4,2X)) |
| FORMAT | (IH ,3H I ,I3,2X ,6F8.3) |
| FORMAT | (IH ,3H I ,I3,3H K ,I3,5H R XC ,F8.3,5H R ZC ,F8.3) |
| FORMAT | (IH ,///,22X,6(2X,1PE11.4,2X)) |

END

SUBROUTINE VM
INTEGER HUPL, CF, CF1, CFB, CFY, CFZ, CFP, CFT, CQF, ERP, TD, VMTP,
1 WTP
REAL NU, LIQ, LIQO, LIQI, LOUT
REAL LIQ, LIQO, LIQI, LIQG, LIQCO
DIMENSION EFRAC(5), ELAM(5), ELAM(5)
DIMENSION CF(1), CQ(1), QCON(1), P(1), RX(1), RZ(1), Q(I), TS(1), U(1),  |
1 W(1), ER(1), PFY(102), FFY(102), PBNTM(2), WO(1), WQ(1), TQO(1),  |
2 TS(1), SIE(1), SIEC(1), CHI(1), CHIO(1) |
A, VAP(1), VAPV(1), LIQ(1), LIQO(1) |
3 , TYMP(25), FN(25), TXMT1(25), TIN(25), TYMT2(25), T2N(25) |
4 COPBA(25), COPBB(25), COPBB(25), COPFB(25), COPFA(25), COPTB(25), COPF(25),  |
5 COPRA(25), COPRB(25), COPFR(25), COPFL(25), COPFL(25), COPLC(25) |
5 RGBM60A 1071
RGBVM60A 1072
RGBVM60A 1073
RGBNM01A 1074
RGBNM60A 1075
RGBNM60A 1076
RGBNM60A 1077
RGBNM60A 1078
RGBNM60A 1079
RGBNM60A 1080

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1 COMMON/COPY, CPYF, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, COPTE, CO
READ (IVDI, 56) (WZSIE(K), WZTQ(K), WZTS(K), WZVP(K), WZLQ(K), WZAP(K), WWRGBVM62A)
ASPI, K=1, npof)
56 FORMAT ('IVDI', 10.5)
WRITE (IVDO, 59) (WZSIE(K), WZTQ(K), WZTS(K), WZVP(K), WZLQ(K), WZAP(K), WWRGBVM62A)
ASPI, K=1, npof)
59 FORMAT ('IVDI', 10.5)
C TRANSFER OF PROFILES BEFORE ANY RESTART CASES
DO 99 K = 2, KBP1
WSP(K) = WSP(K-1)
ZAP(K) = WZAP(K-1)
ZVP(K) = WZVP(K-1)
ZLQ(K) = WZLQ(K-1)
ZSIE(K) = WZSIE(K-1)
ZTQ(K) = WZTQ(K-1)
99 ZTS(K) = WZTS(K-1)
WSP(1) = 0.0
ZAP(1) = 0.0
ZVP(1) = ZVP(2)
ZLQ(1) = ZLQ(2)
ZSIE(1) = ZSIE(2)
ZTQ(1) = ZTQ(2)
ZTS(1) = ZTS(2)
WSP(KBP2) = 0.0
ZAP(KBP2) = 0.0
ZVP(KBP2) = ZVP(KBP1)
ZLQ(KBP2) = ZLQ(KBP1)
ZSIE(KBP2) = ZSIE(KBP1)
ZTQ(KBP2) = ZTQ(KBP1)
ZTS(KBP2) = ZTS(KBP1)
C NOTE: CALCULATION OF CONSTANTS AND PREASSIGNED BRANCHES.
IF ( IRSRT.EQ.0 ) GO TO 100
CALL VRPRM
IF ( IDROU.GT.0 ) DROU = DROU * AIN1(DX, DZ)/AMAX1(UMAX, WMAX, EM6)
IF ( IPRFM.GT.0 ) CALL VRPRM
IRSTR=1
100 ITER-0
ICALI=1
X1=AMAX1( UMAX, WMAX )
VELOLD=1
EPS=EPS0*X1*RLENGH
IF ( X1.LT.VMIN ) EPS=EPS0*VMIN*RLENGH
IF( EPS6.LT.EM6 ) EPS=ABS( EPS0 )
ASSIGN 2000 TO KBC
C NOTE. COMPUTATION OF PNTAU, T1NTAU AND T2NTAU .
PNTAU=SI ( TYM1, FN, TIMET, NFLOW )
T1NTAU=SI ( TYM1, T1N, TIMET, NT1 )
IF(NT2.EQ.0) GO TO 107
T2NTAU=SI ( TYM2, T2N, TIMET, NT2 )
IF(NT3.EQ.0) GO TO 107
T3NTAU=SI ( TYM3, T3N, TIMET, NT3 )
IF(NT4.EQ.0) GO TO 107
T4NTAU=SI ( TYM4, T4N, TIMET, NT4 )
IF(NT5.EQ.0) GO TO 107
T5NTAU=SI ( TYM5, T5N, TIMET, NT5 )
107 CONTINUE
C NOTE. ZERO OUT THE CQ(IF) ARRAY FOR TAU FACTORS IN SIE EQUATION .
I1=2
I2=1BP1
K1=2
K2=KBP1
KK=1
ITANCN=0
DO 109 I=I1,I2
KK=KK + K2NC
LWPC=0
DO 109 K=K1,K2
LWPC=LWPC + NWPC
IK=KK + LWPC
CQ (IK)=0.0
109 CONTINUE
IP( NCYCB.LT.NCYC ) GO TO 1000
C NOTE. CALCULATION OF DIAGNOSTIC CONSTANTS .
ASSIGN 12500 TO KDAGTU

C NOTE. PREASSIGN BRANCHES FOR RESISTANCE EQUATIONS, I.E. RX AND RZ.

RXC = 0.0
RZC = 0.0

ASSIGN 2300 TO KXRZ

IF ( NWPC.GT.13 ) ASSIGN 2250 TO KXRZ

C NOTE. PREASSIGN BRANCHES FOR PLANE - CYL=0.0 - OR CYLINDRICAL COORDINATES.

FCU = 0.0
FCW = 0.0
RL = 1.0
RC = RL
RR = RC
DR = DX
RRL = 1.0
RRC = RRL
RRI = RRC
RRRC = 1.0
RRP = RRRRC
RRR = RRRRC
RRRR = RRRRRC
RRRRR = RRRRRRC
RDR = RDX
RDRS = 1.0/(DR*DR)
RDRM = RDR
RDRP = RDRM
RDRZ = RDRZ
RDRZP = RDRZM

ASSIGN 2400 TO KCLU
ASSIGN 2500 TO KCLW

IF ( CYL.LT.EM6 ) GO TO 120

ASSIGN 2370 TO KCLU
ASSIGN 2470 TO KCLW
ASSIGN 2215 TO KRU

120 ASSTGN 13000 TO KDIAG

IF ( IDIAG.LT.1 ) GO TO 200

ASSIGN 12200 TO KDIAG

IF ( IDIAG.GT.1 ) ASSIGN 12500 TO KDIAG

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200 TSUM=0.0
   TIOSUM=0.0
C
C NOTE. COMPUTATION OF BOUNDARY CONDITIONS.
C
1000 LWPC=1 - NWPC
   IF( KDERBC.LT.1 ) GO TO 1100
C
C NOTE. COMPUTATION OF RIGHT AND LEFT BOUNDARY CONDITIONS.
1100 LWPC=1 - NWPC
   I1=1
   I2=IBP2
   K1=1
   K2=KBP2
   NDERR=0
   NDERL=0
   NCOPR=0
   NCOFL=0
   DO 1289 K=K1,K2
   LWPC=LWPC+NWPC
   IMK=LWPC
   CPL= CP(IMK)
   ICPL=CPL
   IPK=IMK + IKP2
   IPPK=IPK + K2NC
   IMKT=IMK + K2NC
   IPKT=IPK
   CFR= CP(IPPK)
   ICFR=CFR
   IF( CPL.ME.2 ) GO TO 1105
   IF( K.EQ.K2 ) GO TO 1103
   IMKT=IMK + K2NC + NWPC
   IPKT=IPK + NWPC
   CPL= CP(IMK+NWPC)
   CFR= CF(IPPK+NWPC)
   GO TO 1105
1103 IMKT=IMK + K2NC - NWPC
IPKT=IPK - NWPC
CFK= CF(IMK-NWPC)
CFR= CF(IPPK-NWPC)

1175 W(IMK)=W(IMKT)
W(IPPK)=W(IPK)

C NOTE. COMPUTATION OF REFLECTIVE BOUNDARY CONDITIONS ON TQ AND TS.
SIR(IMK)=SIR(IMKT)
SIE(IPPK)=ZSIE(K)
TQ(IMK)=TQ(IMKT)
TQ(IPPK)=ZTQ(K)
TS(IMK)=TS(IMKT)
TS(IPPK)=ZTS(K)
CHI(IMK)=CHI(IMKT)
CHI(IPPK)=0.0
IF (I(IPKT).GT.0.0) CHI(IPPK)=CHI(IPKT)

GO TO (1120,1130,1140,1150),KWL

C NOTE. COMPUTATION OF RIGID LEFT WALL BOUNDARY CONDITION.
1120 U(IMK)=0.0
GO TO 1180

C NOTE. COMPUTATION OF CONTINUATIVE LEFT WALL BOUNDARY CONDITION.
1130 IF (IITER.GT.0) GO TO 1180
U(IMK)=U(IMK+K2NC)
W(IMK)=-W(IMK+K2NC)
W(IMK-NWPC)=-W(IMK+K2NC-NWPC)

