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DEVELOPMENT OF A THREE-DIMENSIONAL
TWO-FLUID CODE WITH TRANSIENT NEUTRONIC
FEEDBACK FOR LWR APPLICATIONS

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A.1 J.E. Kelly, J. Loomis, L. Wolf, "LWR Core Thermal-Hydraulic Analysis--
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A.3 L. Guillebaud, A. Levin, W. Boyd, A. Faya, and L. Wolf, "WOSUB-A
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     M. Granziera, P. Griffith, W. Hinkle (ed.), M. Kazimi, A. Levin,
     M. Manahan, A. Schor, N. Todreas, R. Vilim, G. Wilson, "Development
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B. Papers

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B.1 J.E. Kelly and M.S. Kazimi, "Development of the Two-Fluid Multi-Dimensional Code THERMIT for LWR Analysis," Heat Transfer-Orlando 1980, AIChE Symposium Series 199, Vol. 76, August 1980.

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DEVELOPMENT OF A THREE-DIMENSIONAL TWO-FLUID CODE
WITH TRANSIENT NEUTRONIC FEEDBACK FOR LWR APPLICATIONS

ABSTRACT

The development of a three-dimensional coupled neutronics/thermal-hydraulics code for LWR safety analysis has been initiated. The transient neutronics code QUANDRY has been joined to the two-fluid thermal-hydraulics code THERMIT with the appropriate feedback mechanisms modeled. A literature review of the existing coupled neutronics/thermal-hydraulics codes is presented. It indicates that all of the known codes have limitations in their neutronic and/or thermal-hydraulic models which limit their generality of application and accuracy. It was also found that a tandem coupling scheme was most often employed and generally performed well. A detailed steady-state and transient coupling scheme based on the tandem technique was devised, taking into account the important operational characteristics of QUANDRY and THERMIT. The two codes were combined and the necessary programming modifications were performed to allow steady-state calculations with feedback. A simple steady-state sample problem was produced for the purpose of testing and debugging the coupled code.

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CHAPTER 1. INTRODUCTION

1.1 Background

The analysis of the transient behavior of light water reactors is central to their design, safety analyses, and licensing processes. In order to analyze the spectrum of postulated or anticipated transients successfully, detailed models of the involved phenomena are required. A great deal of effort has been expended in the development of computer codes capable of performing such analyses accurately and economically. As a result, both neutronic and thermal-hydraulic codes are now available to provide detailed three-dimensional time-dependent descriptions of LWR core behavior. However, the various computer codes developed for these purposes are not universally applicable and usually suffer from certain shortcomings. Very often the transient neutronics and thermal-hydraulics are calculated separately, with the inherent feedback mechanisms neglected. Nevertheless, for many reactor transients of interest the feedback between neutronics and thermal-hydraulics is a significant contributor to the transient behavior. It is therefore highly desirable to develop a computer code which includes detailed space- and time-dependent modeling of core neutron physics, fluid dynamics, and heat transfer along with their respective interactive feedback mechanisms. To this end, a research project has been sponsored under the M.I.T. Energy Lab Utilities program to develop a state of the art code to calculate three-dimensional

steady-state and transient neutronics and thermal-hydraulics with feedback for a light water reactor core. As a first step toward this goal, a 12-month project was initiated in January 1980 to incorporate a neutronics model into the two fluid, three-dimensional thermal-hydraulics code THERMIT [1]. This is to be accomplished by uniting THERMIT with QUANDRY [2], an advanced three-dimensional transient neutronics code. The resultant code will be applicable to the analysis of a variety of BWR and PWR transients.

In light of the many codes available for the analysis of LWR transients, it is necessary to justify the development of a new code to analyze such transients. This can be done by examining the existing codes, their limitations and the experience with them. Chapter 2 contains a review of many of the existing coupled neutronics/ thermal-hydraulics codes. The review indicates that no existing and openly available code combines the best available neutronics and thermal-hydraulics models to yield a tool featuring both generality and accuracy. Each coupled code reviewed has important limitations in either the neutronic model or thermal-hydraulics model or both. These limitations restrict the applicability of the codes and may also reduce the accuracy of the results.

An important example of the limitations in the currently available codes is the use of point kinetics neutronics models. These methods are generally characterized by the assumption that the flux shape remains constant during the transient. In fact, in the

standard point kinetics approximation, it is assumed that the flux shape
is unaffected by any reactor perturbation and hence the unperturbed
steady-state flux shapes are used. However, the rigorous calculation
of the reactivity requires the knowledge of the flux shape. If the
flux shape used is in error, it is expected that the calculated reac-
tivities (and related parameters such as reactor power) will also be
in error. Indeed, experience has shown that point kinetics models
are inadequate for many cases of interest [3,4]. Yasinsky and Henry
[3] investigated the application of point kinetics to idealized tran-
sients designed to accentuate non-separable space-time effects. No
feedback effects were accounted for in the prompt critical and below
prompt critical reactivity insertions analyzed. It was found that
the point kinetics model was very poor for large reactors and only
adequate for the below prompt critical transient in a small, "tightly
coupled" core. Figure 1 shows the time behavior of both the reactiv-
ity and amplitude functions for a prompt critical transient in a
large core, as calculated by three different methods. The point
kinetics method is shown to be strikingly inadequate, underpredicting
the maximum amplitude of the transient by a factor of over 10^4. The
results of these numerical experiments led Yasinsky and Henry to
conclude:

> ... the fact that the error in the conventional
> point method is intrinsically so great for the
> large core lends considerable support to the
> view that this model should never be used to
> analyze prompt excursions in large reactors.
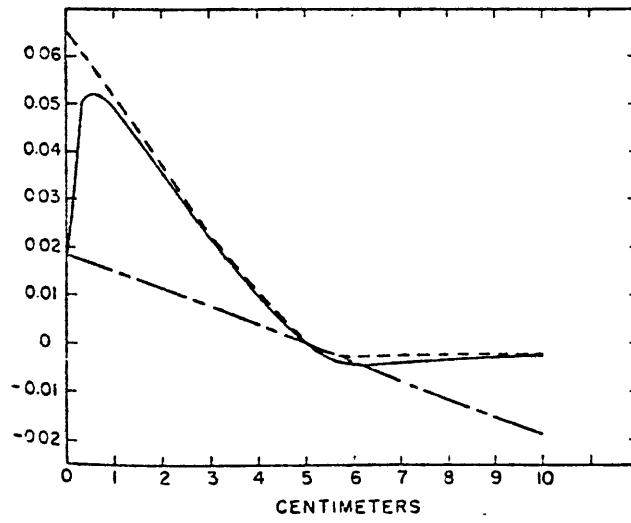
b) for a 240-cm core.

Time behavior of reactivities.
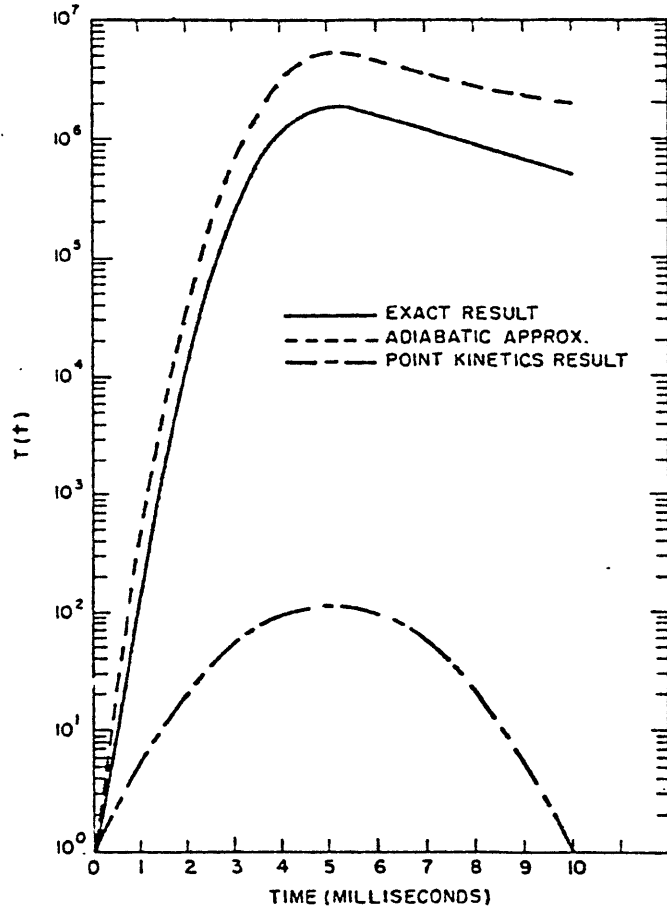
Prompt critical excursion amplitude function
$T(t)$ for 240 cm core.

