

MITNE-243

Availability of the THERMIT Thermal Hydraulic  
Reactor Computer Codes Through M.I.T.

by

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## ABSTRACT

Three of the THERMIT thermal hydraulic reactor computer codes are available through the Department of Nuclear Engineering at MIT. The three available codes are THERMIT-2, for LWR subchannel analysis, THIOD, for BWR analysis and NATOF-2D, for LMFBR sodium boiling analysis.

Descriptive summaries and sample results are given for each code. In addition, a list of THERMIT references is given.

## PREFACE

This document is written for THERMIT users outside of MIT. Code descriptions are given for the three THERMIT versions which are publicly available through the Nuclear Engineering Department.

For THERMIT users at MIT, however, a more detailed description of these three THERMIT reactor computer codes as well as several other versions is found in MITNE-242, "An Introduction to the THERMIT Thermal Hydraulic Reactor Computer Codes at M.I.T."

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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.<sup>(1)</sup> 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  $\Delta z$  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

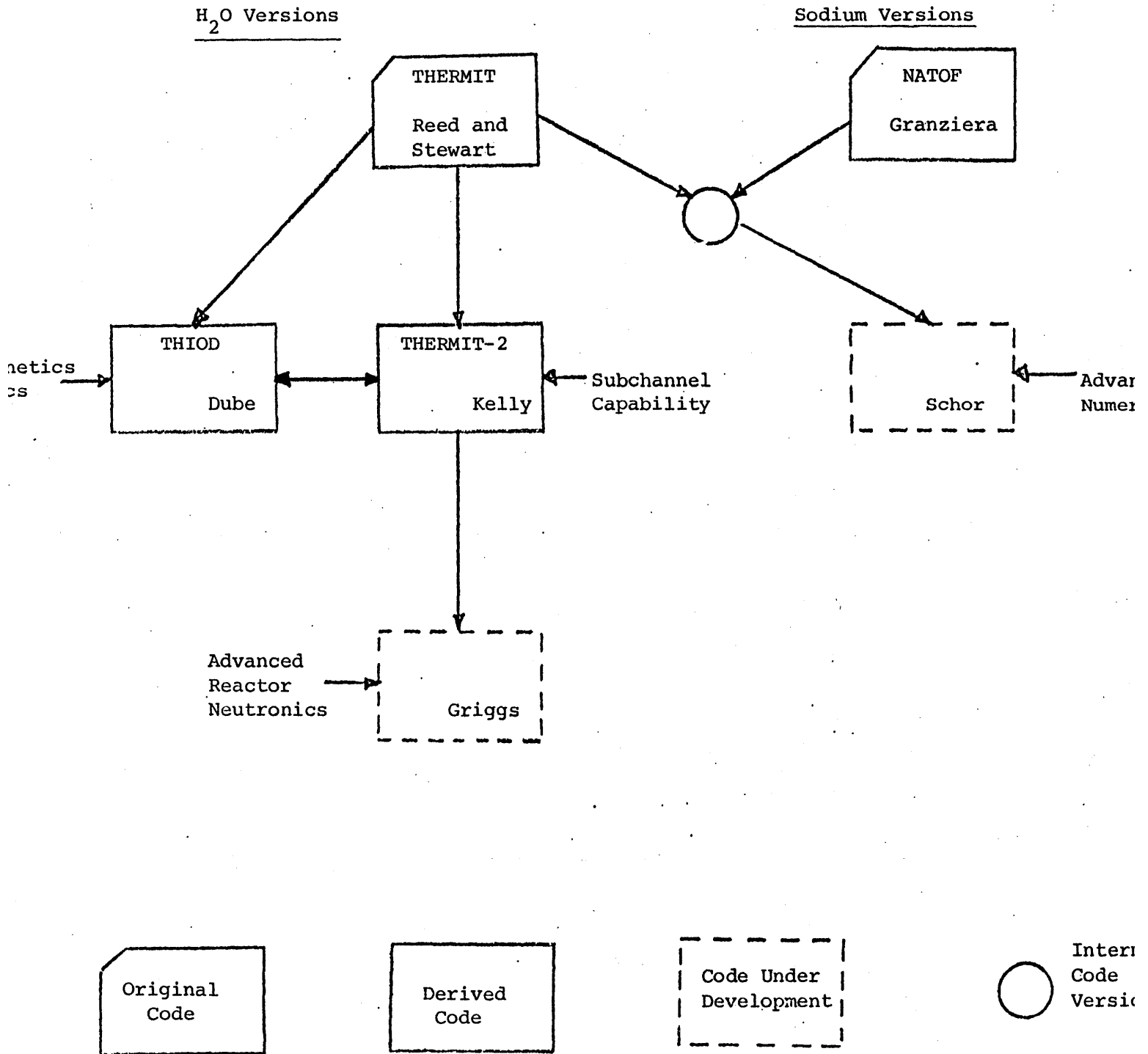
A THERMIT development history is graphically shown in Figure 1. Developmental work is continuing on an advanced coupled neutronics and thermal hydraulic code for LWR analysis and on a more complete sodium version which will have both four and six equation model capability.