GO TO 1180

C NOTE. COMPUTATION OF PERIODIC LEFT WALL BOUNDARY CONDITION.
1140 U(IMK)=U(IPK)
GO TO 1180

C NOTE. VARIABLE BOUNDARY OPTION AT LEFT WALL.
1150 NCPL=CFL-9
GO TO (1152,1130,1155,1160),NCPL

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C NOTE. RIGID BOUNDARY SECTION AT LEFT WALL.
1152 NRIGID=KDERBC + 1
GO TO ( 1120, 1153 ), NRIGID
C NOTE. DERIVED BOUNDARY CONDITION AT LEFT WALL.
1153 WC=W(IMKT)
   IF ( K.EQ.1 ) GO TO 1120
   IF ( K.GE.(KBR+1) ) GO TO 1120
   ICF1=CP(IMKT)
   IF ( ICF1.GE.30 ) GO TO 1120
   QC=TQ(IMKT)
   SC=TS(IMKT)
   NDERL=NDERL + 1
   WSA=USL(NDERL)
   QW=5.*WSA*WSA
   W(IMKT)=WC
   SW = WSA * WSA * HDX/WC
   TQ(IMKT)=2.*QW - QC
   TS(IMKT)=2.*SW - SC
GO TO 1120
C NOTE. CONSTANT INFLOW AT LEFT WALL.
1155 U(IMK)=UBLI
GO TO 1180
C NOTE. VARIABLE OR FUNCTIONAL INFLOW AT LEFT WALL.
1160 IF( ICFL.EQ.2 ) GO TO 1180
   NCOPL=NCOPL + 1
   TI=COPIB(NCOPL)*T1NTAU+COPLC(NCOPL)*T2NTAU
   1+COPLD(NCOPL)*T3NTAU+COPLE(NCOPL)*T4NTAU+COPLE(NCOPL)*T5NTAU
   ASSIGN 1162 TO KIROQC
   SIEX=SIE(IMKT)
GO TO 1500
1162 AREA=3.14159265*FLOAT(2*K-3)*DZ*DZ
   IF ( CYL.LT.1.0 ) AREA=K-DZ
   FLK=COPLA(NCOPL)*PNTAU
   UBAR=FLK/RHOII
   U(IMK)=UBAR/AREA
   IF ( NIV.EQ.1 ) U(IMK)=FLK

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SIE(IMK)=SII
TS(IMK)=TS(IPK)
TQ(IMK)=TQ(IPK)
1180 GO TO (1220,1230,1240,1250),KWR
C NOTE. COMPUTATION OF RIGID RIGHT WALL BOUNDARY CONDITION.
1220 U(IPK)=0.0
GO TO 1280
C NOTE. COMPUTATION OF CONTINUATIVE RIGHT WALL BOUNDARY CONDITION.
1230 IF(ITER.GT.0)GO TO 1280
U(IPPK)=U(IPK-K2NC)
W(IPPK-NWPC)=W(IPK-NWPC)
GO TO 1280
C NOTE. COMPUTATION OF PERIODIC RIGHT WALL BOUNDARY CONDITION.
1240 U(IPPK)=U(IMK+K2NC)
W(IPPK)=W(IMK+K2NC)
GO TO 1280
C NOTE. VARIABLE BOUNDARY OPTION AT RIGHT WALL.
1250 NCFR=CFR-9
GO TO (1252,1230,1255,1260),NCFR
C NOTE. RIGID BOUNDARY SECTION AT RIGHT WALL.
1252 NRIGID=KDERBC+1
GO TO (1220,1253),NRIGID
C NOTE. DERIVED BOUNDARY CONDITION AT RIGHT WALL.
1253 WC=W(IPKT)
IF(K.GT.(KBR+1))GO TO 1220
IF(K.EQ.1)GO TO 1220
ICF2=CF(IPKT)
IF(ICF2.GE.30)GO TO 1220
QC=TQ(IPKT)
SC=TS(IPKT)
NDEPR=NDERR+1
WSA=USR(NDERR)
QW=5.0*WSA*WSA
1256 SW=WSA+WSA*HDX/WC
W(IPPK)=-WC
TQ(IPPK)=2.*QW-QC
TS(IPPK) = 2.0*SWS-SC
GO TO 1220
C NOTE. CONSTANT INFLOW AT RIGHT WALL.
1255 U(IPK) = U(BRI)
GO TO 1280
C NOTE. VARIABLE OR FUNCTIONAL INFLOW AT RIGHT WALL.
1260 IF ( ICPR.EQ.2 ) GO TO 1280
NCOFR = NCOFR + 1
T1 = COFRB(NCOFR)*T1NTAU + COFRC(NCOFR)*T2NTAU
1+COFRD(NCOFR)*T3NTAU+COFRE(NCOFR)*T4NTAU+COFRF(NCOFR)*T5NTAU
ASSIGN 1262 TO KIROBC
SIBK = SIE(IPKT)
GO TO 1500
1262 AREA K = 3.14159265 * 2 * IBR * DR * DZ
IF ( Cyl.LT.1.0 ) AREA K = DZ
FLK = COFRB(NCOFR)*PNTAU
UBAR = FLK/RHOII
U(IPK) = U(IPK)/AREA K
IF(WIV.EQ.1) U(IPK) = FLK
SIEC = SIE(IPKT)
SIEX = SIEX
SIE(IPPK) = (2*SIEX+(ALX-1.0)*SIEC)/(1.0+ALX)
QC = TQ(IPKT)
QW = TQ(IPK) * U(IPK) * U(IPK)
SC = TS(IPKT)
SW = TSW(IPK) * U(IPK) * DZ
SW = ABS(SW)
QW = AMAX1(QW,1.0E-5)
SW = AMAX1(SW,WU)
TQ(IPPK) = (2*QW+(ALX-1.0)*QC)/(1.0+ALX)
TS(IPPK) = (2*SW+(ALX-1.0)*SC)/(1.0+ALX)
1280 CONTINUE
1289 CONTINUE
C NOTE. COMPUTATION OF TOP AND BOTTOM BOUNDARY CONDITIONS.
NDERB = 0
NDERT = 0
NCOPB=0
NCOPT=0
KK=1 + K2NC
DO 1489 I=I1,I2
KK=KK+K2NC
IKM=KK
CPB = CP (IKM)
ICPB=CPB
IKP=IKM + KNC
IKPP=IKP + NWPC
CPT = CP (IKPP)
ICPT=CPT
IKMT=IKM + NWPC
IKPT=IKP
IF ( CFB .NE. 2 ) GO TO 1305
IF ( I .EQ. I2 ) GO TO 1303
IKMT=IKM + K2NC + NWPC
IKPT=IKP + K2NC
CFD = CP (IKM+K2NC)
CFT = CP (IKPP+K2NC)
GO TO 1305
1303 IKMT=IKM - K2NC + NWPC
IKPT=IKP - K2NC
CFB = CF (IKM-K2NC)
CFT = CF (IKPP-K2NC)
1305 U (IKM) = U (IKMT)
U (IKPP) = U (IKP)
C NOTE: COMPUTATION OF REFLECTIVE BOUNDARY CONDITIONS ON TQ AND TS.
SIE (IKM) = SIE (IKMT)
SIE (IKPP) = SIE (IKPT)
TQ (IKM) = TQ (IKMT)
TQ (IKPP) = TQ (IKPT)
TS (IKM) = TS (IKMT)
TS (IKPP) = TS (IKPT)
CHI (IKM) = CHI (IKMT)
CHI (IKPP) = 0.0
IF (W (IKPT) .GT. 0.0) CHI (IKPP) = CHI (IKPT)
VAP (IKM) = VAP (IKMT)
VAP (IKPP) = VAP (IKPT)
LIQ (IKM) = LIQ (IKMT)
LIQ (IKPP) = LIQ (IKPT)
GO TO (1320, 1330, 1340, 1350), KWT
C NOTE. COMPUTATION OF RIGID TOP WALL BOUNDARY CONDITION
1320 W (IKP) = 0.0
GO TO 1380
C NOTE. COMPUTATION OF CONTINUATIVE TOP WALL BOUNDARY CONDITION
1330 IF (ITER .GT. 0) GO TO 1380
W (IKP) = W (IKP-NWPC)
U (IKPP-K2NC) = U (IKP-K2NC)
GO TO 1380
C NOTE. COMPUTATION OF PERIODIC TOP WALL BOUNDARY CONDITION
1340 W (IKP) = W (IKM+NWPC)
U (IKP) = U (IKM+NWPC)
GO TO 1380
C NOTE. VARIABLE BOUNDARY OPTION AT TOP WALL
1350 NCPT = CFT - 9
GO TO (1352, 1330, 1355, 1360), NCPT
C NOTE. RIGID BOUNDARY SECTION AT TOP WALL
1352 NRISID = KDERBC + 1
GO TO (1320, 1353), NRIGID
C NOTE. DERIVED BOUNDARY CONDITION AT TOP WALL
1353 UCT = U (IKP)
IF (.I.EQ.1) GO TO 1320
IF (.I.GE. (IBR + 1)) GO TO 1320
ICP3 = CF (IKP)
IF (ICP3 .GE. 30) GO TO 1320
QCT = TQ (IKP)
SCT = TS (IKP)
NDRT = NDRT + 1
USAT = USAT (NDRT)
QWT = 5. * USAT * USAT
1356 SWT = USAT * USAT * EDZ / UCT

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U(IKPP) = -UCT
TQ(IKPP) = 2. * QWT - QCT
TS(IKPP) = 2. * SWT - SCT
GO TO 1325

C. NOTE CONSTANT INFLOW AT TOP WALL.

1355 W(IKP) = WBTI
GO TO 1380

C. NOTE VARIABLE OR FUNCTIONAL INFLOW AT TOP WALL.

1360 IF( ICFT.EQ.2 ) GO TO 1380
NCOPT = NCOPT + 1
TI = COPTB(NCOPT) * T1NTAU + COPTC(NCOPT) * T2NTAU
1 + COPTD(NCOPT) * T3NTAU + COPTE(NCOPT) * T4NTAU + COPTF(NCOPT) * T5NTAU
ASSGN 1362 TO KIROBC
SIEX = SIE(IKPT)
GO TO 1500