Figure 1:   Assessment of Point Kinetics for Prompt Critical Transient with
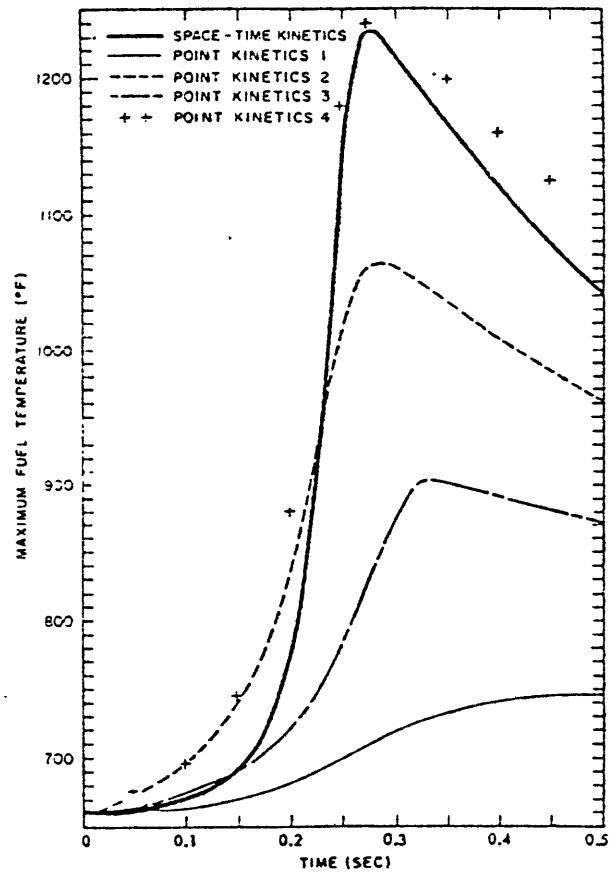No Feedback [3].

Yasinsky [4] investigated the accuracy of point kinetics models in calculating transients with feedback. A group of asymmetric rod-ejection accidents were analyzed with five different point kinetics schemes (using different flux shapes) and compared with an "exact" space-time finite difference solution. It was found that "classical" point kinetics was consistently unable to do a realistic job in calculating either peak power or peak fuel temperature. These key parameters were always underestimated, often by as much as a factor of three. The other methods were neither consistently conservative nor accurate for the transients considered. Figure 2 shows the time behavior of both the reactor power and the fuel temperature as calculated by the different methods. Only one point kinetics method does not underpredict the maximum power. Three of the five point methods underpredict the maximum fuel temperature. These results led Yasinsky to conclude:

> In general we have seen that the accuracy of
> a point model, for rapid, nonseparable tran-
> sients of the type studied here, is extremely
> dependent on the specifics of the particular
> model used (i.e., on the shape functions
> used). It appears to be difficult to assume
> that a given method is conservative; nor can
> we judge the accuracy of the method a priori.

Thus, any coupled neutronics/thermal-hydraulics code which relies upon a point kinetics model should be limited to analyzing transients in which the flux shape is known to remain nearly constant with time.
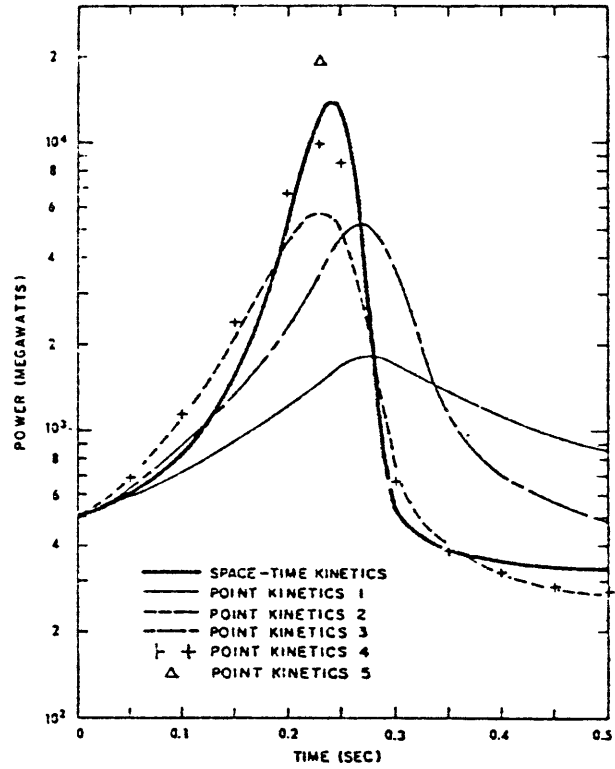
Power for Reactor C rod-ejection accident 1.

Maximum fuel temperature for Reactor C
rod-ejection accident 1.

Figure 2:   Assessment of Point Kinetics for Rod Ejection Transient with
            Feedback [4].

Among the important limitations inherent in many coupled neutron-ics/thermal-hydraulics codes are those related to the treatment of two-phase flow conditions. Several codes have simple lumped parameter models which assume that no boiling can occur. Most of the codes use some variation of the homogeneous equilibrium model, in which the two-phase flow is assumed to be a homogeneous mixture with both phases in equilibrium with each other. The two phases are also assumed to move with the same velocity or to have a constant velocity ratio (slip ratio). There are many situations during reactor transients in which these assumptions are unrealistic, as summarized in Table 1. The homogeneous equilibrium model works best at low and high qualities, since the distribution of phases is more nearly uniform for these regimes. Hence, codes using this model can give adequate results when prudently applied. However, the sensitivity of coupled codes to inadequacies in the two-phase flow model is probably enhanced, since phenomena such as the relative motion of phases and subcooled boiling should affect the void fraction and, hence, the neutronic feedback. When departures from homogeneous equilibrium flow are important, then a model that treats two separate phases and the transfer phenomena between them is necessary. These multi-fluid codes (such as THERMIT) are, in principle, extremely powerful because of the generality of the model and the flexibility to adopt constitutive relations for distinct physical situations.

Many other features of coupled codes serve to limit their applica-

TABLE 1

EXAMPLES OF CASES WHERE ONE-DIMENSIONAL HOMOGENEOUS EQUILIBRIUM THEORY
IS NOT ACCEPTABLE [5]

Multidimensional Effects	Nonequilibrium Effects	Phase Separation
Downcomer region	ECC injection	Small breaks
Break flow	Subcooled boiling	Steam generator
Plena	Post-dryout heat transfer	Horizontal pipe flow
Steam separators	ECC heat transfer	Counter current flow
Steam generators	Low-quality blowdown	PWR ECC Bypass
Reactor core	Reflood quench front	BWR CCFL

bility and accuracy. Some codes assume that fuel and coolant proper-
ties are constants, despite the fact that it has been shown that
temperature-dependent properties are important for the accurate calcu-
lation of many transients [6]. A single gap heat transfer coefficient
is used in many codes, despite the recommendation that space- and
time-dependent gap heat transfer correlations be included in transient
analysis codes [6]. Some thermal-hydraulic models cannot handle re-
verse flow, neglect compressible flow effects, and are limited by
sonic velocity time scales. Codes assuming radial symmetry cannot
model asymmetric transients. MEKIN [7], the most sophisticated pub-
licly available coupled code, is too expensive for many practical
problems of interest. The development of a coupled QUANDRY/THERMIT
should remove most of these limitations.

1.2 QUANDRY

QUANDRY is a neutronic code developed at M.I.T based on an ana-
lytic nodal method to solve space-dependent reactor transients. The
two-group diffusion theory approximation to the neutron transport
equation is utilized and the reactor is modeled as an array of homo-
genized regions (or nodes), for which equivalent diffusion theory par-
ameters must be determined. Either two or three dimensional problems
may be analyzed. The nodal method uses node-averaged fluxes as the
primary unknowns, rather than calculating fine mesh fluxes which are
averaged to give node-averaged fluxes. The analytic nodal method
solves a one-dimensional diffusion equation for each direction to

yield the required flux-current relationships. A quadratic polynomial approximation is used to calculate nodal transverse leakages. A considerable amount of computational time is saved by this approach. Indeed, the computational efficiency of QUANDRY has been shown to be at least two orders of magnitude greater than that of finite difference methods. In addition, QUANDRY has proven to be highly accurate for both static and transient solutions. QUANDRY has a built-in thermal-hydraulic feedback capability, based on a simple lumped heat capacity model with a linear cross-section model. The thermal-hydraulic model does not allow boiling or reverse flow and uses constant thermal properties for the fuel, clad, and coolant. The neutronics and thermal-hydraulics equations are solved in tandem, with all cross-sections treated as linear functions of fuel temperature, moderator temperature, and moderator density. The macroscopic cross-section of type α for calculated volume (i,j,k) is calculated by an equation of the form:

$$\Sigma_{\alpha(i,j,k)} = \Sigma_{\alpha(i,j,k)}^{*} + \left(\frac{\partial \Sigma_{\alpha}}{\partial T^{c}}\right)\left(T_{(i,j,k)}^{c} - T^{c*}\right) + \left(\frac{\partial \Sigma_{\alpha}}{\partial T^{f}}\right)\left(T_{(i,j,k)}^{f} - T^{f*}\right)$$

$$+ \left(\frac{\partial \Sigma_{\alpha}}{\partial \rho^{c}}\right)\left(\rho_{(i,j,k)}^{c} - \rho^{c*}\right) \qquad ,$$

where T^{c} and T^{f} are node average coolant and fuel temperatures, respectively, and ρ^{c} is the node average coolant density. Quantities marked with * indicate user-supplied reference values. This type of relation describes cross-sections accurately over only limited ranges

of temperatures and densities. However, the code assumes that the linear functional form is valid over the entire range of thermal-hydraulic variables so that, if the reference cross-sections and partial derivatives are known, the thermal-hydraulic feedback model can be completely specified.

