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An Introduction to the THERMIT Thermal Hydraulic Reactor Computer Codes at M.I.T.

by

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ABSTRACT

The THERMIT thermal hydraulic reactor computer codes developed at MIT are described. The codes include THERMIT-2, THIOD, NATOF-2D, THERMIT-3, THERMIT-2D-PLENUM, THERFLIBE, THERLIT, THERMIT (sodium) and THERMIT-SIEX. Descriptive code summaries and sample code results from each THERMIT version are given. Finally, a complete THERMIT bibliography is presented.

PREFACE

This document is written for THERMIT users at MIT. Descriptive code summaries for all of the versions of THERMIT are given.

For THERMIT users outside of MIT, a more appropriate guide would be MITNE-243, "Availability of the THERMIT Thermal Hydraulic Reactor Computer Codes at MIT." In that reference, only those versions of THERMIT which are publicly available are described (i.e. THERMIT-2, THIOD, NATOF-2D).

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I. INTRODUCTION

Several versions of the thermal hydraulic reactor code THERMIT have been developed at MIT for various reactor engineering applications. Despite the differences introduced by the various problem specific requirements, most THERMIT versions use the same fundamental engineering approaches developed in the original THERMIT. Therefore, a description of the features of the original THERMIT will provide a basis for understanding the code features generally shared by all versions of THERMIT. Subsequently, descriptive code summaries will be given which will establish the individual code differences.

II. THERMIT DESCRIPTION

THERMIT is a three-dimensional cartesian coordinates computer code originally developed at MIT under EPRI sponsorship for the thermal hydraulic analysis of reactor cores.(1) It employs a two fluid, six equation model for the two phase fluid dynamics. THERMIT also employs a radial heat conduction model of the fuel pins which is coupled to the coolant by a flow regime dependent heat transfer model.

The governing fluid dynamics partial differential equations are solved numerically by a modified version of the I.C.E. method. This method is used in a semi-implicit form which gives rise to a Courant time step stability limit of

$$\Delta t < \frac{\Delta z}{v_{max}}$$

where Δz is the mesh spacing and v_{max} is the maximum fluid velocity of either phase. Due to the mathematical illposedness of the fluid dynamics difference equations, exceedingly fine mesh spacing should be avoided.

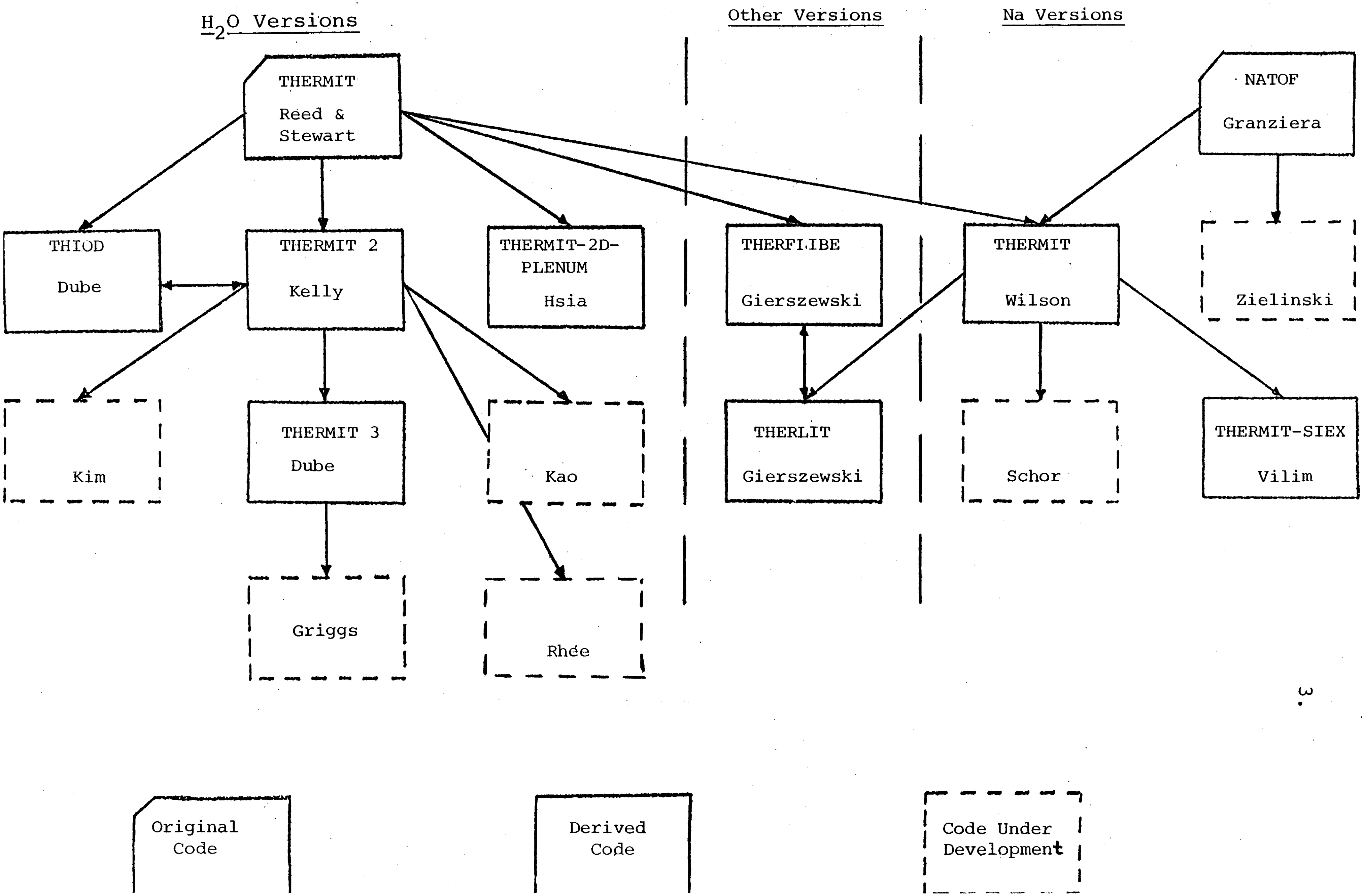
The radial heat conduction equations in the fuel pins are solved using a fully implicit finite difference method. These equations include a gap conductance model between the fuel pellet and cladding.