1362 AREAI = 3.14159265 * PLOA(T(2*I-3)) * DR * DR
IF( CYL. LT. 1.0 ) AREA = DX
PLI = COPTA(NCOPT) * PNNTAU
WBAR = PLI / RhoI

W(IKP) = WBAR / AREAI
IF(NTV.EQ.1) W(IKP) = PLI
SIFC = SIE(IKPT)
SIEW = SIEL
SIF(IKP) = (2 * SIEW + (ALZ - 1.0)) * SIEC / (1.0 + ALZ)
QCT = TQ(IKP)
QWT = TQJET * W(IKP) * W(IKP)
SCT = TS(IKP)
SWT = T5JET * W(IKP) * DR
SWT = ABS(SWT)
QWT = AMAX1(QWT, 1.0E-5)
SWT = AMAX1(SWT, NU)
TQ(IKP) = (2 * QWT + (ALZ - 1.0)) * QCT / (1.0 + ALZ)
TS(IKP) = (2 * SWT + (ALZ - 1.0)) * SCT / (1.0 + ALZ)

1390 GO TO ( 1420, 1430, 1440, 1450 ), KWB

C. NOTE COMPUTATION OF RIGID BOTTOM WALL BOUNDARY CONDITION.

1420 W(IKM) = 0.0
GO TO 1480
C NOTE. COMPUTATION OF CONTINUATIVE BOTTOM WALL BOUNDARY CONDITION.
1430 IF ( ITER.GT.0 ) GO TO 1480
     W (IKM) = W (IKM+NWPC)
     U (IKM) = -U (IKM+NWPC)
     U (IKM-K2NC) = -U (IKM+NWPC-K2NC)
     GO TO 1480

C NOTE. COMPUTATION OF PERIODIC BOTTOM WALL BOUNDARY CONDITION.
1440 W (IKM) = W (IKP)
     GO TO 1480

C NOTE. VARIABLE BOUNDARY OPTION AT BOTTOM WALL.
1450 NCBF = CPB - 9
     GO TO ( 1452, 1430, 1455, 1460 ) , NCBF

C NOTE. RIGID BOUNDARY SECTION AT BOTTOM WALL.
1452 NRIGID = KDERBC + 1
     GO TO ( 1420, 1453 ) , NRIGID

C NOTE. DERIVED BOUNDARY CONDITION AT BOTTOM.
1453 IK = IKM + NWPC
     IF ( I.EQ.1 ) GO TO 1420
     IF ( I .GE. ( IBR + 1 ) ) GO TO 1420
     ICF4 = CF (IK)
     IF ( ICF4.GE.30 ) GO TO 1420
     UCB = U (IK)
     QCB = TQ (IK)
     SCB = TS (IK)
     NDERB = NDERB + 1
     USAB = USB ( NDERB )
     QWB = 5. * USAB * USAB
1456 SWB = USAB * USAB * HDZ / UCB
     U (IKM) = UCB
     TQ (IKM) = 2. * QWB - QCB
     TS (IKM) = 2. * SWB - SCB
     GO TO 1420

C NOTE. CONSTANT INFLOW AT BOTTOM WALL.
1455 W (IKM) = WBI
     GO TO 1480
C NOTE. VARIABLE OR FUNCTIONAL INFLOW AT BOTTOM WALL.

1460 IF( ICPB.EQ.2 ) GO TO 1480
    NCOFBNCOFB + 1
    T1=COFB(NCOFB)*T1NTAU + COFBC(NCOFB)*T2NTAU
    1+COFBD(NCOFB)*T3NTAU+COFBE(NCOFB)*T4NTAU+COFBE(NCOFB)*T5NTAU
    ASSIGN 1462 TO KIROBC
    SIE=SIE(IKMT)
    GO TO 1500
1462 AREA=3.14159265*FLOAT(2*I-3)*DR*DR
    IF( CYL.LT.1.0 ) AREA=DX
    FLI=COFBA(NCOFB)*PNTAU
    WBAR=FLI/RHOII
    W(IKMT)=WBAR/AREA
    IF(NIV.EQ.1) W(IKMT)=FLI
    SIEC=SIE(IK)
    SIEW=SIEII
    SIE(IKMT) = (2*SIEW + (ALZ-1.0)*SIEC)/(1.0+ALZ)
    QCB=TQ(IK)
    QWB=TQJETW(IKMT) *W(IKMT)
    SCB=TS(IK)
    SWB=TSJETW(IKMT) *DR
    QWB=AMAX1(QWB,1.0E-3)
    SWB=AMAX1(SWB,NU)
    TO(IKMT) = (2*QWB + (ALZ-1.0)*QCB)/(1.0+ALZ)
    TS(IKMT) = (2*SWB + (ALZ-1.0)*SCB)/(1.0+ALZ)

1480 CONTINUE
1489 CONTINUE

C NOTE. COMPUTATION OF SIE AND RHO FOR VARIABLE OR FUNCTIONAL INFLOW
C NOTE. AT A BOUNDARY WALL.

1500 TR=TI + 459.7
    GO TO ( 1510,1520,1530,1540 ),MAT

C NOTE. COMPUTATION FOR SODIUM MATERIAL.

1510 SIEII=0.38935*TR - 0.553E-4*TR*TR + 0.1137E-7*TR*TR*TR-29.02
    RHOII=59.566 - 7.9504E-3*TI - 0.2872E-6*TI*TI + 0.06035E-9*TI*TI*TI
    AT=397.17/TR + 1.0203

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TMU = (10.0 * AT/3600.) / TR**0.4925
TH = 0.015085 - 5.2167E-6 * TI + 5.809E-10 * TI * TI
TEMP = -385.27 + 2.6632 * SIEX + 5.9894E-04 * SIEX * SIEX + 1
  1.5575F-06 * SIEX * SIEX * SIEX - 2.9048E-09 * SIEX * SIEX * SIEX * SIEX + 
  2 1.15427E-12 * SIEX * SIEX * SIEX * SIEX * SIEX * SIEX
IF ( ICSPB .GT. 0 ) TI = TEMP
CSUBP = 0.38935 - 1.106E-4 * TI + 0.3411E-7 * TI * TI
GO TO 1550
C NOTE. COMPUTATION FOR WATER MATERIAL.
1520 SIEM = 1.0004 * TI - 32.013
RHOI = 62.742 - 0.372E-2 * TI - 0.44E-4 * TI * TI
BT = 446.0 / ( TI + 207.0 ) - 5.0
TMU = 1.622 * 10. ** BT
TK = 8.369E-5 + 2.368E-7 * TI - 5.89E-10 * TI * TI
TEMP = 0.9996 * SIEX + 32.0002
CSUBP = 1.0004
GO TO 1550
1530 SIEM = AI * TI * TI + BI * TI + CI
RHOI = AR * TI * TI + BR * TI + CR
TMU = AMU * TI * TI + BMU * TI + CMU
TK = AK * TI * TI + BK * TI + CK
CIT = CI - SIEX
TEMP = SI( AI, BI, CIT, -1 )
CSUBP = ACP * TI * TI + BCP * TI + CCP
GO TO 1550
1540 CONTINUE
1550 NU = TMU / RHOI
RPRAN = TK / ( CSUBP * TMU )
GO TO KIROC, ( 1162, 1262, 1362, 1462, 1605, 1615, 1625, 1635, 1736, 1756 )
C NOTE. COMPUTATION OF THE TAU FACTOR FOR USE IN THE SIE EQUATION.
C
C NOTE. FLUID CELL TO THE LEFT OF THE IK OBSTACLE.
1660 ICSPB = 9
IF ( ITAUCN .GT. 1 .OR. NTAU .LT. 1 ) GO TO 1714
ASSIGN 1695 TO KIROC
SIEX=SIF(IMK)
ICSUBP=1
GO TO 1500
1605 NTAU=CFC - 29
RTAU=1./TAU(NTAU)
P(IK)=1./(1.*DT*RTAU)*(P(IK)+DT*RTAU*TEMP)
CQ(IMK)=CSUBPO*RTAU*(TEMP-P(IK))
ICSUBP=0
GO TO 1714
C NOTE. FLUID CELL TO THE BOTTOM OF THE IK OBSTACLE.
1610 ICSUBP=0
IF(ITAUCN.GT.1 .OR. NTAU.LT.1 ) GO TO 1724
ASSIGN 1615 TO KIROBC
SIEX=SIF(IMK)
ICSUBP=1
GO TO 1500
1615 NTAU=CFC - 29
RTAU=1./TAU(NTAU)
P(IK)=1./(1.*DT*RTAU)*(P(IK)+DT*RTAU*TEMP)
CQ(IMK)=CSUBPO*RTAU*(TEMP-P(IK))
ICSUBP=0
GO TO 1724
C NOTE. FLUID CELL TO THE TOP OF THE IK OBSTACLE.
1620 ICSUBP=0
IF(ITAUCN.GT.1 .OR. NTAU.LT.1 ) GO TO 1744
ASSIGN 1625 TO KIROBC
SIEX=SIF(IPK)
ICSUBP=1
GO TO 1500
1625 NTAU=CFC - 29
RTAU=1./TAU(NTAU)
CQ(IPK)=CSUBPO*RTAU*(TIP-PIK)
ICSUBP=0
GO TO 1744
C NOTE. FLUID CELL TO THE RIGHT OF THE IK OBSTACLE.
1630 ICSUBP=0
IF ( ITAUCN.GT.1 .OR. NTAU.LT.1 ) GO TO 1764
ASSIGN 1635 TO KIROBC
SIE=SIE(IPK)
ICSUBP=1
GO TO 1500
1635 NTAU=CFC - 29
RTAU=1./TAU(NTAU)
P(IK)=1./(1.+DT*RTAU)*( P(IK) + DT*RTAU*TEMP )
CQ(IPK)=CSUBPO*RTAU*( TEMP-P(IK) )
ICSUBP=0
GO TO 1764
C
C NOTF. COMPUTATION OF OBSTACLE SUBREGIONS BOUNDARY CONDITIONS .
C
1700 KK=1
ITAUCN=ITAUCN + 1
I1=2
I2=IBP1
K1=2
K2=KBP1
IF( IOBS.EQ.0 ) GO TO 1990
NDERR=0
NDERRL=0
NDEP=0
NDERT=0
NCOPT=0
NCOFR=0
DO 1789 I=I1,I2
KK=KK + K2NC
LWPC=0
DO 1779 K=K1,K2
LWPC=LWPC + NWPC
IK=KK + LWPC
IKM=IK - K2NC
IKP=IK + NWPC
IPK=IK + K2NC
ICFC=CP(IK)
CFC=ICFC
IF( CFC.EQ.1 ) GO TO 1778
CFT=IICFT(IK)+1
CPB=IICPB(IK)+1
CPF=IICPR(IK)+1
CPF=IICPL(IK)+1
IF( CFT.GT.1 ) GO TO 1710
IF( CPB.GT.1 ) GO TO 1710
IF( CPF.GT.1 ) GO TO 1710
IF( CFP.GT.1 ) GO TO 1710
U(IK)=0.0
U(IMK)=0.0
W(IK)=0.0
W(IMK)=0.0
TS(IK)=0.0
TQ(IK)=0.0
SIF(IK)=0.0
GO TO 1770
C NOTE. OBSTACLE BOUNDARY CONDITION AT THE LEFT FACE.
1710 GO TO( 1720, 1600 ),CFL
C NOTE. NON-FLUID CELL TO THE LEFT OF THE IK OBSTACLE.
1712 U(IMK)=0.0
GO TO 1720
C NOTE. FLUID CELL TO THE LEFT OF THE IK OBSTACLE.
1714 U(IMK)=0.0
NRIGID=KDERBC + 1
GO TO ( 1715, 1716 ),NRIGID
C NOTE. RIGID BOUNDARY AT THE LEFT FACE.
1715 W(IK)=PSLIP*W(IMK)
SIF(IK)=SIF(IMK)
TQ(IK)=TQ(IMK)
TS(IK)=TS(IMK)
GO TO 1720
C NOTE. DERIVED BOUNDARY CONDITION AT THE LEFT FACE.
1716 WC=W (IMK)  
QC=TQ(IMK)  
SC=TS(IMK)  
NDERL=NDERL + 1  
WSA=USLOB(NDERL)  
QW=5.*WSA*WSA  
SW=WSA*WSA*HDZ/WC  
W(IK)=-WC  
TQ(IK)=2.*QW - QC  
TS(IK)=2.*SW - SC  
GO TO 1712