### IV. CODE AVAILABILITY

Three versions of THERMIT are currently available through the Nuclear Engineering Department of MIT. All code requests should be directed to Ms. Rachel Morton c/o Nuclear Engineering



Figure 1: Code Development



Department. A tape copy of the requested code with documentation will be sent along with a bill to cover expenses. Code summaries of the three available code versions are given below.

V. 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 subchannels. 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<sup>(2)</sup>. The turbulent mixing model was tested against experimental velocity and quality data from the GE nine-rod bundle tests<sup>(3)</sup> and from the Ispra sixteen rod bundle tests<sup>(4,5)</sup>. 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<sup>(6)</sup>. Sample comparison results from these tests are shown in Figures 3-5.

6. Experience and Code Comparisons: 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.

## 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.

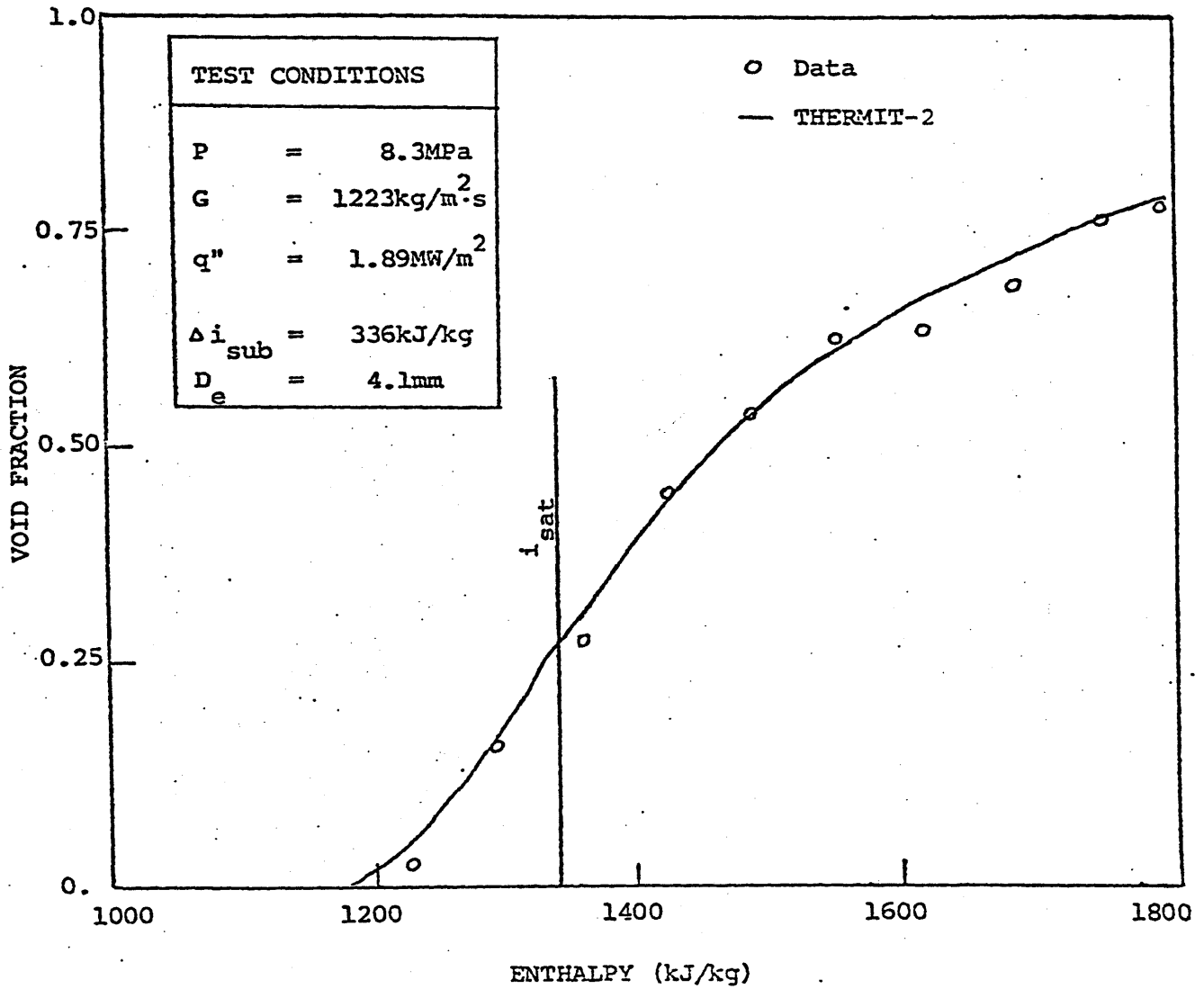


Figure 2: Void Fraction versus Enthalpy - Maurer Case 214-3-5

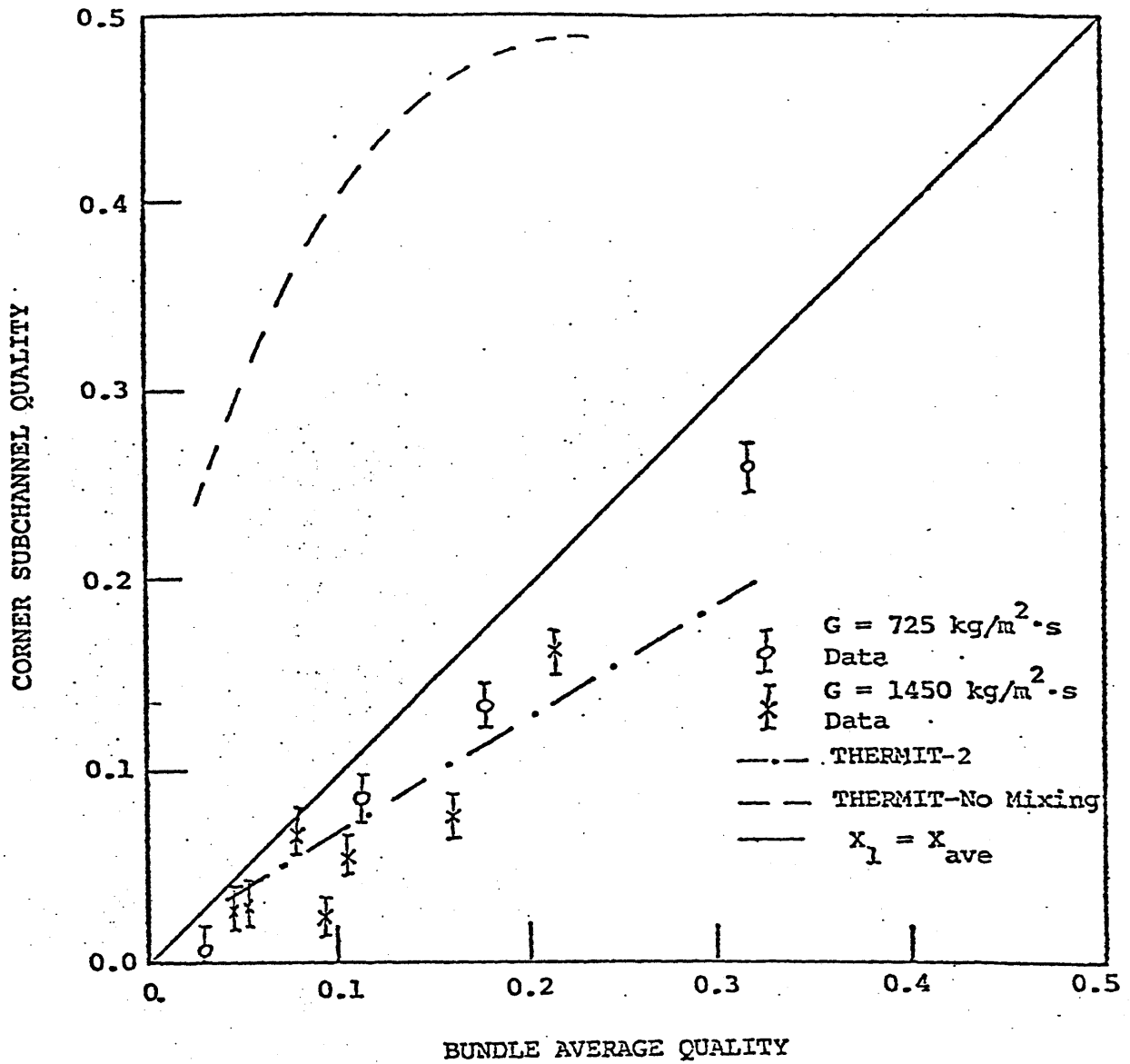


Figure 3: Comparison of Measured and Predicted Exit Quality  
 in Corner Subchannel for G.E. Uniformly Heated  
 Cases