1.3 THERMIT

THERMIT is an advanced two-fluid thermal-hydraulic code capable of performing steady-state and transient analyses of water-cooled nuclear reactors in three dimensions. The two-fluid model uses separate partial differential equations expressing conservation of mass, momentum, and energy for each individual fluid phase. As a result, both thermal and mechanical non-equilibrium between the phases can be realistically modeled. The fluid dynamics model is a distributed resistance (or porous body) model and is well-suited for either core-wide or subchannel analyses. Both PWR and BWR transients may be analyzed in rectangular coordinates. THERMIT can handle complex fluid dynamics conditions, such as natural circulation, blowdown, flow reversal and phase separation. A complete heat transfer package is included which can determine appropriate regimes based on a complete boiling curve. The sophisticated fuel pin model solves the radial heat conduction equation for fuel temperatures, using temperature dependent fuel and clad properties as well as a variable gap heat transfer coefficient model. The combination of a two fluid model with advanced constitutive relations allows for the most detailed

analysis of two phase flow currently available and offers the possibility of being more generally applicable and more accurate.

In addition to having an advanced two-phase flow model, THERMIT also has a very flexible and reliable solution method. A semi-implicit technique is used which is a modification of the ICE method [8]. This method is not limited by the speed or direction of the flow and is thus well suited for severe transients. However, there is a stability limit on the allowed time step size, governed by the Courant condition:

$$\Delta t < \left| \frac{\Delta X}{V_{max}} \right| \qquad ,$$

where ΔX is the axial mesh spacing and V_{max} is the largest fluid velocity. Thus, some calculations may prove to be prohibitively expensive because of time step limitations (but not because of a failure of the solution technique). In fact, the semi-implicit transient solution scheme in THERMIT guarantees convergence of the numerical method (provided a real solution exists). Therefore, THERMIT combines two highly desirable features: an advanced two-phase flow treatment and a reliable numerical method.

1.4 Preview

This introductory chapter has provided background information pertinent to the current work, including descriptions of QUANDRY and THERMIT. Chapter 2 contains a detailed review of existing coupled neutronics/thermal-hydraulic codes. Chapter 3 discusses coupling

strategies employed in existing codes as well as the proposed strategy for coupling QUANDRY and THERMIT. Chapter 4 presents the work that has been done in implementing the coupling strategy discussed in Chapter 3. Finally, Chapter 5 gives a summary of the current project status.

CHAPTER 2. REVIEW OF COUPLED CODES

2.1 Introduction

Coupled neutronics/thermal-hydraulics codes with varying levels of sophistication have been developed and applied to reactor analyses for at least fifteen years. As regulatory pressures have increased and analytical capabilities have grown, these codes have become more complex and rigorous. Some have been designed for rather specific applications, and all contain approximations and compromises in their models which limit applicability and accuracy. It is important to review the existing public codes in order to benefit from previous work and to have a perspective on the current work. Table 2 summarizes the coupled codes investigated.

2.2 CHIC-KIN and PARET

One of the first coupled neutronics/thermal-hydraulics codes developed was CHIC-KIN [9]. It consists of a fairly detailed single channel thermal-hydraulic model coupled to a point kinetics neutronic model. The coupling is achieved through a reactivity feedback loop. The feedback loop includes the effects of moderator density change, moderator temperature change, fuel plate (rod) expansion, and fuel temperature change (Doppler broadening). Fluid dynamics are represented by a momentum integral model which allows zero flow initial conditions, flow reversal, and internal pressure buildup. The fuel element model allows a detailed spatial representation by axial and

TABLE 2

SUMMARY OF NEUTRONIC/THERMAL-HYDRAULIC CODES

	THERMAL-HYDRAULICS	NEUTRONICS
CHIC-KIN [9]	1-D, single channel model	point kinetics
PARET [10]	four channel model	point kinetics
TWIGL [12]	lumped parameter model, no boiling allowed	2-D, 2-group finite difference diffusion theory model
WIGL3 [13]	lumped parameter model, no boiling allowed	1-D, 2-group finite difference diffusion theory model
BNL-TWIGL [14]	time-dependent two-phase model	2-D, 2-group finite difference diffusion theory model
SAS2A (LMFBR) [15]	1-D with sodium bubble model	point kinetics
FX2-TH (LMFBR) [16]	1-D with no boiling	3-D, multi-group diffusion theory, quasistatic method
HERMITE [17]	2-D homogeneous equilibrium model	3-D finite element diffusion theory, 1 to 4 groups
MEKIN [7]	2-D homogeneous equilibrium model	3-D finite difference 2-group diffusion theory
THIOD [27]	1-D, two-fluid model, nonequilibrium	point kinetics
THERMIT-3 [27]	3-D two-fluid model, nonequilibrium	point kinetics
QUANDRY [2]	lumped parameter model, no boiling	3-D, 2-group nodal diffusion theory model
"QUANTHER"	3-D two-fluid, nonequilibrium model for LWR	3-D, 2-group nodal diffusion theory model

radial sectionalization. A subcooled boiling void fraction model is included. The two-phase flow is treated by a homogeneous equilibrium model. A reactor core is represented by a single fuel element and a single coolant channel with the coolant making one pass through the system. Transients may be initiated by reactivity insertion, changes in inlet enthalpy or temperature, changes in inlet flow rate or core pressure drop, or changes in system pressure. Since the neutronics portion is represented by point kinetics, the heat generation is assumed to be a separable function of space and time, with the spatial (axial) function predetermined.

PARET [10] is a very similar code in which the thermal-hydraulic model has been expanded to allow up to four coupled channels. Each channel represents an annular core region and contains a fuel rod (or plate) and its associated coolant. Temperature-dependent thermal properties may be specified for the fuel, gap, clad, and coolant. Heat transfer correlations for subcooled convective-conductive, nucleate-boiling, transition-boiling, and stable film-boiling regimes are included in PARET. The PARET code was successfully applied to analyzing several of the SPERT transient experiments [11]. In addition, CHIC-KIN has been frequently used by utilities to analyze power reactor transients. Both codes are subject to some severe limits of applicability, particularly becuase of the assumptions involved in the point kinetics approximation. The spatial variation of heat generation must be determined in some arbitrary fashion prior to performing a

transient analysis. For CHIC-KIN, only an axial heat generation profile may be included, since the whole reactor is represented by one average channel. Any transient in which the spatial heat generation varies with time cannot be modeled accurately by either code because of the assumption that the spatial shape is independent of time. In addition, the accuracy of the solution is limited by the fact that the feedback is transmitted by a reactivity feedback loop which requires the specification of various reactivity coefficients. These coefficients are left as arbitrary free parameters in the model and are difficult to generate accurately. Finally, a maximum of one or four thermal-hydraulic channels places a severe limit on the detail with which reactor transients can be modeled.

2.3 TWIGL, WIGL3 and BNL-TWIGL

TWIGL [12] is a program which solves the two-dimensional, two-group, space-time neutron diffusion and delayed precursor equations in either x-z or r-z geometry. The thermal-hydraulic model is a lumped heat capacity model which assumes that no boiling occurs and that the coolant makes only one pass through the core. Transients are initiated by specified time variations of the reactor material parameters or by changes in the coolant temperature or flow rate at the core inlet. Feedback is accomplished by a cross-section modification based on the average fuel temperature, the average coolant temperature, and the average coolant density. A related code is WIGL3 [13], which has a one-dimensional, two-group neutronics model and the same thermal-

hydraulic model, but also accounts for xenon and control feedback. A further refinement of this group of codes is seen in BNL-TWIGL [14], in which the two-dimensional (r-z), two-group, time-dependent neutron diffusion equations solution is coupled to a time-dependent two-phase thermal-hydraulic model. Cross-sections are assumed to have a quadratic dependence on the square root of fuel temperature, and a linear dependence on the moderator temperature. These codes represent an improvement over CHIC-KIN and PARET because of the more rigorous neutronic models utilized. However, relatively primitive thermal-hydraulic models constitute a major weakness of these codes. Also, two-dimensional (r-z,x-z) neutronic models do not allow radially asymmetric transients to be realistically calculated.