C NOTE. OBSTACLE BOUNDARY CONDITION AT THE BOTTOM FACE.  
1720 GO TO( 1730,1610 ),CFB  
C NOTE. NON-FLUID CELL TO THE BOTTOM OF THE IK OBSTACLE.  
1722 W(IMK)=0.0  
GO TO 1730  
C NOTE. FLUID CELL TO THE BOTTOM OF THE IK OBSTACLE.  
1724 W(IMK)=0.0  
NRIGID=NDERB + 1  
GO TO( 1725,1726 ),NRIGID  
C NOTE. RIGID BOUNDARY AT THE BOTTOM FACE.  
1725 U(IK)=FSLIP*U(IMK)  
SIE(IK)=SIE(IMK)  
TQ(IK)=TQ(IMK)  
TS(IK)=TS(IMK)  
GO TO 1730

C NOTE. DERIVED BOUNDARY CONDITION AT THE BOTTOM FACE.  
1726 UCT=U(IMK)  
QCT=TQ(IMK)  
SCT=TS(IMK)  
NDERB=NDERB + 1  
USAT=USLOB(NDERB)  
QWT=5.*USAT*USAT  
SWT=USAT*USAT*HDZ/UCT  
U(IK)=-UCT  
TQ(IK)=2.*QWT - QCT
TS(IK) = 2.*SWT - SCT
GO TO 1722

C NOTE. OBSTACLE BOUNDARY CONDITION AT THE TOP FACE.
1730 IF ( CPC.GE.30 ) GO TO 1740
C NOTE. VARIABLE BOUNDARY OPTION AT THE TOP FACE.
NCFT = CPC - 21
GO TO ( 1732, 1734, 1740, 1740, 1740 ), NCFT
C NOTE. CONSTANT INFLOW AT THE TOP FACE.
1732 W(IK) = W0Bi
GO TO 1745
C NOTE. VARIABLE OF FUNCTIONAL INFLOW AT THE TOP FACE.
1734 NCOPF = NCOPF + 1
TI = OPOBTB(NCOPF) * T1NTAU + OPOBTC(NCOPF) * T2NTAU
1+OPOBTD(NCOPF) * T3NTAU + OPOBTB(NCOPF) * T4NTAU + OPOBF(NCOPF) * T5NTAU
ASSIGN 1736 TO KIROBC
SIEX = SIE(IKP)
GO TO 1500
1736 AREA = 3.14159265*FLOAT(2*I-3)*DR*DR
IF ( CYL. LIM. 1.0 ) AREA = DX
FLI = OPOBTB(NCOPF) * FNTAU
WBAR = FLI / RHOII
W(IK) = WBAR / AREA
IF ( NIV. EQ. 1 ) W(IK) = FLI
SIEC = SIE(IKP)
SIFW = SIE(IKP)
SIE(IK) = (2*SIEW + (ALZ-1.0)*SIEC) / (1.0 + ALZ)
QCT = TQ(IKP)
QWT = TQJET * W(IK) * W(IK)
SCT = TS(IKP)
SWT = T5JET * W(IK) * DR
QWT = AMAX1(QWT, 1.0E-5)
SWT = AMAX1(SWT, NU)
TQ(IK) = (2*QWT + (ALZ-1.0)*QCT) / (1.0 + ALZ)
TS(IK) = (2*SWT + (ALZ-1.0)*SCT) / (1.0 + ALZ)
U(IK) = PSLIP*U(IKP)
GO TO 1750