THERMIT was developed using MULTICS on a Honeywell 6180, but conversion to IBM machines is possible. THERMIT makes exclusive use of SI units. Like other thermal hydraulic reactor codes, THERMIT allows either the conventional pressure or velocity boundary conditions at the top and bottom of the reactor core.

III. CODE DEVELOPMENT

A THERMIT development history is graphically shown in Figure 1. Developmental work is continuing on an advanced coupled neutronics and thermal hydraulic code for LWR analysis and on a more complete sodium version which will have both four and six equation model capability. Other areas under research and development are steam generator modelling, CHF assessment, vapor draft phenomena and improved methods of sodium boiling simulation.

Figure 1: Code Development



IV. CODE SUMMARIES

A. THERMIT-2

1. Author: John Kelly

2. Advisor: Mujid S. Kazimi

3. Relationship to Other Versions of THERMIT: THERMIT-2 was developed directly from the original THERMIT.

4. Capabilities and Features: THERMIT-2 was developed primarily to give the original THERMIT the capability of LWR subchannel analysis. This was done by a modification of the coolant to fuel rod coupling which allows coolant centered sub-channels. In addition, three other major modifications to THERMIT were made. First, the liquid vapor interfacial exchange terms were improved. Second, a two phase mixing model was added to predict turbulent mixing effects between mesh cells. Finally, the heat transfer models and CHF correlations were improved.

5. Verification Tests: During the assessment of the modifications made to THERMIT, numerous comparisons with reported experimental measurements were made. The liquid vapor interfacial mass exchange model was tested against some 30 void fraction experiments. For example, Figure 2 shows a comparison between THERMIT and the data of Maurer(2). The

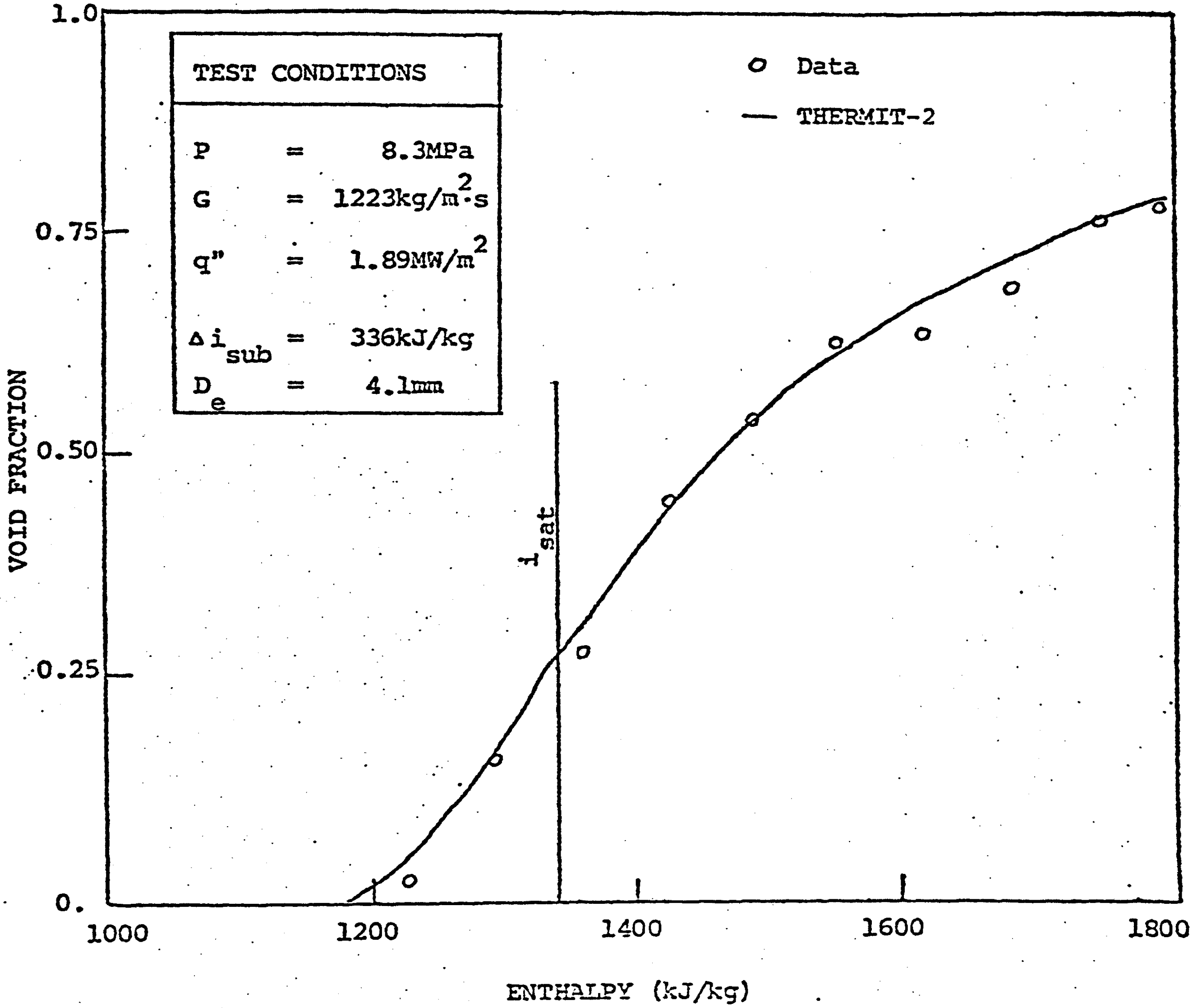


Figure 2: Void Fraction versus Enthalpy - Maurer Case 214-3-5

turbulent mixing model was tested against experimental velocity and quality data from the GE nine-rod bundle tests[3] and from the Ispra sixteen rod bundle tests[4,5]. The heat transfer models were tested against experimental wall temperature and CHF data from the GE nine rod transient CHF measurements and from the steady state experiments of Bennett[6]. Sample comparison results from these tests are shown in Figures 3-5.

6. <u>Experience and Code Comparisons</u>: THERMIT-2 was the first two-fluid reactor thermal-hydraulics computer code which included a turbulent mixing model to have been shown to correctly predict the thermal-hydraulic behavior of rod bundles. Other codes which are similar in function are listed and compared with THERMIT-2 on Table 1.