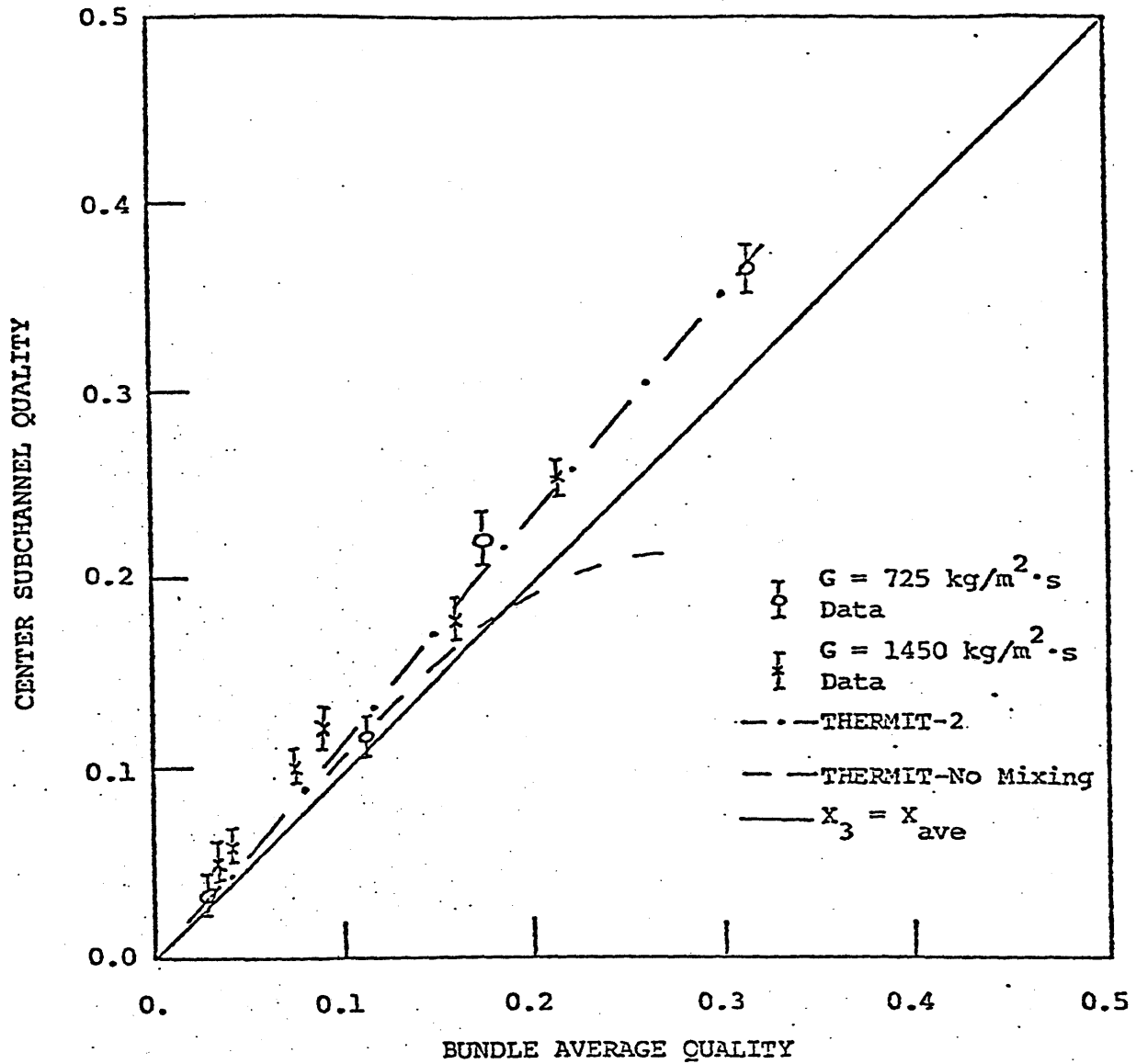


Figure 4: Comparison of Measured and Predicted Exit Quality in Center Subchannel for G.E. Uniformly Heated Cases