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C NOTE. OBSTACLE BOUNDARY CONDITION AT THE TOP FACE.
1740  GO TO ( 1750, 1620 ), CFT
C NOTE. NON-FLUID CELL TO THE TOP OF THE IK OBSTACLE.
1742  W(IK)=0.0
      GO TO 1750
C NOTE. FLUID CELL TO THE TOP OF THE IK OBSTACLE.
1744  W(IK)=0.0
      WRIGID=KDERBC + 1
      GO TO ( 1745, 1746 ), WRIGID
C NOTE. RIGID BOUNDARY AT THE TOP FACE.
1745  U(IK)=-U(IKP)
      S1E(IK)=S1E(IKP)
      TQ(IK)=TQ(IKP)
      TS(IK)=TS(IKP)
      GO TO 1750
C NOTE. DERIVED BOUNDARY CONDITION AT THE TOP FACE.
1746  UCT=U(IKP)
      QCT=TQ(IKP)
      SCT=TS(IKP)
      NDERT=NDERT + 1
      USAT=USTOB(NDERT)
      QWT=5.*USAT*USAT
      SWT = USAT * USAT + 3DZ/UCT
      U(IK) = -UCT
      TQ(IK)=2.*QWT - QCT
      TS(IK)=2.*SWT - SCT
      GO TO 1742
C NOTE. OBSTACLE BOUNDARY CONDITION AT THE RIGHT FACE.
1750  IF( CFC.GE.30 ) GO TO 1760
C NOTE. VARIABLE BOUNDARY OPTION AT THE RIGHT FACE.
1751  NCPR=CFC - 21
      GO TO( 1776, 1776, 1776, 1752, 1754 ), NCPR
C NOTE. CONSTANT INFLOW AT THE RIGHT FACE.
1752  U(IK)=UGI
      GO TO 1765
C NOTE. VARIABLE OR FUNCTIONAL INFLOW AT THE RIGHT FACE.
1754 NCOFR=NCOFR + 1
1755 TI=FOBRE (NCOFR) * T1NTAU + OPOBRC (NCOFR) * T2NTAU
1756 1+OPOBRE (NCOFR) * T3NTAU + OPOBRE (NCOFR) * T4NTAU + OPOBRE (NCOFR) * T5NTAU
1757 ASSIGN 1756 TO KBM01A
1758 GO TO 1500
1759 AREAK = 3.14159265 * 2*(I-1) * DR * DZ
1760 IF ( CYL. LT. 1.0 ) AREAK = DZ
1761 FLK=FOBRA (NCOFR) * FNTAU
1762 UBAR=FLK/RHOII
1763 U (IK) = UBAR/AAREAK
1764 IP(NIV.EQ.1) U (IK) = FLK
1765 SIEC=SIP(IPK)
1766 SIEW=SIEEK
1767 SIP (IK) = (2*SIEW + (ALX-1.0)*SIEC)/(1.0+ALX)
1768 QC = TQ(IPK)
1769 QW = TQJET * U (IK) * U (IK)
1770 SC = TS(IPK)
1771 SW = TSJET * U (IK) * DZ
1772 QW=AMAX1(QW,1.0E-5)
1773 SW=AMAX1(SW,NU)
1774 TQ (IK) = (2*QW + (ALX-1.0)*QC)/(1.0+ALX)
1775 TS (IK) = (2*SW + (ALX-1.0)*SC)/(1.0+ALX)
1776 W (IK) = PSLIP*W(IPK)
1777 GO TO 1770
1778 C NOTE. OBLIQUE BOUNDARY CONDITION AT THE RIGHT FACE.
1779 C NOTE. NON-FLUID CELL TO THE RIGHT OF THE IK OBSTACLE.
1780 U (IK) = 0.0
1781 GO TO 1770
1782 C NOTE. FLUID CELL TO THE RIGHT OF THE IK OBSTACLE.
1783 U (IK) = 0.0
1784 NRIGID=KDEBRC + 1
1785 GO TO( 1765, 1766 ) , NRIGID
1786 C NOTE. RIGID BOUNDARY AT THE RIGHT FACE.
1787 W (IK) = PSLIP*W(IPK)
SIE (IK) = SIE (IPK)
TQ (IK) = TQ (IPK)
TS (IK) = TS (IPK)
GO TO 1770
C NOTE. DERIVED BOUNDARY CONDITION AT THE RIGHT FACE.
1766 WC = W (IPK)
QC = TQ (IPK)
SC = TS (IPK)
NDEF R = NDER R + 1
WSA = 0.5 ROB (NDER R)
QW = 5. * WSA * WSA
SW = WSA * WSA * MDX/WC
W (IK) = -WC
TQ (IK) = 2. * QW - QC
TS (IK) = 2. * SW - SC
GO TO 1762
1770 IF ( CF R.EQ.2 .AND. CPC.GE.30 ) W (IK) = 0.0
1776 IF ( CF R.EQ.2 .AND. CPC.LT.25 ) U (IK) = 0.0
1778 CONTINUE
1779 CONTINUE
1789 CONTINUE
1999 GO TO 1630, ( 2000, 2990, 4100, 5000, 5060 )
C
C NOTE. CHECKS FOR INITIAL CYCLES PRINTS, I.E. NPRT=0 NO PRINT,
C NOTE. NPRT=1 CYCLE 0 PRINT AND NPRT=2 CYCLE 0,1 PRINTS.
C
2000 IF ( NCYC.LT.NPRT ) GO TO 2010
GO TO 2030
C
2010 CALL VRPT
IF ( IPRF M.GT.0 ) CALL VRPLM
C NOTE. CALL TO THE VARIABLE RESISTANCE SUBROUTINE.
C NOTE. BEGIN THE N PASS PHASE OF THE TILDE EQUATION SECTION.
2030 DO 2999 NTE=1, NTPAS
   IF ( NWPC.GT.11 ) CALL WREQ
C
C NOTE. U AND W TILDE VELOCITY EQUATIONS SECTION.
   PAGE 54
C
C NOTE. TRANSFERS VELOCITIES TO STORAGE ARRAY ( AT TIME=N ).
K1=1
K2=KB2
LWPC=1-NWPC
DO 2109 K=K1,K2
LWPC=LWPC+NWPC
IK=LWPC
IKS=I2K2 + IK
SIE(IKS)=SIE(IK)
U(IKS)=U(IK)
W(IKS)=W(IK)
TQ(IKS)=TQ(IK)
TS(IKS)=TS(IK)
CHI(IKS)=CHI(IK)
VAP(IKS)=VAP(IK)
LIQ(IKS)=LIQ(IK)
2109 CONTINUE
II=2
I2=IBP1
K1=2
K2=KB2
KK=0
KKL = 0
DO 2989 I=I1,I2
KK=KK+K2NC
KKL = KKL + K2NC
LWPC = 1
IKMS=I2K2 + 1
SIE(1)=SIE(IKMS)
U(1)=U(IKMS)
W(1)=W(IKMS)
TQ(1)=TQ(IKMS)
TS(1)=TS(IKMS)
CHI(1)=CHI(IKMS)
VAP (1) = VAP (IKMS)
LIQ (1) = LIQ (IKMS)
SIE (IKMS) = SIE (KK+1)
U (IKMS) = U (KK+1)
W (IKMS) = W (KK+1)
TQ (IKMS) = TQ (KK+1)
TS (IKMS) = TS (KK+1)
CHI (IKMS) = CHI (KK+1)
VAP (IKMS) = VAP (KK+1)
LIQ (IKMS) = LIQ (KK+1)
GO TO KRU, (2215, 2222)

C NOTE. COMPUTATION OF RADIUS CONSTANTS IN THE I DIRECTION.

2215 RR = FLOAT (I-1) * D X
RC = RR - HD X
RL = RR - D X
RRR = 1. / RR
RRC = 1. / RC
RRC1 = RR + HD X
RERRC = 1. / RRC1
RRP = RR + DR

2220 DO 2979 K = K1, K2
C NOTE. COMPUTATION OF CELL INDICES.
LWPC = LWPC + NWPC
IK = KK + LWPC
LWPC1 = LWPC1 + NWPC1
IKL = KKL + LWPC1
DCR = DFFCO (IKL)
DCT = DFFCO (IKL+1)
DCI = DFFCO (IKL+2)
DCB = DFFCO (IKL+3)

C NOTE. BYPASS OBSTACLE CELLS.
CF = CF (IK)
IPK = IK + K2 MC
IKP = IK + NWPC
IMKS = I2K2 + LWPC
IKMS = IMKS - NWPC

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UR=U (IPK)
UC=U (IK)
UL=U (IMKS)
WT=W (IPK)
WC=W (IK)
WB=W (IMKS)
PC=P (IK)
PR=P (IPK)
PT=P (IKP)
SIEC=SIE (IK)
SIFR=SIE (IPK)
SLET=SIE (IKP)
SIEL=SIE (IMKS)
SIEB=SIE (IKMS)
SIECO=SIEO (IK)
UCO=UO (IK)
WCO=WO (IK)

C NOTE: COMPUTATION OF TQ AND TS CONSTANTS.

TQC=TQ (IK)
TQR=TQ (IPK)
TQT=TQ (IKP)
TQL=TQ (IMKS)
TQB=TQ (IKMS)
TQC0=TQO (IK)
TSC=TS (IK)
TSR=TS (IPK)
TST=TS (IKP)
TSL=TS (IMKS)
TSB=TS (IKMS)
TSCO=TSO (IK)
CHIC=CHI (IK)
CHIR=CHI (IPK)
CHIT=CHI (IKP)
CHIL=CHI (IMKS)
CHIB=CHI (IKMS)
CHICO=CHIO (IK)
VAPC=VAP (IK)
VAPR=VAP (IPK)
VAPT=VAP (IKP)
VAPL=VAP (IKMS)
VAPB=VAP (IKMS)
VAPCO=VAP (IK)
LIQ=LIQ (IK)
LIQR=LIQ (IPK)
LIQT=LIQ (IKP)
LIQL=LIQ (IKMS)
LIQB=LIQ (IKMS)
LIQO=LIQ (IK)

IF ( CPC.RE.1 ) GO TO 2700
TSR=.25*(TSR + TSC + TST + TS(IPK+K2NC))
TSBR=.25*(TSR + TSC + TSB + TS(IPK-NWPC))
TSL=.25*(TSL + TSC + TST + TS(IMKS+NWPC))

IF ( ICALI.EQ.2 ) GO TO 2500
GO TO 2700

C NOTE. STORAGE OF SUBSCRIPTED RX(), RZ() TO CONSTANT RXC AND RZC.

2250 RXC=RX (IK)*ABS( UC )**NRESEX
RZC=HZ (IK)*ABS( WC )**NRESEX

C NOTE. COMPUTATION OF U TILDE FLUXES.

2300 URA=.5*(UC+UR)
URAA=ABS(URA)
ULA=.5*(UL+UC)
ULAA=ABS(ULA)

FUZ=.5*RX*( URA*(UC+UR) + ALX*URAA*(UC-UR) - ULA*(UL+UC)
-ALX*ULAA*(UL-UC) )

WTA=.5*(WC+W(IPK))
WTAA=ABS(WTA)
WBA=.5*(WB+W(IPK-NWPC))
WBAA=ABS(WBA)

FUZ=.5*RDZ*( WTA*(UC+U(IPK)) + ALZ*WTAA*(UC-U(IPK))
- WBA*(U(IMKS)+UC) - ALZ*WBAA*(U(IMKS)-UC) )

C NOTE. CALCULATION OF THE U TILDE DIFFUSION TERMS.

DURR=RDRP*RRPC*TSR*( RRP*UR - RR*UC )
C NOTF. COMPUTATION OF THE U TILDE CYLINDRICAL FLUX TERM.
2370 FCU=.5*RRC*( URA*URA + UL*ULA + .5*ALX*URAA*(UC-UR) + .5*ALX*URAA*(UL-UC) ) VM 237002
C NOTF. COMPUTATION OF W TILDE FLUXES.
2400 UTA=.5*(UC+U(IPK)) VM 240002
UTAA=ABS(UTA)
ULT=.5*(UL+U(IMKS+WP)) VM 240006
UTA=ABS(ULT)
WTA=.5*(WC+WT)
WTAA=ABS(WTA)
WBA=.5*(WB+WC)
WBAA=ABS(WBA)
FWX=.5*RDZ*( UTA*(WC+W(IPK)) + ALX*UTAA*(WC-W(IPK)) )
1 - ULT*(W(IMKS)+WC) - ALX*ULTA*(W(IMKS)-WC) ) VM 240012
FWZ=.5*RDZ*( WTA*(WC+WT) + ALX*WTAA*(WC-WT) )
1 - WBA*(WB+WC) - ALX*WBAA*(WB-UC) ) VM 240014
C NOTF. CALCULATION OF THE W TILDE DIFFUSION TERMS.
DWR=RDWP*RP*TSTR*(W(IPK)-WC)
DWR=RDMP*RP*TSTL*(WC-W(IMKS))
DWR=RDRC*RDC*( DWRR - DWR )
DZ=RDZ*{ TST*(WT-WC) + RDZ - TSC*(WC-WB) *RDZ )
PWT=DWR + DWZ
GO TO KCLW, ( 2470, 2500 )
C NOTF. COMPUTATION OF THE U TILDE CYLINDRICAL FLUX TERM.
2470 FCW=.25*RRC*( UTA*(WC+W(IPK)) + ULT*(W(IMKS)+WC) )
1 + ALX*UTAA*(WC-W(IPK)) + ALX*ULTA*(W(IMKS)-WC) ) VM 240016
C NOTF. COMPUTATION OF BOTH Q AND SIGMA TURBULENCE QUANTITIES.
2500 TOBA=.5*(TOC+TQR)
IF(ICALI.EQ.1) GO TO 2591
TQLA=.5*(TOC+TQL)
TQTA=.5*(TOC+TQT)
TQA = .5*(TQC+QTB)
TSA = .5*(TSC+TSR)
TSL = .5*(TSC+TSL)
TST = .5*(TSC+TST)
TSA = .5*(TSC+TST)