THERMIT-2 is the most widely used of the THERMIT codes at MIT. It has been applied to a wide range or problems and considerable experience has been gained.

Convergence problems were encountered when THERMIT-2 was applied to a mixed convection-natural circulation problem[12]. When applied to steam generator modelling, however, THERMIT-2 showed convergence when the original THERMIT could not. That particular problem has been traced to a faulty subscript in the relative velocity term of the

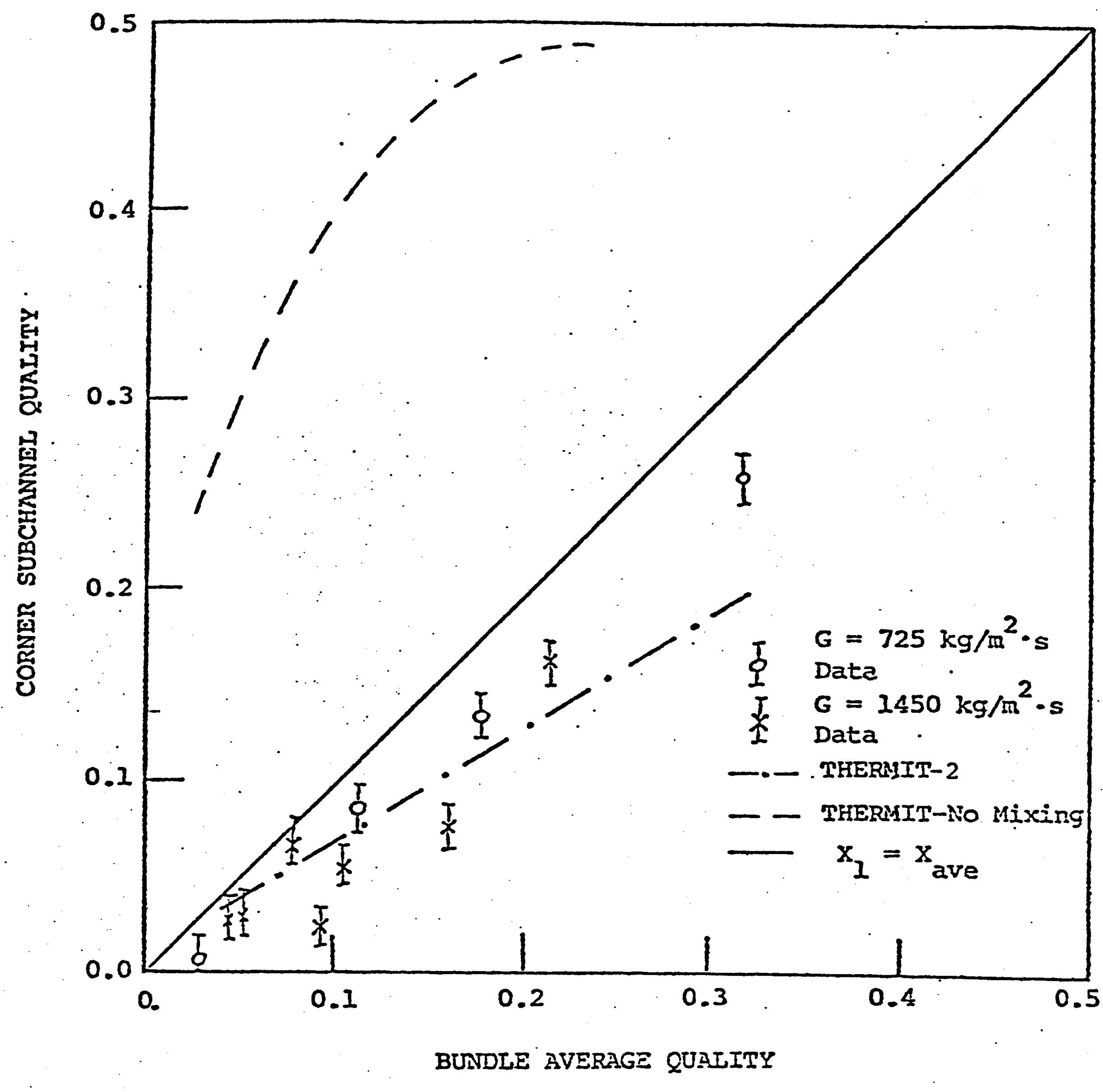


Figure 3: Comparison of Measured and Predicted Exit Quality in Corner Subchannel for G.E. Uniformly Heated Cases