2.4 SAS2A

The need for a code to analyze LMFBR accidents led to the development of the SAS2A [15] coupled neutronics/thermal-hydraulics code. SAS2A calculates the initial consequences of an accident, from steady-state, pre-accident conditions up to the point of large-scale fuel motion or disassembly. The thermal-hydraulics portion assumes one-dimensional fluid flow and calculates transient temperatures in the fuel, cladding, and coolant, transient coolant pressures and flow rates, and transient stresses and strains in the fuel and cladding. Additional models allow the calculation of sodium boiling, film dry-out, cladding melting, and fuel melting. The neutronic portion of the code is calculated with a point-kinetics approximation. Transients

are initiated by a power level, reactivity, or flow rate per-
turbation as specified by the user. The thermal-hydraulic and neu-
tronic portions are coupled by a reactivity feedback loop which ac-
counts for changes in fuel temperature, fuel thermal thermal expan-
sion, sodium voiding, fuel slumping, and scram. It should be clear
that SAS2A is a rather sophisticated code which has been designed for
a very specific task and is thus very limited in its applicability.

2.5 FX2-TH

Another coupled code developed for LMFBR transient analysis is
FX2-TH [16]. The code combines a two-dimensional, time-dependent
multigroup neutron diffusion theory solution technique with a one-
dimensional thermal-hydraulics model which does not allow boiling or
flow reversal. The time-dependent diffusion equations are solved by
the improved quasistatic method, in which the point kinetics equa-
tions are solved with a periodic recalculation of the time-dependent
multigroup neutron fluxes. The main function of the thermal-hydrau-
lics model is to calculate average fuel and coolant temperatures in
each reactor region in order to provide feedback to the neutronic por-
tion. The heat conduction equations are solved to give the tempera-
ture distribution through the fuel pin, clad, and coolant. The cool-
ant in each reactor region is assumed to be isolated from the coolant
in any other regions modeled. As previously mentioned, the model
assumes that the coolant does not boil, and flow reversal is not
allowed. Coolant and fuel properties are modeled as polynomial functions

of the coolant and fuel temperatures, respectively. The fuel

pin model assumes that heat generation in the fuel is radially uni-

form and axial and azimuthal heat transfer are neglected. The average

temperatures calculated by the thermal-hydraulics portion of the code

are used to calculate the macroscopic cross-sections for each reactor

region. Changes in the average fuel temperature result in changes in

the microscopic capture and fission cross-sections. Changes in the

average coolant temperature are reflected by a linear variation of the

coolant atom density. In this way, the macroscopic capture, removal,

scattering, and transport cross-sections of the coolant are dependent

on the average coolant temperature.

2.6 HERMITE

Of the codes presented thus far, all have been limited to one- or

two-dimensional representations of a reactor core. However, a number

of more advanced three-dimensional codes have been developed which can

perform coupled neutronics/thermal-hydraulics calculations. One of

these is HERMITE [17], a proprietary multi-dimensional space-time de-

pendent code developed by Combustion Engineering as a benchmark code.

HERMITE is a very flexible code, in that the neutronic and thermal-

hydraulic portions can be used independently or coupled with feedback.

The neutronic portion utilizes a finite element method to solve the

neutron diffusion equations with from one to four energy groups in

one, two, or three dimensions. A full core can be modeled, as well as

half and quarter core symmetry sections. The solution method allows

arbitrary mesh spacings and zero flux or zero current boundary condi-
tions. In addition to steady-state and transient analyses, HERMITE
can also perform depletion calculations. The thermal-hydraulic model
solves a three-dimensional, variable area coolant continuity, lateral
and axial momentum, and energy conservation equations for a homo-
geneous mixture. The core may be modeled with open or closed channels,
for which coolant inlet conditions of flow and enthalpy or temperature
may be individually prescribed. The code will also accept inlet and
outlet pressure distribution boundary correlations. A finite differ-
ence fuel pin model allows an arbitrary number of nodes in the fuel
and clad and includes temperature-dependent material properties. Im-
portant constitutive relations include several two-phase void fraction
models and models for nucleate boiling and forced convection to sub-
cooled water heat transfer regimes. During a transient calculation,
channel inlet conditions may vary independently and core-wide ambient
pressure may also vary. Decay heat may be represented as a component
of the static power distribution. Feedback is accomplished by means
of a linear cross-section model which accounts for any combination of
fuel temperature, moderator temperature, moderator density, and solu-
ble boron concentration. In addition, there is an explicit exposure
and depletable boron calculation included. HERMITE is clearly a very
flexible and sophisticated code for the calculation of reactor tran-
sients. Among the approximations apparently made in the thermal-hy-
draulics portion are a homogeneous equilibrium mixture representation

of the fluid dynamics with an incomplete momentum equation (not)
fully three-dimensional).

2.7 MEKIN

Another advanced code is MEKIN [7], a three-dimensional light
water reactor transient analysis code with feedback. MEKIN was devel-
oped at M.I.T. under EPRI sponsorship to be a benchmark code for veri-
fying the analyses of simpler codes. MEKIN is the only known non-
proprietary code for three-dimensional LWR transient analysis that
couples neutronic and thermal-hydraulic calculations. The code oper-
ates in a tandem fashion, with information being exchanged between
individual neutronic and thermal-hydraulic solution schemes. Both
steady-state and transient problems can be analyzed. The neutronic
portion utilizes a finite difference solution to the three-dimensional
neutron diffusion equations, either in one or two energy groups.
Full, half, and quarter core symmetric sections may be modeled with
fuel assembly sized volumes (divided axially) of equal dimensions.
The neutronic solution accepts zero flux, zero current, or albedo
boundary conditions. A transient can be initiated by a perturbation
of the base cross-sections. In addition, a scram can be simulated
during a transient, initiated by overpower, reactor period, or
elapsed time. The thermal-hydraulic model is based upon the code
COBRA III C/MIT [18], a steady-state and transient code capable of
both subchannel analysis and lumped channel calculations. This model
allows a three-dimensional thermal-hydraulic model with either open or

closed flow channels, but requires a uniform axial mesh. Steady-state
inlet conditions of coolant flow rate and enthalpy (or temperature)
may be specified for each channel. During a transient, the time-de-
pendence of inlet conditions must be the same for all channels. Core
outlet pressure may vary during a transient. Under two-phase condi-
tions, the coolant is modeled as a single fluid with the two phases
well mixed (at equilibrium) and uniformly distributed throughout each
other. The inclusion of slip ratio correlations allows the vapor and
liquid phases to move at different speeds. The code permits a choice
of two-phase void fraction models. A one-dimensional finite differ-
ence fuel pin model allows an arbitrary number of nodes in the fuel
pellet, one node in the clad, and assumes constant material proper-
ties. Correlations are included for the forced convection to sub-
cooled water and nucleate boiling heat transfer regimes. The solution
method is a semi-explicit marching type scheme which allows any value
of time step size and axial mesh size without numerical instabilities.
The coupling logic begins with the calculation of cross-sections for
each calculational volume which are appropriate for the current
thermal-hydraulic parameters. A neutronic calculation is then per-
formed, taking into account any external neutronic perturbations.
The fluxes thus calculated are then used to determine new volumetric
heat generation rates, the thermal-hydraulic portion is updated, and a
complete thermal-hydraulic calculation (one time step in a transient
calculation) is performed, including any externally supplied thermal-

hydraulic perturbations. An updated set of cross-sections for the new

thermal-hydraulic conditions is then generated, and the cycle is

repeated. In the steady-state this process continues until selected

convergence criteria are satisfied. For a transient calculation, one

such cycle is used per time step. The cross-section calculation is

based on a linear variation with respect to changes in fuel tempera-

ture, moderator temperature, and moderator density. The reference

cross-sections and their partial derivatives are constants supplied

by the user.

MEKIN has undergone a considerable amount of investigation [6, 19, 20,

21, 22, 23, 24, 25, 26] and assessment. As a result, many of its oper-

ational characteristics and limitations have been documented. Some of

these limitations are inherent in the models and were recognized when

the code was developed, while others have been discovered through ex-

perience. Many of the inherent limitations are due to the thermal-

hydraulics model. Two such limitations are the lack of a pressure

drop boundary condition option and the inability to calculate a re-

verse flow situation. The mathematical model neglects sonic velocity

propagation and as a result only transients in which the time scale is

greater than the time for a sonic wave to pass through the channel may

be analyzed. Treating the coolant as a single homogeneous fluid is

quite adequate for single phase, low quality, and very high quality

two-phase flow. However, it is much less appropriate for annular flow

regimes that are often encountered in BWR analyses. The assumption

of equilibrium between the phases may result in inaccurate results when extreme power transients are analyzed. Many of the thermal-hydraulic models employed by MEKIN were originally devised for subchannel analysis, rather than for the lumped channel application typical of a MEKIN analysis. Thus it has been observed that a large channel model provides accurate prediction of hot channel parameters only if the hot assembly is divided into several smaller channels [20]. The major disadvantage associated with the neutronics portion of MEKIN is the high cost associated with the fine mesh finite difference solution technique. A fully-converged neutronics solution requires a tight neutronic mesh size (on the order of 2 cm.), resulting in the necessity for a small neutronic time step. It has been estimated that the calculation of a full core PWR rod ejection transient, with accurate neutronic convergence, would require months of computer time [24]! Even modeling a partial core could take days of continuous computer time. Thus it is that the primary application of MEKIN is likely to be the calculation of small three-dimensional benchmark problems, rather than the analysis of transients needed for licensing.