C NOTE. CALCULATION OF THE SIJ TERM, I.E. THE SOURCE TERM.
SIJ = RDR*(UC-UL)**2 + RDZ*(WC-WB)**2 + .25*CYL*(RRC*(UC+UL))**2 +
1 0.03125*(RDZ*(U(IPK)+U(IMKS+NWPC)-U(IMKS)-U(1))
2 + RDR*(W(IPK)+W(IMK-NWPC)-W(IMKS)-W(1))**2

C NOTE. CALCULATION OF THE Q EQUATION CONVECTION TERMS.
CQR = -.5*RRC*RDR*(RR*(UC*(TQC+TQR)+ALX*ABS(UC)*(TQC-TQR))
1 - UL*(TQL+TQC) + ALX*ABS(UL)*(TQL-TQC))

C NOTE. CALCULATION OF THE Q EQUATION DIFFUSION TERM.
DQRR = RRC*RDR*(RR*TSRA*(TQR-TQC))*DCR
DQRL = RRC*RDR*(RL*TSLA*(TQC-TQL))*DCL
DQR = RDR*(DQRR-DQRL)
DQST = RDR*(TSTA*(TQT-TQC))*DCT
DQZB = RDR*(TSA*(TQC-TQB))*DCB
DQZ = RDR*(DQST-DQZB)

C NOTE. CALCULATION OF THE Q EQUATION DECAY TERM.
DQ = 4.*ALP*TQC/(TSC+1.E-20)

C NOTE. CALCULATION OF THE NEW Q AT TIME N+1.
TQ(I,K) = (1./(1.*DT*DQ))*{(TQC0+DT*(CQR+CQZ+2.*TSC*SIJ+
1 + GAM*(DQR+DQZ))}

C NOTE. COMPUTATION OF SIJMA QUANTITIES.

C NOTE. CALCULATION OF THE SIGMA EQUATION CONVECTION TERMS.
CSR = -.5*RRC*RDR*(RR*(UC*(TSC+TSR)+ALX*ABS(UC)*(TSC-TSR))
1 - RL*(UL*(TSL+TSC)+ALX*ABS(UL)*(TSL-TSC))

CSZ = -.5*RDZ*(WC*(TSC+TST)+ALX*ABS(WC)*(TSC-TST)
1 - WB*(TSB+TSC)+ALX*ABS(WB)*(TSC-TST))

C NOTE. CALCULATION OF THE SIGMA EQUATION DIFFUSION TERM.
IF( I+LT.I2 ) GO TO 2502
IFLG5 = 0
IFLSQ = 0
IF( TQR.LT.0.0 ) IFL3.Q=1
IF( TSR.LT.0.0 ) IFLGS=1
IFLG1=IFLGQ+IFLGS
IF( IFLG1.EQ.2 ) TQR=-TQR
2502 IF( K.LT.K1 ) GO TO 2504
IFLS=0
IFLGQ=0
IF( TQB.LT.0.0 ) IFL3.Q=1
IF( TSB.LT.0.0 ) IFLGS=1
IFLG1=IFLGQ + IFLGS
IF( IFLG1.EQ.2 ) TQB=-TQB
2504 IF( K.LT.KBP1 ) GO TO 2506
IFLS=0
IFLGQ=0
IF( TQT.LT.0.0 ) IFL3.Q=1
IF( TST.LT.0.0 ) IFLGS=1
IFLG1=IFLGQ + IFLGS
IF( IFLG1.EQ.2 ) TQT=-TQT
2506 IF( I.LT.I1 ) GO TO 2508
IFLS=0
IFLGQ=0
IF( TQL.LT.0.0 ) IFLGQ=1
IF( TSL.LT.0.0 ) IFLGS=1
IFLG1=IFLGQ + IFLGS
IF( IFLG1.EQ.2 ) TQL=-TQL
2508 CONTINUE
DSRR = RRC * RDR * ( RF * T3RA * ( TQR/TSR - TQC/TSC )) * DCR
DSRL = RRC * RDR * ( RL * TQI * ( TQC/TSC - TQL/TSL )) * DCL
DSR = RDR * ( DSRR - DSRL)
DSZT = RDZ * ( TQT * ( TQT/TST - TQC/TSC )) * DCT
DSZE = RDZ * ( TQBA * ( TQC/TSC - TQB/TSB )) * DCR
DSZ = RDZ * ( DSZT - DSZE)
C DIJ=GM*TS/CQC+(DQR+DQZ) - GAM1*TS/CQC+TS/CQC+TQC*(DSR+DSZ) RGBVW000
C DIJ=GM*TS/CQC+(DQR+DQZ) - GAM1*TS/CQC+TS/CQC+TQC**(DSR+DSZ)
C DS=4.*ALP*TQC/(TS+1.0E-20)
DS=ALP*TQC/(TS+1.0E-20)
C NOTF. CALCULATION OF THE NEW SIGMA AT N+1.

\[
\begin{align*}
TS(IK) &= (1.0 / (1.0 + TS(IC) * TS(TS(TS(K))))) \times (TSC0 + DT(CSR + CSZ + TSC + TSC + TQC + SIJ + DIJ)) \\
IF(TQ(IK) + LT.ZTQ(K)) &= TQ(IK) = ZTQ(K) \\
IF(PS(TS(IK).LT.ZTS(K)) &= TS(IK) = ZTS(K)
\end{align*}
\]

C CALCULATION OF TERMS IN THE VAP TRANSPORT EQUATION

\[
\begin{align*}
CVR &= 0.5 * RR * RDZ * (RR * UC*(VAPC + VAPB) + ALZ*ABS(UC) * (VAPC - VAPB)) \\
1 &= RL*(UL*(VAPC + VAPC) + ALZ*ABS(UL) * (VAPC - VAPC)) \\
CVZ &= 0.5 * RDZ * (WC*(VAPC - VAPC) + ALZ*ABS(WC) * (VAPC - VAPC)) \\
1 &= WB*(VAPC + VAPB) - ALZ*ABS(WB) * (VAPB - VAPC)
\end{align*}
\]

\[
\text{VAP}(IK) = \text{VAPCO} + DT * (-CVR - CVZ + DVR + DVZ)
\]

C CALCULATION OF TERMS IN THE LIQ TRANSPORT EQUATION

\[
\begin{align*}
CLR &= 0.5 * RR * RDZ * (RR * UC*(LIQF + LIQR) + ALZ*ABS(UC) * (LIQF - LIQR)) \\
1 &= RL*UL*(LIQF - LIQF) + ALZ*ABS(UL) * (LIQF - LIQF) \\
CLZ &= 0.5 * RDZ * (WC*(LIQF + LIQT) + ALZ*ABS(WC) * (LIQF - LIQT)) \\
1 &= WB*(LIQF + LIQF) - ALZ*ABS(WB) * (LIQF - LIQF)
\end{align*}
\]

\[
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\text{DLR} = \text{RDZ} + (RR * GAML * TSRA * DCR * (LIQF - LIQF)) \\
\]

\[
\text{LIQ}(IK) = \text{LIQCO} + DT * (-CLR - CLZ + DLR + DLZ)
\]

C EQUILIBRIUM MOISTURE THERMODYNAMICS SECTION

\[
\begin{align*}
\text{CIT} &= \text{CSC} \\
\text{TEMP} &= \text{SI} (\text{AI}, \text{BI}, \text{CIT}, -1) \\
\text{RHOC} &= \text{AR} * \text{TEMP} * \text{TEMP} + \text{BR} * \text{TEMP} + \text{CR}
\end{align*}
\]

C CALCULATE THE ABSOLUTE THERMODYNAMIC TEMPERATURE (DEG C)

\[
\begin{align*}
\text{ABT} &= (\text{TEMP} + 459.7) * ((\text{ZAP}(K) / 1000.) * 2856) / (1.0 * 0.61 * \text{VAP}(IK) / \text{RHOC}) / 1.3 \text{BAW} \text{BAW} \\
\text{A} &= \text{BAW} \text{BAW}
\end{align*}
\]