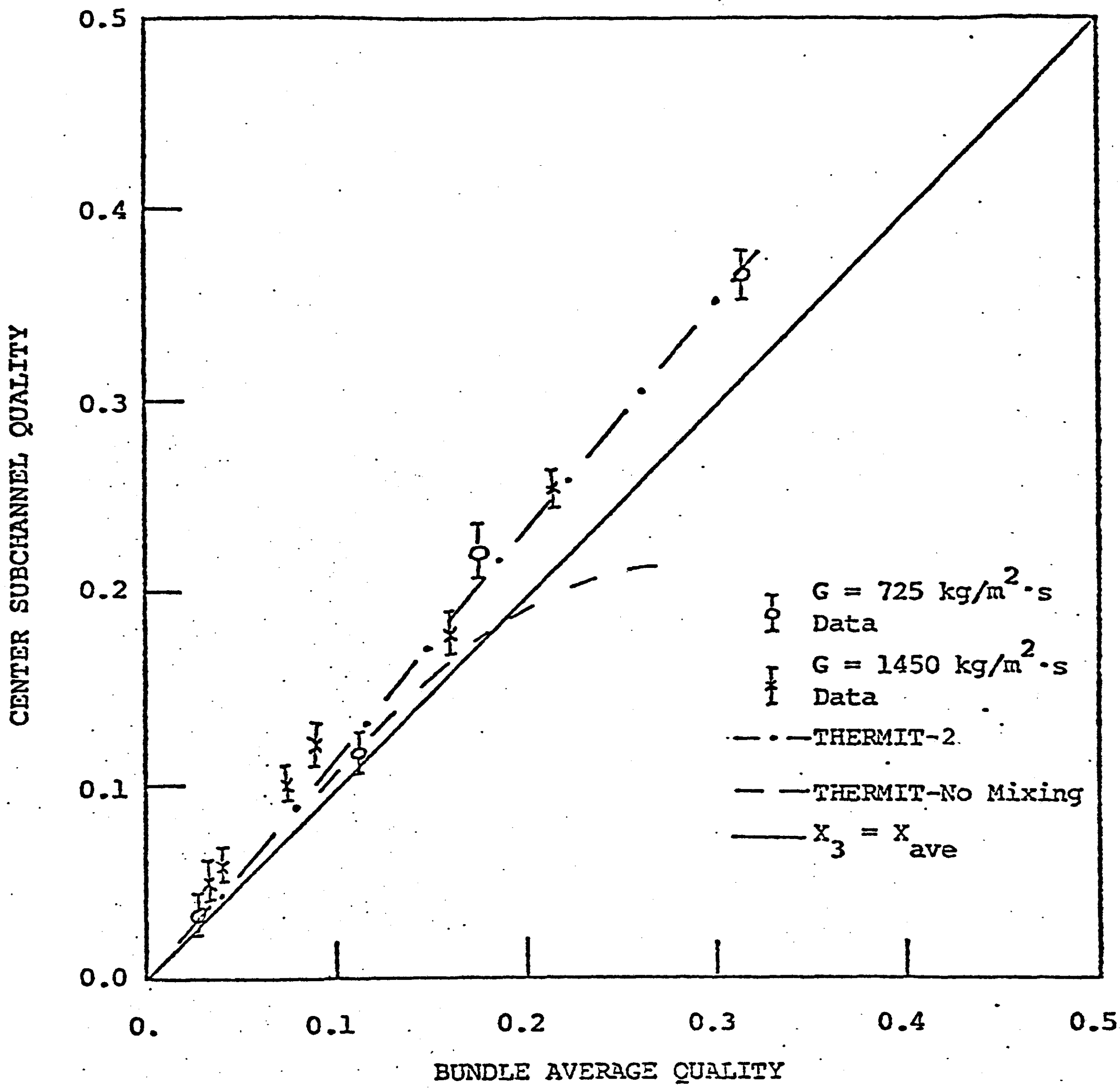


Figure 4: Comparison of Measured and Predicted Exit Quality in Center Subchannel for G.E. Uniformly Heated Cases

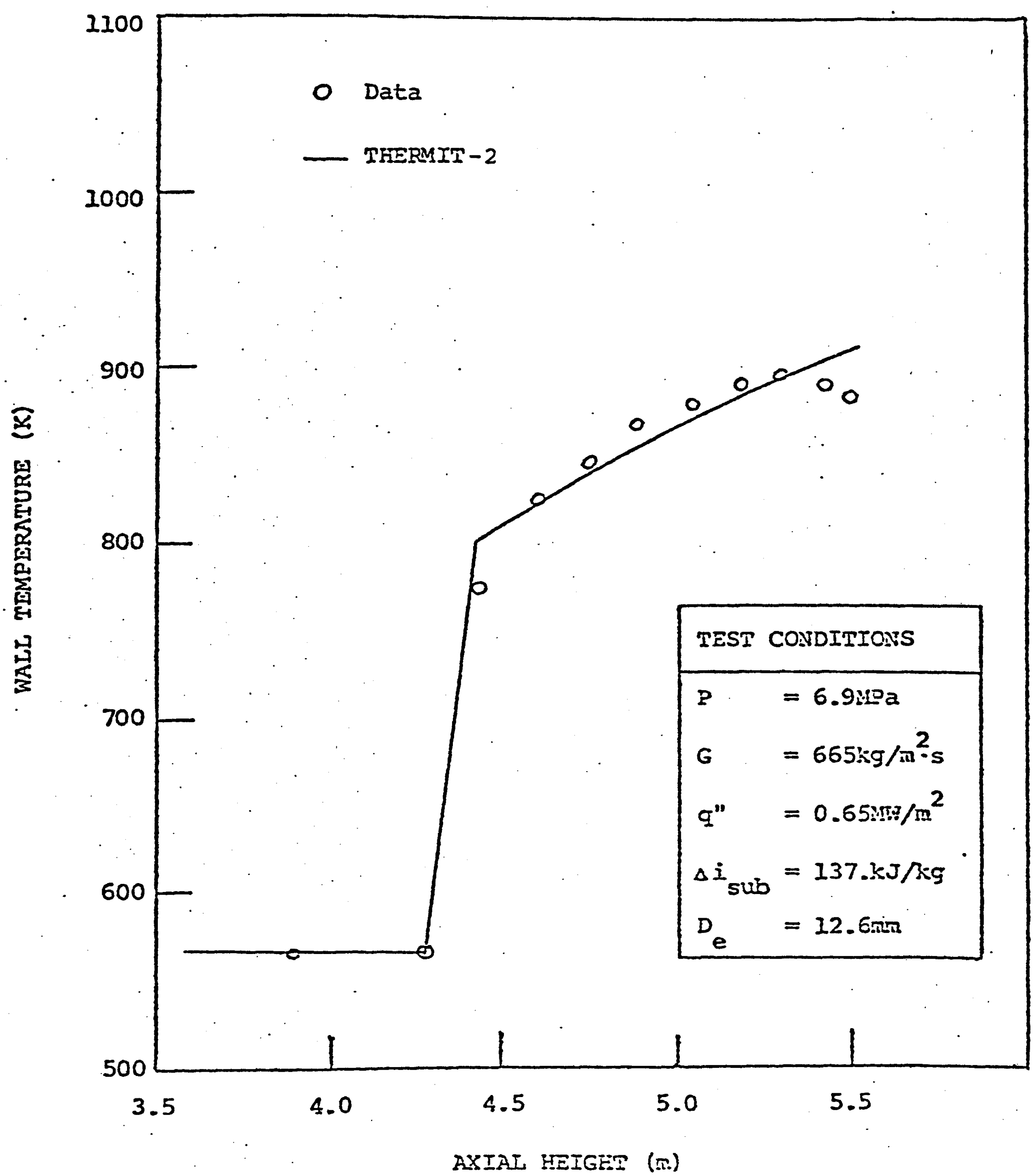


Figure 5: Wall Temperature Comparisons for Bennett Case 5332

(Length = 5.56m)

TABLE 1

Features of Some Thermal-Hydraulic Computer Codes

Computer Code	Type of Analysis	Method of Analysis	Two-Phase Flow Model	Solution Technique
COBRA IIIC (7)	Component	Subchannel	Homogeneous Equilibrium	Marching Method
COBRA IV (8)	Component	Subchannel	Homogeneous Equilibrium	Marching Method or I.C.E. Method
WOSUB (9)	Component	Subchannel	Drift Flux	Marching Method
COMMIX-2 (10)	Component	Distributed Resistance	Two-Fluid	I.C.E. Method
THERMIT	Component	Distributed Resistance	Two-Fluid	I.C.E. Method
TRAC (11)	Loop	Distributed Resistance	Two-Fluid or Drift Flux	I.C.E. Method

momentum conservation equation[13].