2.8 THIOD and THERMIT-3

Two coupled codes strongly related to the current work have been recently developed at M.I.T. by Dube [27]. THIOD, a one-dimensional fully implicit version of THERMIT, has been coupled to a point kinetics model via a reactivity feedback loop. In addition, the identical point kinetics model was coupled to THERMIT, resulting in a new version

that is designated THERMIT-3. These two codes are significant
for the current work in that they represent the first attempt at com-
bining reactivity feedback with two-fluid thermal-hydraulics.

The main goal of Dube's work was to develop a numerical solution
technique for solving the two-fluid conservation equations in one
dimension that would be faster and more accurate than the THERMIT
methodology. To achieve this end, the application of the new tech-
nique was limited to steady-state and mild transient cases, with an
emphasis on BWR analyses. In addition, a simple point kinetics model
was implemented to investigate the applicability of two-fluid two-
phase models to transients with reactivity feedback.

The major effort in increasing the speed and accuracy of the
THERMIT code was in modifying the solution technique. Constructing
a strictly one-dimensional formulation of the two-fluid conservation
equations reduced the number of scalar equations and unknowns from
10 to 6 per calculational volume. However, all of the conservation
equations and constitutive relations in THIOD remained functionally
identical to those in THERMIT. Hence, the numerical solution strategy
of THERMIT came under scrutiny for possible changes which could satis-
fy the goals stated earlier. As discussed in Chapter 1, the semi-
implicit technique used in THERMIT places limitations on the time step
size according to the Courant stability limit. This limit may often
require very small time steps, with typical maximum time step sizes on
the order of 80 msec for PWRs and 16 msec for BWRs [27]. Even with a

very efficient solution technique, the necessity of taking such small
time steps can make THERMIT calculations rather expensive. In order
to relax this time step limitation, THIOD was developed with a fully
implicit finite difference technique. In theory, there is no restric-
tion on the maximum time step that may be chosen with this numerical
approach. However, since all of the expressions in the THIOD differ-
ence equations are evaluated at the advanced time step, it is neces-
sary to solve simultaneously for all the basic unknowns at each axial
node. Hence, greater calculational effort is required per time step
than in the semi-implicit formulation of THERMIT. Indeed, a simple
direct solution method was found to converge too slowly to be practi-
cal and was abandoned in favor of a marching solution method. In this
technique, the algebraic difference equations are solved for one cal-
culational volume at a time, using the most updated values at neigh-
boring volumes as the coupling from volume to volume. This method
gave substantial savings in computing time over the direct solution
method. The method was shown to give the same solutions as calculated
by THERMIT with several orders of magnitude better convergence. In
addition, for one-dimensional problems within its scope of applicabil-
ity, THIOD was found to be about 4 to 5 times faster than THERMIT.
However, this gain was not without its cost. The marching solution
scheme assumes that the flow is in one direction as the procedure
moves from one calculational volume to the next. As a result, reverse
flow conditions cannot be treated by THIOD. This was an acceptable

sacrifice, since the scope of application had been limited to steady-state and mild transients where reverse flow conditions should not be encountered. It should be noted that an unsuccessful attempt was made to extend the one-dimensional marching method to three dimensions for steady-state calculations. Table 3 gives a comparison of the THERMIT and THIOD solution methods.

Despite the fact that THIOD models thermal-hydraulics as a strictly one-dimensional phenomenon, three-dimensional reactors may be analyzed if the flow channels can be considered to be uncoupled from their neighbors in terms of the exchange of mass, momentum, and energy. THIOD can handle a very appropriate BWR core model in which many "isolated" one-dimensional flow channels are coupled to each other through a common upper and lower plenum pressure field. Indeed, THIOD allows two types of boundary conditions for BWR problems: 1) specification of the inlet and outlet pressures, and 2) specification of the total inlet mass flow rate and the outlet pressure.

A point kinetics model GAPOTKIN [28] was coupled to both THIOD and THERMIT and a number of transients were analyzed with feedback. These analyses are discussed in Chapter 3. GAPOTKIN solves the space independent kinetics equations for a very general form of the reactivity function. The code operates rapidly, allows varying time steps, and is numerically unconditionally stable for all values of the reactivity or time step. The reactivity is specified as functions of time to simulate control rod motion, as well as functions of thermal-

TABLE 3

COMPARISON OF THERMIT AND THIOD NUMERICS
[27]

	THERMIT	THIOD
# of Dimensions	3	Multi 1-D
Reactor Types	PWR, BWR	BWR
# of Fluid Conservation Equations	10	6
# Equations of State	4	4
# Basic Unknowns (reduced)	14(10)	10(6)
Heat Transfer Model	Modified "BEEST"	Same
Fuel Pin Model	Temp. Depend., Fully Implicit	Same
Spatial Differencing	Staggered Mesh, Donor Cell	Same
Temporal Differencing	Semi-Implicit	Fully-Implicit
Theoretical Stability Condition	$\Delta t < \left\| \dfrac{\Delta x}{v_{max}} \right\|$	None
Numerical Methods		
a) Linearization	Newton-Raphson	Newton-Raphson
b) Solution Technique	Gauss-Seidel Iteration for Pressures	Direct Inversion for 6 Unknowns
Boundary Conditions	1) Inlet/Outlet Pressures	1) Inlet/Outlet Pressures
	2) Inlet Velocity/ Outlet Pressure	2) Outlet Pressure/ Total Inlet Mass Flow
	3) Inlet Pressure/ Outlet Velocity	

hydraulic parameters such as void fraction, coolant temperature, and fuel temperature. The coupling was by a reactivity feedback loop, requiring the calculation of core-averaged coefficients of reactivity. If available, reactivity coefficients for core regions can be specified and flux-squared weighting is used to generate core-averaged coefficients.

2.9 Summary

A number of coupled neutronics/thermal-hydraulics codes have been reviewed. All known non-proprietary codes of this type have been seen to have important limitations in either their neutronics or thermal-hydraulics models or both. The coupling of QUANDRY and THERMIT represents an increased level of generality, sophistication, and physical rigor over the existing codes. The coupling of a point kinetics model to THERMIT provides a good first step toward the full space-time coupling of QUANDRY and THERMIT.

CHAPTER 3. COUPLING STRATEGIES

3.1 Introduction

As seen in Chapter 2, a number of coupled neutronics/thermal-hydraulics codes have been developed. The coupling strategies in these codes are variations on the tandem method, in which the neutronics and thermal-hydraulics calculations are performed alternately, with feedback information passed between each segment as required. These feedback loops are either reactivity or cross-section feedback loops. The purpose of this chapter is to present strategies for coupling neutronic and thermal-hydraulic codes, with an emphasis on choosing a strategy for the coupling of QUANDRY and THERMIT. To this end, a review of the work of Dubé [27] will be presented. Dubé linked THERMIT and its fully implicit version, THIOD, to a point kinetics model via a reactivity feedback loop. The results obtained with these coupled codes will give impetus to the selection of a coupling strategy for QUANDRY and THERMIT. In addition, the coupling strategies of several other codes will be detailed. Finally, the strategy selected for coupling QUANDRY and THERMIT will be presented.

3.2 Reactivity Feedback Calculations with THERMIT and THIOD

As described in Chapter 2, a point kinetics model was connected to THERMIT and THIOD via a reactivity feedback loop. For both codes, no feedback is considered in steady-state calculations, since the initial reactor power is assumed to be known. As previously discussed

THIOD is a fully implicit version of THERMIT which allows time
step sizes to be selected independently of numerical stability con-
straints. The solution technique of THIOD is less efficient than that
of THERMIT for one time step, but the possibility of taking larger
time steps with THIOD can lead to computational savings. For tran-
sients which change rapidly, however, large time steps may not give
accurate results, thereby nullifying the advantages of the implicit
method. In addition, THIOD cannot calculate reverse flow situations
because of the marching method used in solving the equations. Final-
ly, THIOD assumes that the flow is strictly one-dimensional.