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C CALCULATE THE SATURATION VAPOR PRESSURE (MB)
    EVAP=10.*( ( 293.7-4/ABT-4.9283*ALOG10(ABT) ) +23.5518 )
C CALCULATE THE VAPOR DENSITY AT SATURATION (LBM/CU FT)
    RHOS=RHOC*.61*EVAP/ZAP(K)
    IF(VAP(IK).LT.RHOS) GO TO 300
    IF(VAP(IK).EQ.RHOS) GO TO 320
C CONDENSE VAPOR AND RELEASE LATENT HEAT
    LIQ(IK)=LIQ(IK)+VAP(IK)-RHOS
    CQ(IK)=CQ(IK)-((VAP(IK)-RHOS)*1075.0)/(DT*RHOC)
    VAP(IK)=RHOS
    GO TO 320
C EVAPORATE LIQUID AND ABSORB LATENT HEAT
   300 IF(LIQ(IK).LE.3.0) GO TO 320
    IF(LIQ(IK).LE.RHOS-VAP(IK)) GO TO 310
    LIQ(IK)=LIQ(IK)-RHOS+VAP(IK)
    CQ(IK)=CQ(IK)+((RHOS-VAP(IK))*1075.0)/(DT*RHOC)
    VAP(IK)=RHOS
    GO TO 320
   310 CQ(IK)=CQ(IK)+((LIQ(IK)*1075.0)/(DT*RHOC)
    VAP(IK)=VAP(IK)+LIQ(IK)
    LIQ(IK)=0.0
   320 CONTINUE
C
C NOTE. COMPUTATION OF SPECIFIC INTERNAL ENERGY.
C
C NOTE. CALCULATION OF THE SIE EQUATION CONVECTION TERMS.
2590 CIR=.5*RRC*RDR*( PR*( UC*(SIEC+SIER) + ALX*ABS(UC)*(SIEC-SIER) )
      1 - RL*( UL*(SIEL+SIEC) + ALX*ABS(UL)*(SIEL-SIEC) ) )
    CIZ=.5*RZ*( WC*(SIEC+SIET) + ALZ*ABS(WC)*(SIEC-SIET)
      1 - WB*(SIER+SIEC) - ALZ*ABS(WB)*(SIER-SIEC) )
C NOTE. CALCULATION OF THE SIE EQUATION DIFFUSION TERMS.
    GAMD=GAM
    IF( TSC.LE.NU ) GAMD=RPPAN
    DDIR=RDR*(RR*GAMD*TSRA*DCR*(SIER-SI EC))
    DIFL=RDR*(RL*GAMD*TSLA*DCL*(SIEC-SI EL))
DIP = RRC * RDR * (DIRR-DIRL)
DIZT = RDZ * (GAMT*TSTA*DCT*(SIET-SIET))
DIZB = RDZ * (GAMT*TSBA*DCB*(SIET-SIB))
DIZ = RDZ * (DIZT-DIZB)

C CALCULATION OF DECAY HEAT (BTU/LBM*SEC)

DECH = 1.50934E10 * CHI (IK) * SER / (RHOC * WMOLX)

C NOTE. COMPUTATION OF THE NEW SPECIFIC INTERNAL ENERGY AT N+1.

SIET (IK) = SIETO + DT * (-CIR - CIZ + DIZ - CQ (IK) + DECH)

C ELECTRIC FIELD IN THE CHI TRANSPORT EQUATION

CIR = .5 * RRC * RDR * (RR + UC * (CHIC+CHIR) + ALX*ABS (UC) * (CHIC-CHIR))
CIZ = .5 * RDZ * (WC * (CHIC+CHIT) + ALX*ABS (WC) * (CHIC-CHIT))

GOTO 2650

C NOTE. CALCULATION OF SPECIFIC MATERIAL FOR TEMPERATURE AND DENSITY.

C NOTE. RELATIVE DENSITY.

GO TO (2592, 2594, 2596, 2598) MAT

C NOTE. CALCULATION OF SODIUM MATERIAL FOR TEMPERATURE AND RHO.

TEMPC = -385.27 + 2.6602 * SIET + 5.9894E-04 * SIET * SIET +
1 1.5575E-06 * SIET ** 3 - 2.9048E-09 * SIET ** 4 +
2 1.15427E-12 * SIET ** 5

TEMP = -385.27 + 2.6602 * SIET + 5.9894E-04 * SIET * SIET +
1 1.5575E-06 * SIET ** 3 - 2.9048E-09 * SIET ** 4 +
2 1.15427E-12 * SIET ** 5

TEMPR = -385.27 + 2.6602 * SIER + 5.9894E-04 * SIER * SIER +
1 1.5575E-06 * SIER ** 3 - 2.9048E-09 * SIER ** 4 +
2 1.15427E-12 * SIER ** 5

RHOC = 59.566 - 7.9504E-3 * TEMPC - 0.2872E-6 * TEMPC * TEMPC +
1 0.06035E-9 * TEMPC * TEMPC * TEMPC

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C NOTE. CALCULATION OF WATER MATERIAL FOR TEMPERATURE AND RHO.

RHO=59.566 - 7.9504E-3*TEMP - 0.2872E-6*TEMP*TEMP +
 1         0.06035E-9*TEMP*TEMP*TEMP*TEMP
RHOR=59.566 - 7.9504E-3*TEMP - 0.2872E-6*TEMP*TEMP +
 1         0.06035E-9*TEMP*TEMP*TEMP*TEMP
RHOA=0.5*( RHC + RHO )
RHOAX=0.5*( RHC + RHOR )
RHOX=( RHOA-RHO0 )/RHO0
RHOZ=( RHOA-RHO0 )/RHO0
GO TO 2600

2594 TEMPC=0.9996*SIELC + 32.0002
TEMP=0.9996*SIELT + 32.0002
TEMPR=0.9996*SIER + 32.0002
RHC=62.742 -0.372E-2*TEMPC - 0.44E-4*TEMPC*TEMPC
RHOT=62.742 -0.372E-2*TEMP - 0.44E-4*TEMP*TEMP
RHOA=0.5*( RHC + RHO )
RHOAX=0.5*( RHC + RHOR )
RHOX=( RHOA-RHO0 )/RHO0
RHOZ=( RHOA-RHO0 )/RHO0
GO TO 2600

2596 CIT=CI - SIELC
TEMP=SI( AI,BI,CIT,-1 )
CIT=CI-SIELT
TEMP=SI( AI,BI,CIT,-1 )
CIT=CI-SIER
TEMP=SI( AI,BI,CIT,-1 )
RHC=AR*TEMPC*TEMPC + BR*TEMPC + CR
RHOT=AR*TEMP*TEMP + BR*TEMP + CR
RHOR=AR*TEMPR*TEMPR + BR*TEMPR + CR
RHOA=0.5*( RHC + RHOT )
RHOZ=( RHOA-RHO0 )/RHO0
RHOA=0.5*( RHC + RHOR )
RHOZ=( RHOA-RHO0 )/RHO0
GO TO 2600

2598 CONTINUE
C NOTE. COMPUTATION OF FULL TILDE EQUATIONS AT TIME=N+1.

2600 IF ( ICALI.EQ.2 ) GO TO 2650

   U (IK) = (1./ (1. + DT*RXQ) ) * ( UC0 + DT* ( RDX* (PC-PR) ) + RHOX*GX
       1             - PUZ - FUX - PCU + PUT )

   W (IK) = (1./ (1. + DT*RZQ) ) * ( WCO + DT* ( RDZ* (PC-PT) ) + RHOZ*GZ
       1             - PWZ - FWX - FCW + FWT )

2650 IF ( ICALI.EQ.1 ) GO TO 2700

C NOTE. UPDATE THE Q EQUATION WITH THE RESISTANCE FACTORS.

   RXC = RX (IK) * ABS ( UO (IK) ) ** NRESEX
   RXL = RX (IKM) * ABS ( UO (IKM) ) ** NRESEX
   RZC = RZ (IK) * ABS ( WO (IK) ) ** NRESEX
   RZB = RZ (IKM) * ABS ( WO (IKM) ) ** NRESEX

2700 U (1) = U (IMKS)
   W (1) = W (IMKS)
   TQ (1) = TQ (IMKS)
   TS (1) = TS (IMKS)
   SIE (1) = SIE (IMKS)
   CHI (1) = CHI (IMKS)
   VAP (1) = VAP (IMKS)
   LIQ (1) = LIQ (IMKS)
   SIE (IMKS) = SIEC
   U (IMKS) = UC
   W (IMKS) = WC
   TQ (IMKS) = TQC
   TS (IMKS) = TSC
   CHI (IMKS) = CHIC
   VAP (IMKS) = VAPC
   LIQ (IMKS) = LIQC

2979 CONTINUE
2989 CONTINUE
   ASSIGN 2990 TO KBC
   IF ( NTE.LT.NTPAS ) GOTO 1100

2990 CONTINUE
2999 CONTINUE
   IF ( ICALI.EQ.2 ) GO TO 5050

C NOTE. IMPLICIT PRESSURE ITERATION.
**C NOTE. BEGIN PRESSURE ITERATION AFTER SETTING BOUNDARY CONDITIONS.**

4100  I1=2
     I2=IBP1
     K1=2
     K2=KBP1
     KK=K1
     DO 4469 I=I1,I2
     KK=KK+K2NC
     LWPC=0
     RRADD=(FLOAT(I)-1.5)*DX
     RRADD=1./RRADD
     IF ( CYL.LT.E6 ) RRADD=0.0
     DO 4479 K=K1,K2
     LWPC=LWPC+NWPC
     IK=KK+LWPC
     IMK=IK-K2NC
     IKM=IK-NWPC
     CFC=CF(IK)
     IF ( CFC.NE.1 ) GO TO 4479
     D=RDX*(U(IK)-U(IMK)) + RDZ*(W(IK)-W(IMK)) + .5*RRADD*(U(IK)+U(IMK))
     DTP=-BETA*D
     RXC=RX(IK)*ABS(UO(IK))**NRESEX
     RXL=RX(IMK)*ABS(UO(IMK))**NRESEX
     RZC=RZ(IK)*ABS(WO(IK))**NRESEX
     RZB=RZ(IMK)*ABS(WO(IMK))**NRESEX
     U(IK)=U(IK) + RDX*DTP/(1.+DT*RXC)
     U(IMK)=U(IMK) - RDX*DTP/(1.+DT*RXL)
     W(IK)=W(IK) + RDZ*DTP/(1.+DT*RZC)
     W(IMK)=W(IMK) - RDZ*DTP/(1.+DT*RZB)
     P(IP)=P(IP) + RDT*DTP