At least one restriction on the flexibility of THERMIT-2 has been found which is not mentioned in the user's manual. THERMIT-2 is programmed to accept only four different types of fuel rods for any one problem.

A few problems still remain to be resolved. When THERMIT-2 is applied to air-water systems, no heat transfer coefficient between the air and water is specified[13]. This makes thermal equilibrium difficult to model. Also, inconsistencies have been found in the definitions and use of the film and vapor temperatures[14].

B. THIOD

1. Author: Don Dube
2. Advisor: David D. Lanning
3. Relationship to Other Versions of THERMIT: Even though THIOD was developed from the original THERMIT, a major numerical revision effort was required.
4. Capabilities and Features: THIOD (thermal-hydraulic; implicit; one-dimensional) was developed primarily to address the restrictive Courant time step stability limit of THERMIT. The two fluid six equation model difference equations used in THERMIT were rewritten into a fully implicit one-dimensional form. In addition, a point kinetics neutronic package was coupled to the thermal-

hydraulics via some simple reactivity feedback loops. However, THIOD does not have the capability to handle flow reversals. Therefore, THIOD is a useful code for the analysis of mild reactor transients which are of a one-dimensional nature. Examples of this kind of transient are BWR feedwater water failures, flow coastdowns or turbine trips. THIOD may also be used to model one-dimensional flow experiments, steam generator tubes or other reactor system components.

5. Verification Tests: Although the primary verification effort for THIOD involved comparisons with THERMIT-2, one of the supplemental assessment efforts performed was a modelling of the Peach Bottom 2 turbine trip measurements. While most of the experimental data was available(15), critical data on the reactivity coefficients was proprietary(16). Typical reactivity coefficients for end of cycle conditions were therefore used. Neutron flux squared weighting of the void reactivity coefficients was also found necessary.

   Figure 6 shows a comparison between the measured turbine trip results and the THIOD calculations for the reactor power. Within the limitations of the point kinetics model, good agreement is seen.

6. Experience and Code Comparisons: Comparisons between THERMIT-2 and THIOD were made in sufficient numbers to validate the THIOD code for thermal hydraulic calculations. The solution technique used in THIOD

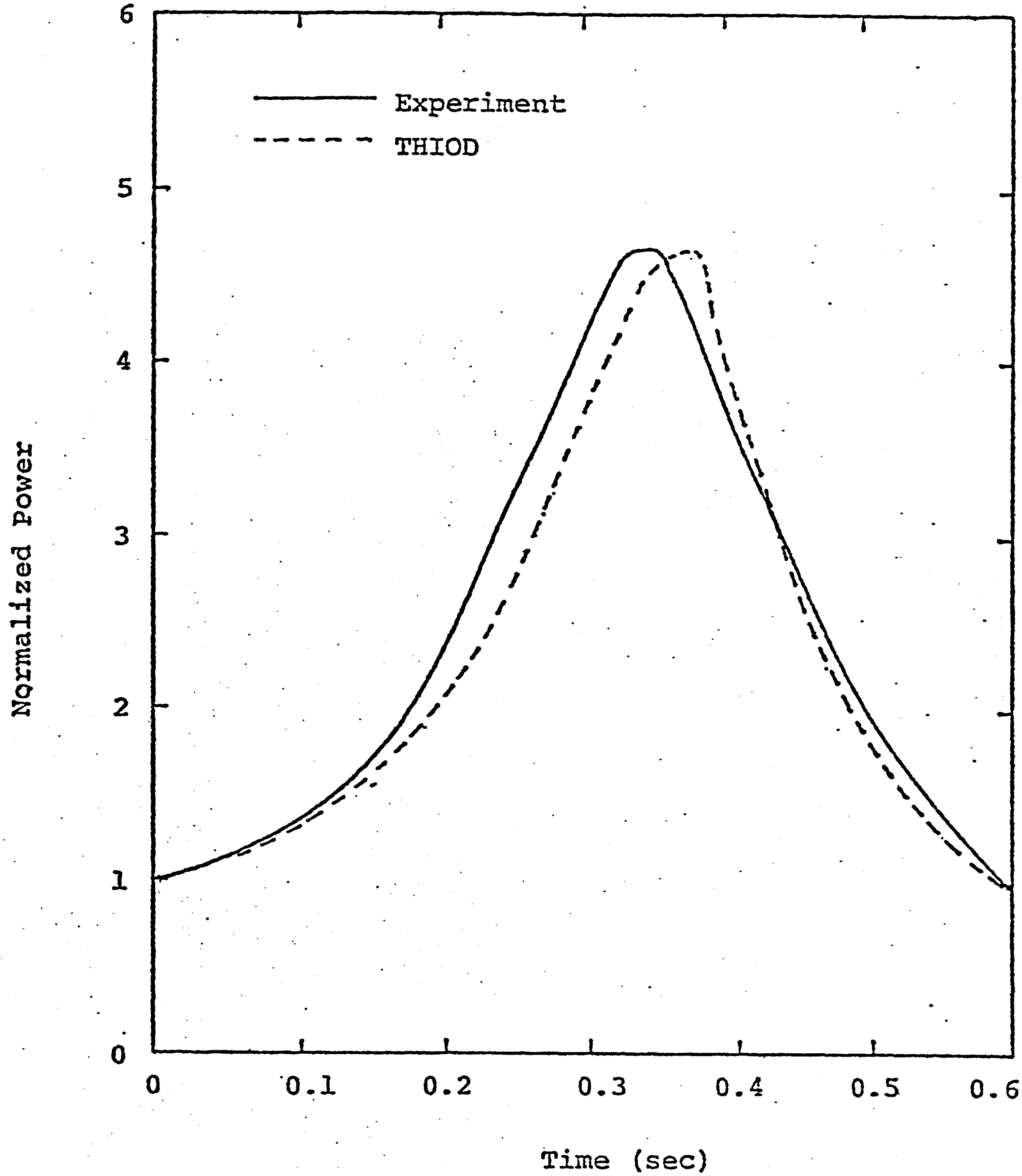


Figure 6: Peach Bottom Turbine Trip 1 Power History

was found to generate steady state solutions about five times faster than the semi-implicit method used in THERMIT-2. Additionally, levels of convergence several orders of magnitude greater than the THERMIT-2 results were attained. For mild thermal hydraulic transients, time step sizes up to about twenty times larger than the Courant limit were found to yield admissibly accurate results.