Since the point kinetics model was coupled to THERMIT and THIOD
in a tandem fashion, the reactor power is held constant during each
thermal-hydraulic time step. At the completion of each thermal-hy-
draulic time step, a new reactor power is calculated by the point ki-
netics model by including fuel temperature, coolant temperature, and
coolant density reactivity feedback as well as external reactivity
contributions. As mentioned, with THIOD it is desirable to use large
time steps because of the great computational effort per time step.
However, it is necessary to update the reactivity values often enough
to keep step changes in reactor power from being too dramatic, resul-
ting in unrealistic results. To reconcile these conflicting impera-
tives, a linear reactivity extrapolation was programmed into the THIOD
feedback loop. This model calculates an initial reactivity for the
feedback calculation based on a linear extrapolation of the reactivity

calculated prior to the previous thermal-hydraulic calculation. This method generally works well, but it was found that when time step sizes are too large, extrapolation of the reactivity can actually render the solution procedure unstable.

Dubé used THIOD and THERMIT-3 (THERMIT-3 refers to THERMIT with point kinetics) to perform two groups of reactivity feedback analyses. The first group consisted of four simulated BWR transients. The second group consisted of two "benchmark" calculations. Most of these calculations involved THIOD rather than THERMIT-3. The first group began with a simulated BWR flow transient in which an exponential decrease in core inlet flow was modeled with THIOD. It was found that the maximum calculated errors in reactor power could be as large as 18% if the time steps were large and/or the transient time constants were small. However, it was found that even relatively large deviations in power did not cause large discrepancies in void fraction or fuel temperature. Hence, although smaller time steps may be necessary to calculate accurately the transient reactor power, the important thermal-hydraulic variables of interest such as maximum fuel and clad temperatures and minimum CHFR can be calculated quite accurately with relatively large time step sizes. A second set of transient analyses with THIOD resulted in an operational map of core power as a function of rated core flow for a BWR plant. The values were determined by performing several flow transients until the neutral void reactivity effect reestablished a steady-state condition. These calculations

matched the reference power versus flow curve very well. THIOD was
then used to analyze a simulated BWR feed water heater transient. In
this accident, decreased inlet temperature results in decreased boil-
ing and a very gradual power rise because of the negative void coef-
ficient of reactivity. The final power increase calculated was in
very good agreement with the reference value. However, some difficul-
ties were experienced when large time steps (3 and 4 seconds) were
used. The solution became unstable, apparently because the thermal-
hydraulic updates were too infrequent.

The final calculation in the first group was that of a BWR rod
drop accident. For this problem, THERMIT was used with a single
assembly modeling the core. The reactor was assumed to be at full
power when a high worth control rod dropped out of the core. The
reactivity insertion was assumed to occur at a constant rate. The
reactor was scrammed at 0.2 seconds after core power reached 120% of
the rated value. The negative reactivity insertion was also assumed
to occur at a constant rate. Temperature-dependent fuel properties
were used in the calculation. The reactor power was calculated to
increase to 2.6 times the steady-state value before being turned
around by the scram. It was found that changes in fuel temperature
and void fraction were negligible contributors to the transient behav-
ior between time of the rod drop and the scram. About 2% of the total
energy produced was deposited directly into the coolant, contributing
somewhat to the void reactivity feedback. The magnitude of the void

reactivity feedback was found to be about twice as great as that due to the Doppler effect. No verification of the accuracy of these results was given.

The first of the benchmark cases was an analysis of a reactivity insertion transient experiment performed with the SPERT III E-Core reactor. This reactor was essentially a small PWR in which the fuel was enclosed in cans. Because of the severity of the transient, small time steps were deemed necessary and hence THERMIT-3 was used. The calculated results were in excellent agreement with the experimental measurements. The calculated peak power was within the uncertainty of the experimentally measured value and occurred only 0.005 seconds later than the measured peak. The second benchmark case was a calculation of the first Peach Bottom-2 turbine trip experiments. Three pressurization transients were performed at the BWR plant in April 1977 in which the turbine was manually tripped at different power levels and near rated core flow. An intentional delay in the scram circuit logic permitted limited neutron flux increases as a result of the void collapse caused by the core pressurization. The signal to scram was eventually initiated by a high neutron flux level. The reactor was modeled by a single average-powered assembly and THIOD was used for the analysis. A major problem in specifying the problem was the unavailability of the core average coefficients of reactivity needed for the feedback calculation. Published reactivity coefficients which appeared to be the best available were used, but it was

found that the results were extremely sensitive to the value of
the void reactivity coefficient. It was assumed that 1.86% of the
total power was directly deposited in the moderator. Core inlet
flow and outlet pressure boundary conditions were used as calculated
by RETRAN and adjusted for use in MEKIN. After the turbine trip, the
pressure remained constant for approximately 0.35 seconds and rose
thereafter. The transient was analyzed using several different time
steps. A time step of 0.05 seconds was found to be too large; so
calculations with time steps of 0.02 and 0.01 seconds were performed.
These small time steps were not required by stability considerations,
but rather by the accuracy of the calculated results. One result of
this was that THERMIT-3 would have been more appropriate than THIOD
for this analysis. The measured peak power and time to peak power
could not be matched with the reference reactivity coefficients, so
the void reactivity coefficient was "fine-tuned" until the calculated
results agreed well with the measurements. This emphasizes a major
problem with reactivity feedback loop. The feedback calculation is
only as good as the reactivity coefficients used in the model. Core
average reactivity coefficients are limited in their accuracy and are
difficult to calculate. Even when the calculation matched the exper-
mental peak power and time of peak power fairly well, the total energy
deposited during the transient was significantly less than the experi-
ment indicated. This was largely due to a more gradual power increase
calculated by THIOD. Dubé explained this discrepancy as a combination

change in local power and maximum fractional change in k-effec-
tive. When the input convergence limits are met, the neutron flux is
converged to a higher precision to complete the steady-state calcula-
tion.

The code FX2-TH also iterates on local power while using a "re-
laxed" neutronic convergence criterion for the steady-state calcula-
tion. When the change in local powers is small enough, tightly con-
verged neutron fluxes are then calculated, as well as the final set of
thermal-hydraulic conditions. This iterative process will always con-
verge if the temperature coefficients of reactivity for both fuel and
coolant are negative.

3.4 Coupling of QUANDRY and THERMIT

The investigation of other coupled codes indicated that a tandem
solution procedure has been frequently used and has been generally
sucessful. This approach seems particularly appropriate for the task
at hand, since two existing codes with rather different solution
schemes are to be coupled. For these reasons, it was decided to pur-
sue a simple tandem coupling of OUANDRY and THERMIT while considering
many of the following important characteristics of the two codes:

1) Both codes can model a nuclear reactor core as a collection
   of large homogenized volumes or nodes. As a result, it is
   assumed that the same geometric model will be used for both
   neutronic and thermal-hydraulic calculations.

2) There is no convenient way to get a steady-state solution

of two problems: an inadequate reactor model and the existence of multidimensional effects which could not be accounted for.

3.3 Details of Coupling Strategies

Though all the codes reviewed utilized a tandem method, there are differences in the details of how this is applied to specific cases. This is particularly true for the steady-state solution procedures. For example, in BNL-TWIGL the coupled steady-state solution is obtained by iterating on the thermal-hydraulic region power until the largest fractional change is less than 10^{-4}. The spatial fluxes are then converged to within 10^{-6} fractional change. The steady-state is then considered to have been achieved. In MEKIN, a relaxation scheme was built into the steady-state procedure to correct problems encountered when certain calculations developed oscillations and would not converge. Cook conjectured that the problems were the result of representing cross-section changes as step perturbations, a fundamental characteristic of tandem strategies. Initially, no damping or smoothing terms other than reactor feedback effects were built into the code. The relaxation scheme takes the local powers after each neutronic calculation and averages them with the local powers of the preceding iteration, transmitting the averaged values to the thermal-hydraulics portion. This procedure has a significant impact in that it enables problems to converge without oscillations, at the expense of slightly longer running times. The steady-state calculation iterates on maximum fractional change in local power and maximum fractional

in THERMIT. Steady-state solutions are obtained by running an
unperturbed transient from an initial guess of thermal-hydrau-
lic conditions, which eventually converges to a solution which
changes little from time step to time step. This limitation
cannot be removed without making THERMIT fully implicit, a
major effort in and of itself. Running a problem with THERMIT
is a two-step process. When a steady state solution has been
obtained, the conditions are written to a disk file where they
are preserved for the transient calculation. The transient
calculation is a separate problem, beginning with reading the
initial conditions stored on the tape.

3) QUANDRY has a separate static (steady-state) solution proce-
dure which is very fast and convenient to use. A transient
solution follows immediately after the completion of the
static solution, continuing until the specified transient time
has elapsed. Thus, the modes in which QUANDRY and THERMIT
operate are not consistent.

4) For calculations involving feedback, the QUANDRY static calcu-
lation utilized the simple thermal-hydraulic model to deter-
mine cross-sections before and during the calculation. Thus,
the feedback effects are included in the static calculation as
well as in a transient calculation. The simple thermal-hy
draulic model cannot calculate boiling conditions.