**C NOTE. CHECKS FOR CONVERGENCE OF PRESSURE FIELD.**

IF ( ABS(D).GT.EPS ) IFC=1

4470    CONTINUE
4479 CONTINUE
4489 CONTINUE
4499 ITPE=ITER + 1
      IF(ITER.LT.1500) GO TO 4510
C NOTF. PRESSURES FAILED TO CONVERGE WITHIN 999 ITERATIONS.
      WRITE(IVDO,50)
      EPF=AMIN1(1.0, .1*NCYC)
      GO TO 4600
4510 IF( IFC.EQ.1 ) GO TO 4050
4600 ASSIGN 5000 TO KBC
      ITER=ITER
      ITER=0
      GO TO 1100
C NOTF. COMPUTES THE DIVERGENCE ERRORS - ER(IK) .
C
5000 ICALI=2
      GO TO 2330
5050 ASSIGN 5060 TO KBC
      GO TO 1100
5360 ITER=ITPE
      I1=1
      I2=IBP2
      K1=1
      K2=KBP2
      KK=1 - K2 NC
      DMX= 0.0
      TSMAX=-1.E+20
      TMAX=TSMAX
      WMAX=TMAX
      UM= xmax
      TMIN=+1.E+20
      WMIN=TMUX
      UMIN=WMN
      PMAX=-1.E+20
      TQMAX=PMAX

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DO 5729 I=I1,I2
KK=KK + K2NC
LWPC=-NWPC
RRADD=1./((FLOAT(I)-1.5)*DX)
DO 5019 K=K1,K2
LWPC=LWPC + NWPC
IK=KK + LWPC
IMK=IK - K2NC
IKM=IK - NWPC
CPC=CP(IK)
IF( CFC.NE.1 ) GO TO 5001
EF(IK)= RDX*( U(IK)-U(IMK)) + RDZ*( W(IK)-W(IMK))
DMX=AMAX1( DMX,ABS(E(IK)) )
+ .5*CYL*RRADD*( U(IK)+U(IMK))
5001 SIEO(IK)=SIE(IK)
TQO(IK)=TQ(IK)
TSO(IK)=TS(IK)
UO(IK)=U(IK)
WO(IK)=W(IK)
SIEO(IK)=SIE(IK)
CHIO(IK)=CHI(IK)
VAPC(IK)=VAP(IK)
LIQC(IK)=LIQ(IK)
SIEC=SIE(IK)
IF( CFC.GE.30 ) GO TO 5018
GO TO( 5002,5004,5006,5008 ),MAT
C NOTE. COMPUTATION OF TEMPERATURE FOR SODIUM MATERIAL .
5772 TEMP = -385.27 + 2.6602*SIEC + 5.9894E-04*SIEC*SIEC +
1 1.5575E-06*SIEC**3 - 2.9048E-09*SIEC**4 +
? 1.15427E-12*SIEC**5
GO TO 5010
C NOTF. COMPUTATION OF TEMPERATURE FOR WATER MATERIAL .
5094 TEMP=0.9996*SIEC + 32.0002
GO TO 5010
5796 CIT=CI-SIEC
TEMP=SI( AI, BI, CIT, -1 )
GO TO 5010
5008 CONTINUE
5017 UMAX=AMAX1(UMAX,U(IK))
WMAX=AMAX1(WMAX,W(IK))
TMAX=AMAX1(TMAX,TEMP)
TSMAX=AMAX1(TSMAX,TS(IK))
UMIN=AMIN1(UMIN,U(IK))
WMIN=AMIN1(WMIN,W(IK))
TMIN=AMIN1(TMIN,TEMP)
TQMAX=AMAX1(TQMAX,TQ(IK))
PHMAX=AMAX1(PHMAX,P(IK))
IF(I.EQ.IDG.AND.K.EQ.KDG) GO TO 5012
GO TO 5018
5012 UDG=U(IK)
WDG=W(IK)
TDG=TEMP
TIM=TIMET+DT
5018 CONTINUE
5019 CONTINUE
5029 CONTINUE
IF (ERPL.LT.1) GO TO 10000
CALL VRPRT
IF(IPRFM.GT.0) CALL VRFLM
RETURN
C
C NOTE. UPDATES TIME AND NUMBER OF CYCLES.
C
10000 TIMET=TIMET+DT
NCYC=NCYC+1
SNSIE=0.0
SMCHI=0.0
FCHI=0.0
VELCHI=0.0
C
COMPUTE PLUME CENTER AND SIGMA (HEIGHT) FOR CHI DISTRIBUTION
DO 11150 K=2,KBP1
DO 11160 I=2,IBP1
IK=1+NWPC*(((I-1)*KBP2)+K-1)
CIT=CJ-SIE(IK)
TEMPC=SI(AI,BI,CIT,-1)
RHOC=A*R+TEMPC*TEMPC+BR*TEMPC*CR
SMSIE=SMSIE+RHO*CZ*DS*SIE(IK)
SMCHI=SMCHI+(CHI(IK)-BKGND)
PCHI=PCHI+(FLOAT(K)-1.5)*DZ*(CHI(IK)-BKGND)
VELCHI=VELCHI+WSF(K)*{(CHI(IK)-BKGND)
11160 CONTINUE
11150 CONTINUE
YPUME=PCHI/SMCHI
VELCHI=VELCHI/SMCHI
DWDNS=DWDNS+VELCHI*DT
IF(IDIAG.GT.0) WRITE(IVDO,51) TIMET,NCYC,ITER,DT,DMX
IF(IDIAG.EQ.0) GO TO 11000
C NOTE: CHECKS ON TIME WHEN TO PRINT AND/OR PLOT FLM.
IF(IDATIN.EQ.1) GO TO 11001
11000 IF(TIMET+1.0E-5.LT.TPRT) GO TO 11100
TPRT=TPRT+TPR
CALL VRPRT
GO TO 11100
11001 TPRT=TPRT+TPR
11100 IF(IPRFM.LT.1.OR.TIMET+1.0E-5.LT.TPLT) GO TO 11200
TPLT=TPLT+TPL
WRITE(IVDO,60) YPUME,VELCHI,DWDNS
60 FORMAT(' ',15HPLUME CENTER AT,F8.2,6H FEET.,15H PLUME SPEED IS,
1F8.2,22H DOWNWIND DISTANCE IS,F6.0)
WRITE(IVDO,63) SMSIE
63 FORMAT(4H ,TOTAL ENERGY ON MESH IS ',E12.5)
WRITE(IVDO,51) TIMET,NCYC,ITER,DT,DMX
CALL VRPLM
11200 CONTINUE
C TIMING SECTION FOR RESTARTING PROGRAM ON A COARSER MESH
11300 IF(TIMET+1.0E-5.LT.TRSTRTR(NRSTRT)) GO TO 11400
CALL COARSE
NRSTRT=NRSTRT+1
DR=DX
RDR=RD?
RD=1/(DR*DR)
RDM=RDR
RDP=RDM
RDZC=RDZ
RDZP=RDM
WRITE(1,40) TIMET, DX, DZ
40 FORMAT (22H PROGRAM RESTART AT, P10.3,12H SECONDS', DX = ',I6.2,', DZ = ',I6.2)
CALL VRPR
do CONTINUE
C NOTE. CHECKS ON TIME WHEN TO WRITE MAG TAPE FILE.
12000 IF( TWD.GE.1.E+5) GO TO 12100
   IF( (TIMET+1.0E-5 .LT. TWD) ) GO TO 12100
   TWD=TWD+TTD
   CALL TAPWRI
   GO TO 12100
12101 TWD=TWD+TTD
C NOTE. COMPUTATION OF SPECIFIC DIAGNOSTIC VARIABLES.
12100 GO TO KDAG,( 12200, 12500, 13000)
C NOTE. OUTPUT OF DIAGNOSTIC VARIABLES IF IDIAG=1 FROM CARD NO. 3.
12200 WRITE(IYDO,54) IDG,KDG,UDG,WDG,TDG,UMAX,UMIN,WHAX,WHIN,TMAX,TMIN
1,TSMAX, EPS
C
C NOTE. COMPUTATION OF TIMING IN VARIOUS PORTIONS OF THE PROGRAM.
C
12500 IF( TIMET+1.E-10 .LT. TFIN) GO TO 13000
C
C NOTE. CHECKS ON TIME WHEN TO FINISH.
C
13000 IF( TSTFP.LT.EM6) GO TO 13010
   IF( MCYC.LT.2) GO TO 13010
   ALEN=A1MIN1( DX, DZ )
   VEL=A1MAX1( UMAX,WHAX )
IF ( VEL_GT_EM6 ) DT=TSTEP*ALENG/VEL
DTDF=TSTEP*RDXZS/TSMAX
VELNEW=AMAX1( UMAX, WMAX )
TAUDT=0.2*VELNEW/( VELNEW-VELOLD+EM6 )
TAUDT=ABS( TAUDT )
DT=0.51( DT,DTDF,TAUDT )
RDT=1./DT
13010 IDATIN=0
IF( TIMET+1.0E-5 .LT. TFIN ) GO TO 100
RETURN
C   * FORMATS *** FORMATS ***** FORMATS ***** C
50 FORMAT(1H ,75H *** ERROR 004 - PRESSURES FAILED TO CONVERGE WITHIN
1 1500 ITERATIONS . *** )
51 FORMAT(1H ,5H TIME=,1PE12.4,3H , ,14HCYCLE NUMBER =,I5,3H ,
1 289 PRESSURE ITERATION NUMBER =,I4,3H , ,4HDT =,E12.4,3H ,
2 16HMAX DIVERGENCE =,E12.4)  
52 FORMAT(1H ,5X,62H THE FOLLOWING DIAGNOSTICS OCCUR AFTER TIME HAS B
1EEN UPDATED )
54 FORMAT(1H ,5X,2H I=,I3,3H K=,I3,4H U=,1PE12.5,4H W=,E12.5,
1 4H T=,E12.5,3H * ,6H UMAX=,E12.5,6H UMIN=,E12.5/6H WMAX=,E12.5,
2 6H WMIN=,E12.5,17X,7H Tmax=,E12.5,7H TMIN=,E12.5,7H TSmax=,
3 E12.5/TH EPS=,E12.5)  
55 FORMAT(1H ,5X,10HTIME/CYC =,1PE10.3,10H TOT TIME=,E10.3,
1 10H I/O T/CYC=,E10.3,10H TOT I/O =,E10.3)
END