When the neutronic feedback was included, however, it was found that time step sizes only somewhat larger than the Courant limit could be used. This was due primarily to a lack of accuracy observed in the results and not particularly due to any stability concerns.

THIOD is compared to other coupled neutronic and thermal hydraulic reactor codes on Table 2. Of all the codes, THIOD appears best suited for long slow BWR transients such as flow coastdowns and feedwater heater failures.

TABLE 2: Summary of Neutronic-Thermal-Hydraulic Codes

	THERMAL-HYDRAULICS	NEUTRONICS
CHIC-KIN (17)	1-D, single channel model	point kinetics
PARET (18)	four channel model	point kinetics
TWIGL (19)	Lumped parameter model, no boiling allowed	2-D, 2-group finite difference diffusion theory model
BNL-TWIGL (20)	time-dependent two-phase model	2-D, 2-group finite difference diffusion theory model
FX2-TH (LMFBR) (21)	1-D with no boiling	3-D, multi group diffusion theory, quasistatic method.
SAS2A (LMFBR) (22)	1-D with sodium bubble model	point kinetics
HERMITE (23)	2-D homogeneous equilibrium model	3-D finite element diffusion theory, 1 to 4 groups
MEKIN (24)	2-D homogeneous equilibrium model	3-D finite difference 2 group diffusion theory
THIOD	1-D, two fluid, non-equilibrium model for LWR	point kinetics
THERMIT-3 (25)	3-D, two fluid model, non-equilibrium	point kinetics
QUANDRY (23)	lumped parameter model, no boiling	3-D, 2 group nodal diffusion theory model

C. NATOF-2D

1. Author: Mario Granziera

2. Advisor: Mujid S. Kazimi

3. Relationship to Other Versions of THERMIT: NATOF was developed independently of THERMIT, but it makes use of many of the same methods used in THERMIT.

4. Capabilities and Features: NATOF was developed for the analysis of LMFBR fuel assemblies under non-uniform radial flow conditions. This is possible either during sodium boiling or at low coolant flow rates.

   NATOF is a two-dimensional code written in R-Z coordinates. Like THERMIT, it employs two-fluid six-equation thermal hydraulics difference equations in a semi-implicit form. Some of the constitutive relationships and correlations used in NATOF were developed at MIT. The interfacial mass exchange rate correlation is based on the kinetic theory of boiling and condensation[27]. The interfacial momentum exchange rate correlation was empirically based on the KFK experiments in Karlsruhe[28]. A relationship for the interfacial heat exchange rate was developed from theoretical principles[29].

5. Verification Tests: Two experimental tests were simulated with NATOF as part of its code assessment

effort. The first test simulated was the P3A experiment of the Sodium Loop Safety Facility in Idaho[30]. Table 3 compares the experimental results with the NATOF predictions. SOBOIL[31] results are also given. The second test simulated was the steady state predictions of BACCHUS of the GR19 experiment performed in France[32]. Table 4 compares the experimental measurements of the maximum coolant temperatures with the NATOF predictions as a function of flow rate.

6. Experience and Code Comparisons: It has been found that NATOF is very sensitive to the interfacial mass exchange rate correlation. This is due to the density difference between the two phases of sodium.

NATOF provides a two-dimensional analysis capability for the analysis of LMFBR fuel assemblies under non-uniform radial flow conditions. Such capability is not available in the widely used code SAS[22]. Other comparable codes which are also under further development are COMMIX[10], SABRE (U.K.)[33], BACCHUS (France)[32] and an advanced sodium version of THERMIT.

TABLE 3

P3A Experiment Event Sequence Times (s)

	Experimental Data	NATOF-2D	SOBOIL
Boiling inception	8.8	8.9	8.9
Boiling at DAS 23 (35.7 in., interior)	10.0	9.7	9.5
Boiling at DAS 12 (32.7 in., edge)	10.0	9.9	9.9
Inlet flow reversal	10.15	10	9.9

TABLE 4

Mass Flow Rate
and Temperatures for the GR19 Experiment

Flow (kg/sec)	T_{max}(°C) (measured)	T_{max}(°C) (NATOF-2D)
.606	693	694
.476	766	768
.405	825	827
.350	890	892
.329	918	920 (Boiling)
.311	923	921
.293	926	921
.277	926	922
.265	926	925
.260	944	927