5) There is a large difference in time scales between the re-
sponse of the neutronic component and the thermal-hydraulic
component during a transient. Therefore, it is likely that
the appropriate neutronic and thermal-hydraulic time steps
will be different during a transient calculation.

6) Because of "Courant" stability limitations, THERMIT is design-
ed to choose the proper time step sizes (within user-supplied
upper and lower limits) during the calculation of a transient.
Thus, it is not possible to know exactly what thermal-hydrau-
lic time step sizes will be used prior to running the actual
problem. As a result, the neutronic time steps cannot be pre-
dicted either.

7) Transients which may be of interest may be initiated by either
neutronic or thermal-hydraulic perturbations and may include
additional contributions from either component during a trans-
ient (i.e., control-rod movement during a loss of flow acci-
dent).

8) Simple tandem solution techniques result in step changes in
cross-sections and local powers which may give rise to errors
and/or oscillatory behavior.

9) THERMIT requires a set of initial conditions to be supplied as
input to the code. Among these initial conditions are the av-
erage coolant temperatures for each node, which must be deter-
mined from some auxiliary calculation or simply guessed. A

realistic set of initial coolant temperatures can lead to improved steady-state convergence for calculations with feedback [29]. As a result, the simple QUANDRY thermal-hydraulics model will be retained to calculate the initial coolant temperatures and to set the first cross-sections.

All of these factors had to be considered in designing the coupling strategy. The steady-state coupling procedure selected is as follows:

1) Read in input data. All data arrays are placed in a container array and read in free format.

2) Perform initializations. The initial thermal-hydraulic conditions are calculated with the simple QUANDRY model and the initial cross-sections are calculated.

3) Perform an entire static neutronics calculation with no feedback.

4) Calculate the nodal powers and pass these to the thermal-hydraulics segment.

5) Perform the thermal-hydraulics calculation for one unperturbed time step (time step size determined by THERMIT subroutine).

6) Check for convergence, based on nodal power fractional change. If not converged, check for exceeding maximum time. If converged, the steady-state conditions are written on disk file for transient use. If not, continue.

7) Recalculate cross-sections using latest averaged thermal-hydraulic parameters.

8) Return to 3.

To date, this procedure has not been fully implemented. Convergence based on nodal powers has not yet been incorporated, so the current version simply calculates to the end of the specified time period. Experience with performing coupled steady-state calculations is needed to establish the proper convergence criteria. Programming is incomplete for writing the converged steady-state solution on the disk file, so only steady-state calculations are now feasible. The programming necessary to perform a transient calculation has not been incorporated and will be added only after adequate demonstration of the steady-state coupling methodology.

The proposed transient coupling scheme is as follows:

1) Read steady-state conditions from disk file. Read transient input data from input source.

2) Determine thermal-hydraulic time step, using THERMIT subroutine to satisfy Courant numerical stability requirements. Calculate the neutronic time step as an integral function of the thermal-hydraulic time step.

3) Begin the tandem calculation procedure, starting with either the neutronics or the thermal-hydraulics segments, depending on the type of transient initiation.

4) Following neutronic calculations spanning one thermal-hydrau-
lic time step, nodal powers are calculated and updated in the
thermal-hydraulics segment. Following a thermal-hydraulic
time step, the average coolant temperature, coolant density,
and average fuel temperature is calculated for each volume.
The linear cross-section model then adjusts the cross-sections
for each volume and the next neutronic time step begins.

5) The procedure described in 4 continues until the transient
time has elapsed. Figures 3 and 4 show the steady-state and
transient coupling strategies, respectively.

3.5 Summary

The work of Dubé showed that THERMIT is amenable to being coupled
to a neutronics model and can give good results within the limitations
of the neutronics model. The investigation of coupling strategies
showed that the tandem formulation is most often used and generally
works well. However, certain problems encountered in other codes may
be anticipated for the current work. The detailed coupling strategy
developed for QUANDRY/THERMIT attempts to accommodate the different
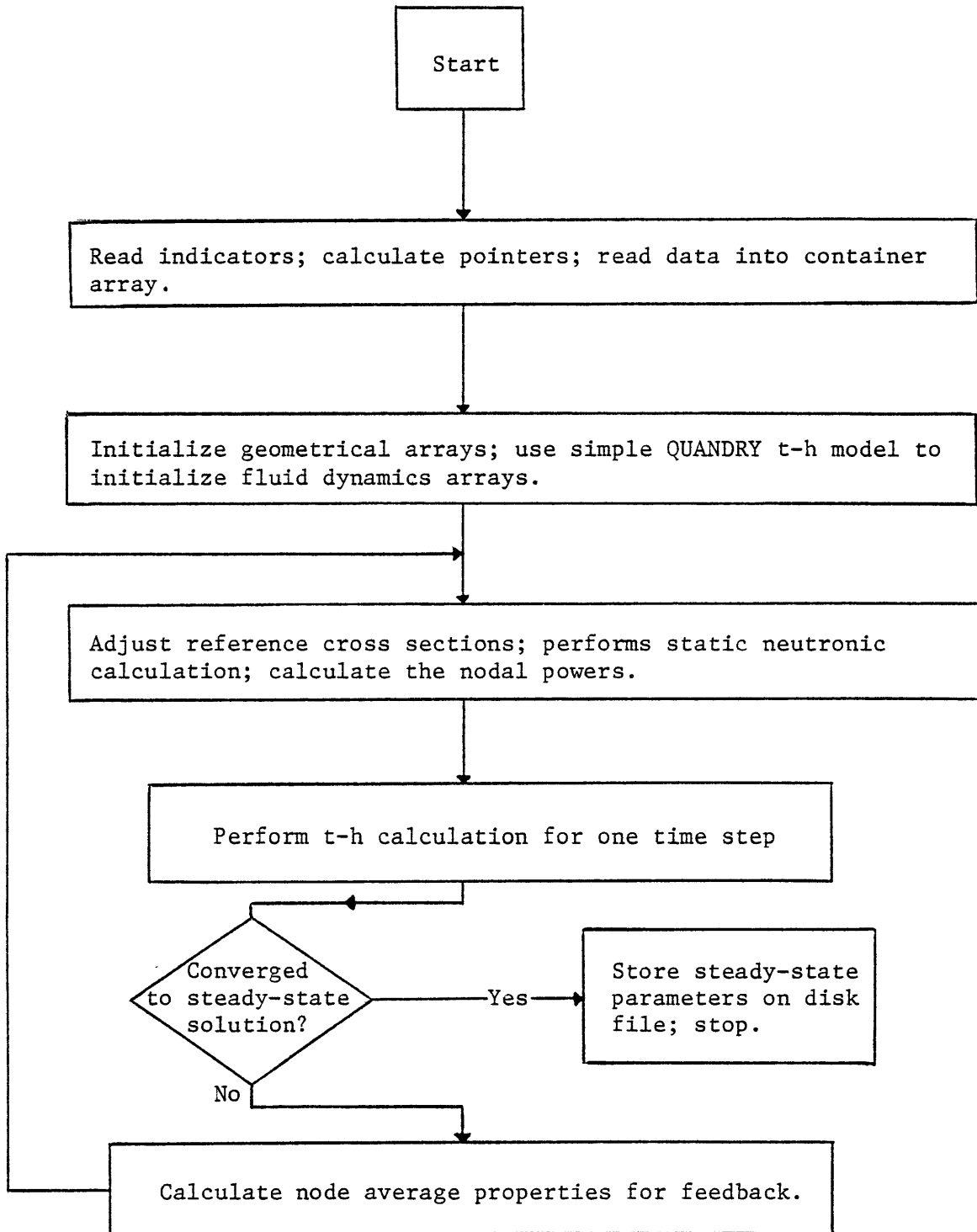solution schemes and operational characteristics of the two codes.