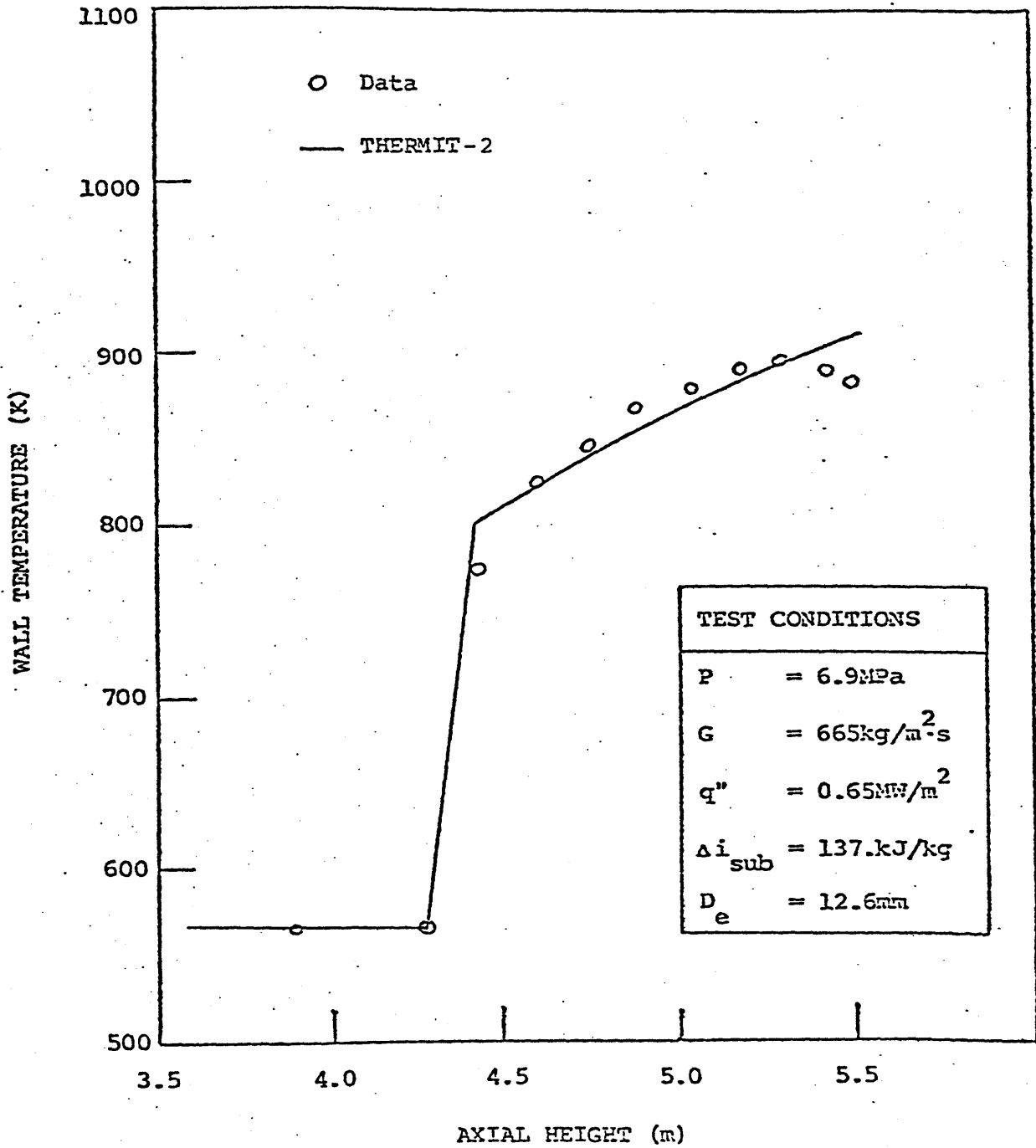


Figure 5: Wall Temperature Comparisons for Bennett Case 5332  
(Length = 5.56m)

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



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 on THIOD was a modeling of the Peach Bottom 2 turbine trip measurements. While most of the experimental data was available<sup>(12)</sup>, critical data on the reactivity coefficients was proprietary<sup>(13)</sup>. 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 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 in Table 2. Of all the codes, THIOD appears best suited for long slow BWR transients such as flow coastdowns and