D. THERMIT-3

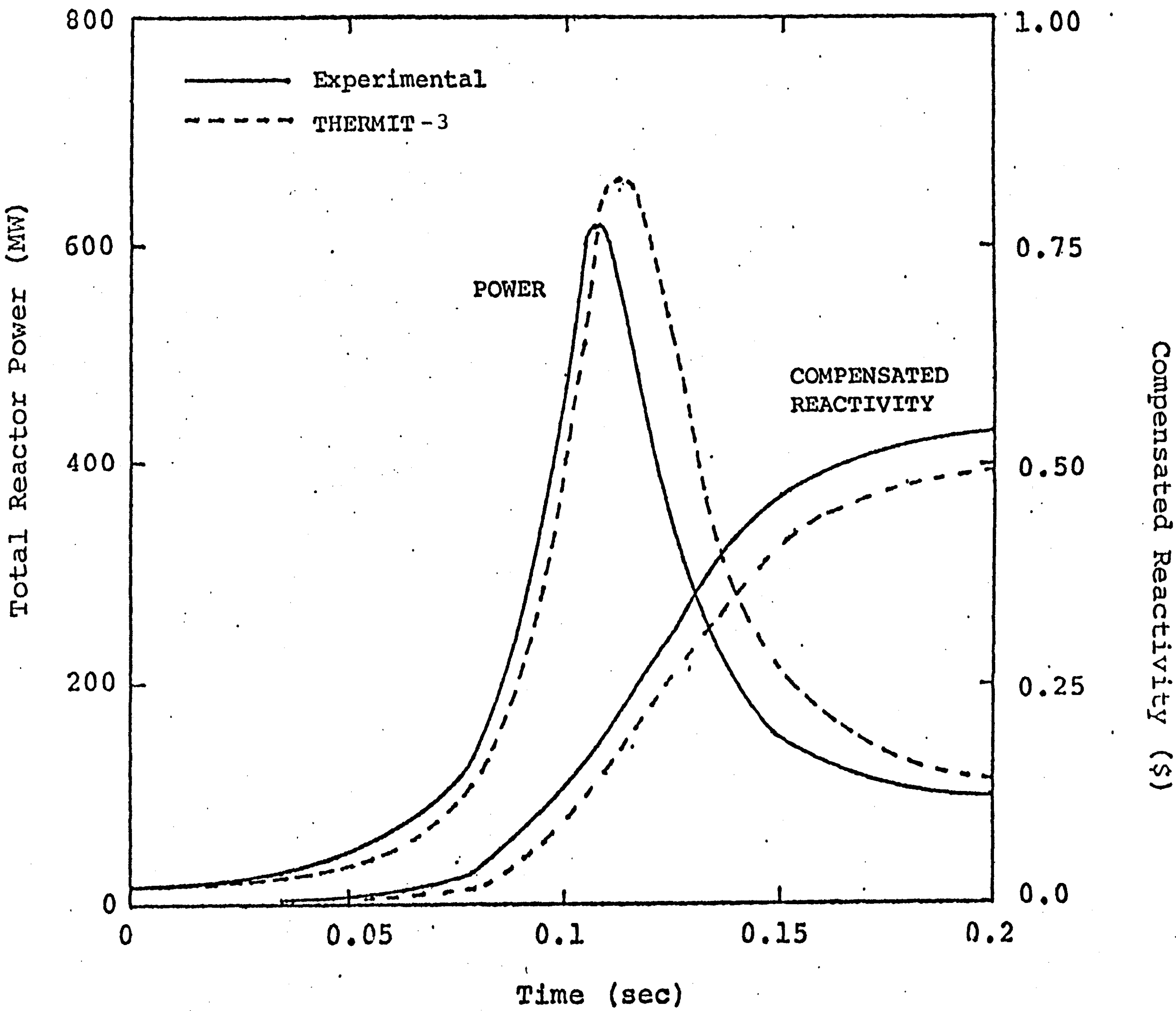
1. Author: Don Dube

2. Advisor: David D. Lanning

3. Relationship to Other Versions of THERMIT: THERMIT-3 was developed directly from THERMIT-2.

4. Capabilities and Features: THERMIT-3 is the result of a coupling of the point kinetics neutronic model GAPOKIN[(34)] with the thermal hydraulic code THERMIT-2. THERMIT-3 is therefore a three-dimensional coupled neutronics and thermal hydraulics reactor engineering code. It is well suited for the simulation of combined neutronic and thermal hydraulic reactor transients with characteristic time constants less than one second. Examples of this kind of transient are rod drop or turbine trip accidents.

5. Verification Tests: The principle code assessment effort of THERMIT-3 was a simulation of the SPERI-III E-core reactor transient test 86[(35)]. In that experiment there was a rapid insertion of $1.17 of reactivity into a critical core. A comparison of the measured reactor power and the THERMIT-3 calculations is shown in Fig. 7. Possible causes for the slight discrepancy seen in the results are the lack of a fuel rod expansion model in THERMIT-3 and shortcomings in the reactivity insertion models.



'igure 7: SPERT III E-Core Test 86:. Experimental and THERMIT-3 Predictions

6. Experience and Code Comparisons: THERMIT-3 is listed with several other coupled neutronic and thermal hydraulic codes on Table 2. THERMIT-3 is a precursor of an advanced coupled code which will combine QUANDRY[26] with THERMIT-2.

   THERMIT-3 has been extensively compared with THIOD. It has been found that THERMIT-3 is computationally slower than THIOD, but more capable of handling severe reactor transients.

E. THERMIT-2D-PLENUM

1. Author: Der-Yu Hsia
2. Advisor: Peter Griffith
3. Relationship to Other Versions of THERMIT: THERMIT-2D-PLENUM was derived from the original THERMIT.
4. Capabilities and Features: THERMIT-2D-PLENUM is the result of the application of THERMIT to steam generator flow instability modeling. The primary purpose was an analytical comparison to the experimental results from a steam generator model. The principle code modification which was made was a transformation of the top and bottom boundary conditions in THERMIT to side boundary conditions more appropriate for steam generator geometry.
5. Verification Tests: None
6. Experience and Code Comparisons: It was found that the interfacial momentum exchange term caused

divergent solutions to be calculated when THERMIT-2D-PLENUM was applied to the experiment. Convergent solutions could be obtained only by increasing either the interfacial drag or wall friction terms by a factor of about 70. Unfortunately, these solutions gave inaccuracies in the void fraction results. Therefore, a different interfacial drag model was implemented into the code. It gave better but not altogether satisfactory results.

The principle problem appears to be the lack of an accurate model for the vortex and secondary flow seen in the experimental tests.

F. THERFLIBE and THERLIT:

1. Author: Paul Gierszewski
2. Advisor: Neil E. Todreas
3. Relationship to Other Versions of THERMIT: THERFLIBE was developed from the original THERMIT written by Reed and Stewart. THERLIT was developed from the original sodium version of THERMIT written by Wilson.
4. Capabilities and Features: THERFLIBE and THERLIT were developed to model fusion blanket thermal hydraulics. The basic LWR geometry of THERMIT limits the modelling of complex fusion blanket geometries. The primary programming changes were the addition of static uniform magnetic field effects and the change in liquid properties from water and sodium to flibe and lithium.

5. Verification Tests: None

6. Experience and Code Comparisons: THERFLIBE and THERLIT have been used to make scoping calculations of the relative importance of natural circulation in fusion blankets[36]. The codes functioned satisfactorily over a wide range of magnetic field strengths.

G. THERMIT (The original sodium version)

1. Author: Greg Wilson

2. Advisor: Mujid S. Kazimi

3. Relationship to Other Versions of THERMIT: The original sodium version of THERMIT was developed directly from the original THERMIT written by Reed and Stewart.

4. Capabilities and Features: The primary revision required to produce the sodium version of THERMIT was a change of the fluid properties, friction factor, and interfacial exchange rate correlations from water to sodium. In addition, the fuel pin model was given greater flexibility. Mechanisms for heat lost to the structure and radial heat loss through the coolant were also included.

5. Verification Tests: The sodium version of THERMIT was tested by a simulation of the THORS Bundle 6A experiments performed at Oak Ridge[37]. Figure 8 is a sample comparison of the experimental results

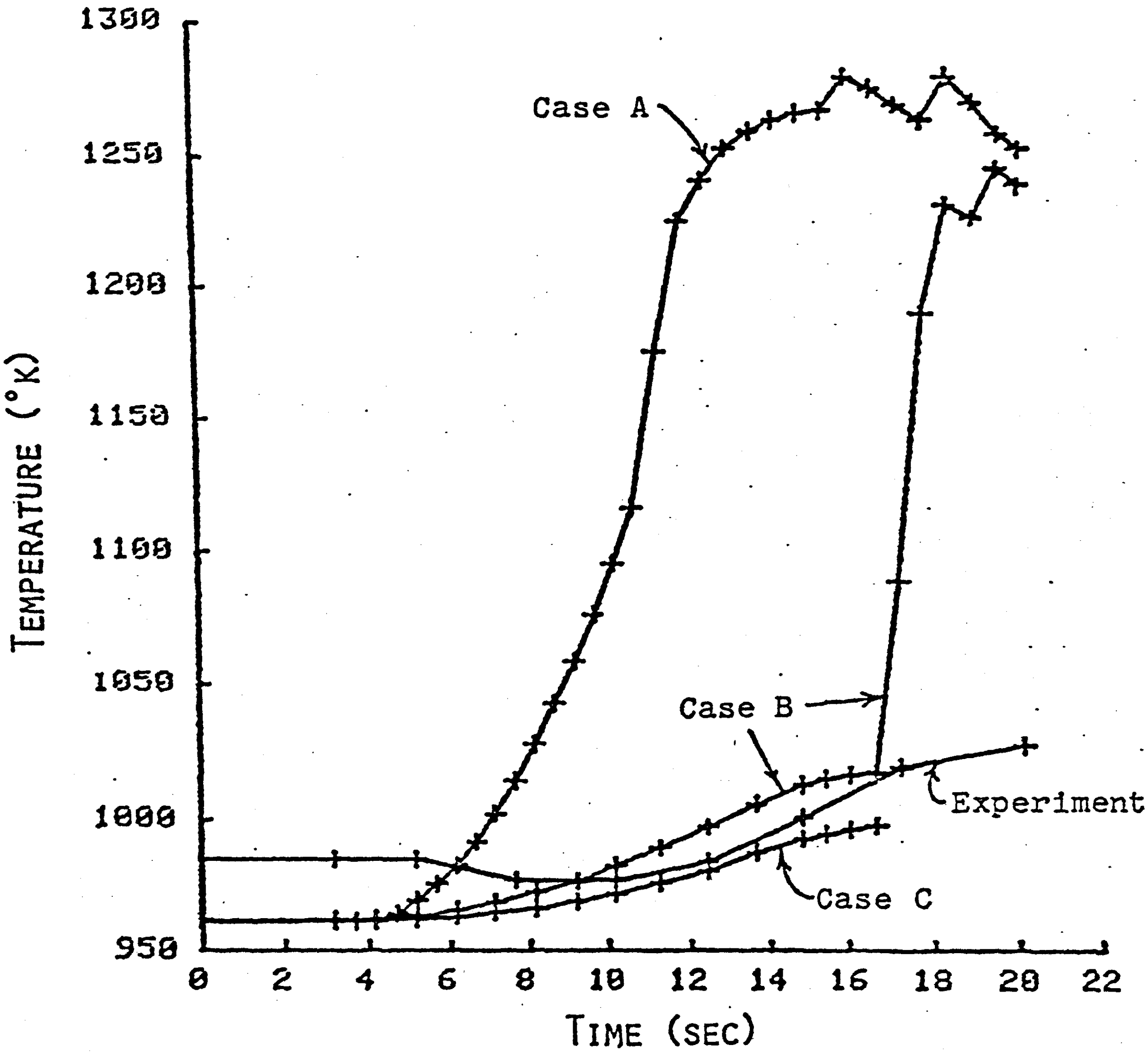


Figure 8: THORS Bundle 6A - Temperature History at z=54 inches (Test 71h, Run 101)

with the THERMIT predictions. Case A does not include either the radial heat loss through the coolant. Case B includes only the radial heat loss through the coolant. Case C includes both heat loss mechanisms. It is seen that the inclusion of the two heat loss mechanisms improve the THERMIT predictions substantially.

6. Experience and Code Comparisons: Certain numerical problems were encountered with the onset of sodium boiling which were never fully resolved. However, more advanced versions of THERMIT are being developed specifically for sodium boiling.

H. THERMIT-SIEX

1. Author: Rick Vilim
2. Advisor: Mujid S. Kazimi
3. Relationship to Other Versions of THERMIT: THERMIT-SIEX was developed from the original sodium version of THERMIT.
4. Capabilities and Features: Since LMFBR fuel pin properties change significantly over time, the fuel performance code SIEX[38] was coupled to the sodium version of THERMIT to produce a code capable of steady state and transient thermal hydraulic analysis at any time during the fuel lifetime. Burn-up induced changes such as fuel pin dimensions and gap conductivity which are computed by SIEX are passed

free of user intervention to THERMIT. THERMIT is then allowed to execute normally.

5. Verification Tests: No experimental tests have ever been simulated with THERMIT-SIEX. However, tests have been made which verify that all of the input and output variables of SIEX are passed correctly to and from THERMIT.

6. Experience and Code Comparisons: None

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