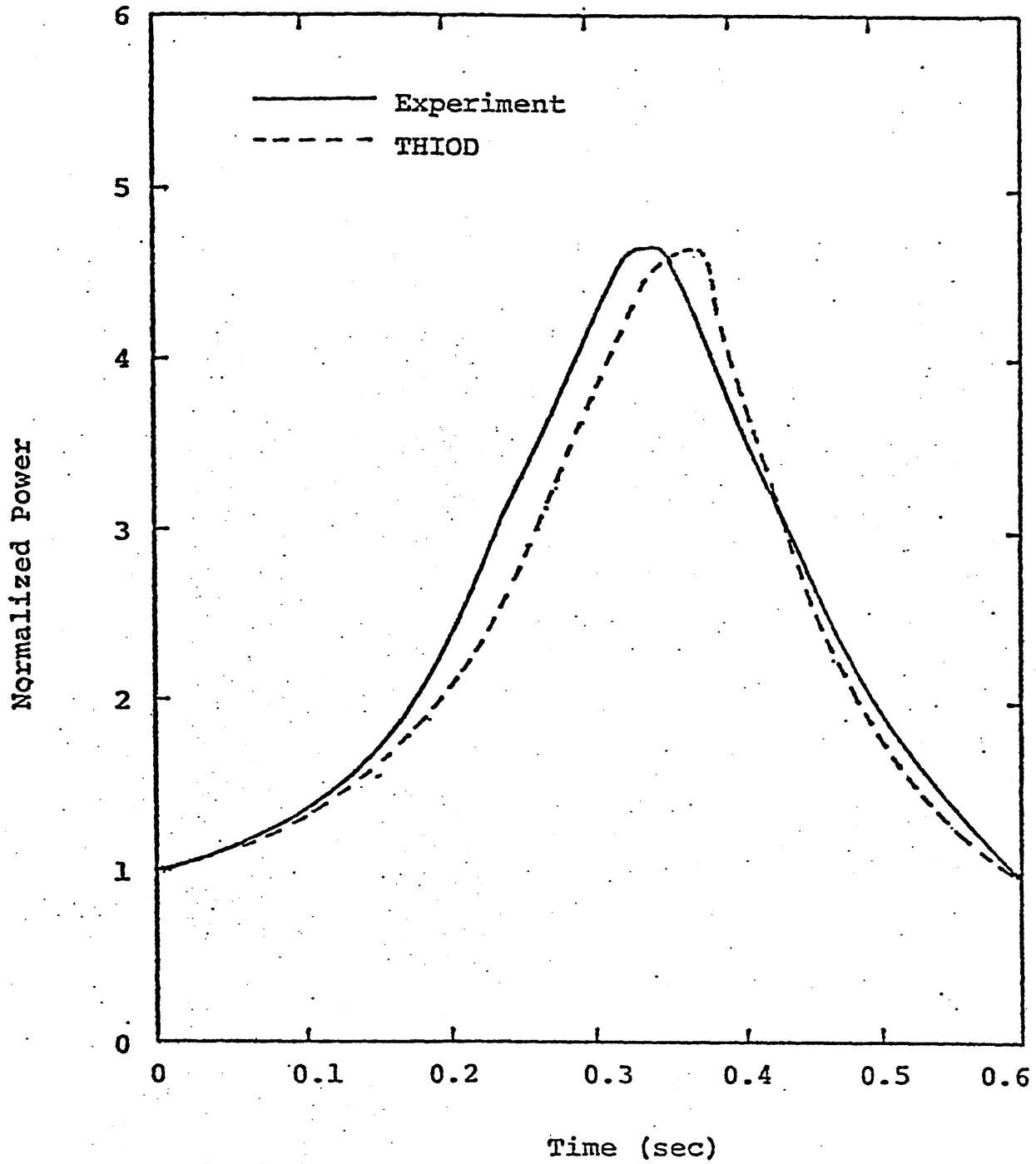


Figure 6: Peach Bottom Turbine Trip 1 Power History

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

feedwater heater failures.

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<sup>(24)</sup>. The interfacial momentum exchange rate correlation was empirically based on the KFK experiments in Karlsruhe<sup>(25)</sup>. A relationship for the interfacial heat exchange rate was developed from theoretical principles<sup>(26)</sup>.

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<sup>(27)</sup>. Table 3 compares the experimental results with the NATOF predictions. SOBOIL<sup>(28)</sup> results are also given. The second test simulated was the steady state predictions of BACCHUS of the BR19 experiment performed in France<sup>(29)</sup>. 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<sup>(19)</sup>. Other comparable codes which are also under further development are COMMIX<sup>(10)</sup>, SABRE (U.K.)<sup>(30)</sup>, BACCHUS (France)<sup>(29)</sup> and an advanced sodium version of THERMIT.

TABLE 3P3A 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 4Mass Flow Rate  
and Temperatures for the GR19 Experiment

<u>Flow (kg/sec)</u>	<u>T<sub>max</sub>(°C) (measured)</u>	<u>T<sub>max</sub>(°C) (NATOF-2D)</u>
.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

Supplemental THERMIT References

The ongoing development of the THERMIT computer codes at MIT has given rise to the publication of a considerable number of papers in the open literature. This bibliography is given to facilitate further research and document previous work on THERMIT.

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