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                                ▼
┌─────────────────────────────────────────────────────────────────┐
│ Read indicators; calculate pointers; read data into container    │
│ array.                                                           │
└─────────────────────────────────────────────────────────────────┘
                                │
                                ▼
┌─────────────────────────────────────────────────────────────────┐
│ Initialize geometrical arrays; use simple QUANDRY t-h model to   │
│ initialize fluid dynamics arrays.                                │
└─────────────────────────────────────────────────────────────────┘
                                │
            ┌───────────────────┤
            │                   ▼
┌───────────┴─────────────────────────────────────────────────────┐
│ Adjust reference cross sections; performs static neutronic       │
│ calculation; calculate the nodal powers.                         │
└─────────────────────────────────────────────────────────────────┘
                                │
                                ▼
      ┌─────────────────────────────────────────────────┐
      │ Perform t-h calculation for one time step        │
      └─────────────────────────────────────────────────┘
                                │
                   ╱◆╲
              ╱ Converged ╲              ┌──────────────────────┐
             ╱ to steady-state ╲──Yes──▶│ Store steady-state    │
             ╲  solution?      ╱         │ parameters on disk    │
              ╲              ╱           │ file; stop.           │
                   ╲◆╱                   └──────────────────────┘
                    │ No
                    ▼
┌─────────────────────────────────────────────────────────────────┐
│ Calculate node average properties for feedback.                  │
└─────────────────────────────────────────────────────────────────┘
```
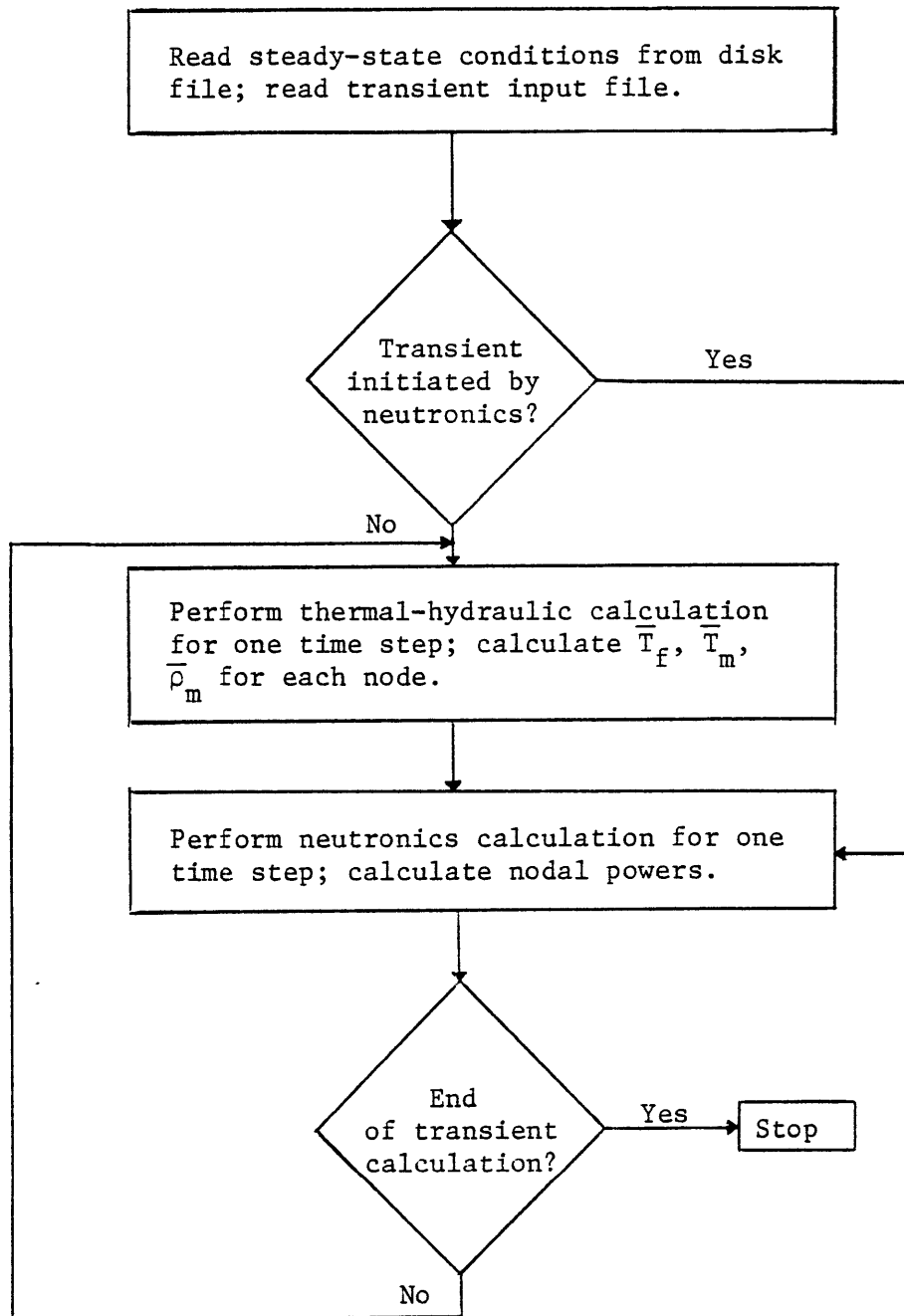
Figure 3: Steady-State Coupling Strategy

```
┌─────────────────────────────────────────┐
│ Read steady-state conditions from disk   │
│ file; read transient input file.         │
└─────────────────────────────────────────┘
```

Transient initiated by neutronics?

Yes

No

Perform thermal-hydraulic calculation for one time step; calculate $\overline{T}_f$, $\overline{T}_m$, $\overline{\rho}_m$ for each node.

Perform neutronics calculation for one time step; calculate nodal powers.

End of transient calculation?

Yes

Stop

No

Figure 4: Transient Coupling Strategy

CHAPTER 4. CODE DEVELOPMENT

4.1 QUANDRY Conversion

Before the coupling methodology could be implemented, it was necessary to convert QUANDRY from an IBM version to a MULTICS version. MULTICS is an interactive computer system at MIT incorporating a Honeywell computer and an extensive complement of software features. In addition, the MULTICS system has considerable cost advantages over the other available MIT system (IBM 370/168), an important consideration for developmental work. Finally, essentially all of the THERMIT developmental work has been performed on the MULTICS system, so that the working versions of THERMIT are all on MULTICS. This conversion was accomplished and a number of sample problems have been run to verify that the code is working properly. The conversion proved to be much more difficult than was anticipated, because of subtle differences between the handling of entry points in the two systems. The important changes to QUANDRY involved in making the MULTICS version were:

    1) Removal of IBM data management package;

    2) Explicit dimensioning of all arrays;

    3) Removal of all entry points;

    4) Reduction of argument lists length for several subroutines;

5) Addition of several common blocks;

6) Addition of function subprograms for the calculation of
   hyperbolic functions.

4.2 Steady-State Coupling

QUANDRY and THERMIT have been reprogrammed so that they will now
function as one program in calculating steady-state problems with
feedback as described in Chapter 3. Accomplishing this required nu-
merous changes in both codes. These changes may be summarized as fol-
lows:

1) The first category of changes involved the reading of input
   data and the handling of subscripted variables (arrays). In
   THERMIT, all arrays are placed in a single container array and
   a pointer system locates the indices of the particular values
   of interest. This is done to allow object-time dimensioning
   of the arrays, preventing the wasted storage space associated
   with explicitly dimensioned arrays. In fact, object-time di-
   mensioning is not done in the current version, since the vir-
   tual memory of MULTICS allows the container array to have a
   dimension of unity and yet can address an essentially unlimi-
   ted number of data values placed in the array. To take advan-
   tage of this feature, all QUANDRY arrays were placed in this
   container array and new pointers corresponding to the QUANDRY
   arrays were added. In addition, the reading of many of the
   QUANDRY data constant was moved into THERMIT subroutine INPUT.

2) The second category of changes involves the transfer of data among the various subroutines. This required the creation of several new common blocks and the addition of existing common blocks to certain subroutines. The variables passed through subroutine argument lists were expanded in certain cases. Some dimension statements had to be augmented as well.

3) The QUANDRY subroutines MAIN and SSTATE were eliminated. These subroutines were primarily responsible for controlling the flow of the program. These functions were transferred to THERMIT subroutines INPUT, INIT, INITFD, and TRANS.

4) The fluid dynamics initialization procedure was modified so that the simple thermal-hydraulics model in subroutine SSTH calculates the initial coolant temperatures prior to specifying the fluid temperatures in INITFD. The coolant temperatures are then set equal to the calculated value for each volume. Since the simple model does not calculate a pressure drop, the existing input pressure initialization is retained.

5) The axial and transverse power shape functions used by THERMIT to calculate local powers have been replaced by a single array which stores the calculated local power for each node.

6) A subroutine CONTROL has been added which is the interface between the static solution procedure of QUANDRY and the transient calculational procedure of THERMIT.

7) A subroutine LUMPTH has been added which calculates the average fuel temperature, average coolant density, and average coolant temperature for each volume following each thermal-hydraulic time step. LUMPTH also initiates the calculation of new cross sections for each volume in preparation for the next neutronic calculation.

A large number of other miscellaneous changes were made, all of which will be documented in the eventual thesis report. Figure 5 is a flow chart of the coupled steady-state code. As was mentioned in Chapter 3, the programming for the transient solution has not been completed, pending adequate demonstration of the steady-state technique. However, the achievement of the steady-state coupling includes the most significant of the coding changes needed for transient coupling.

4.3 Sample Problem

A sample steady-state problem has been prepared for testing and debugging. This problem consists of two shortened BWR bundles (based on Brown's Ferry). The problem has already been analyzed with an updated version of QUANDRY capable of calculating feedback with boiling. The problem has the virtues of being simple and of having the results verifiable.
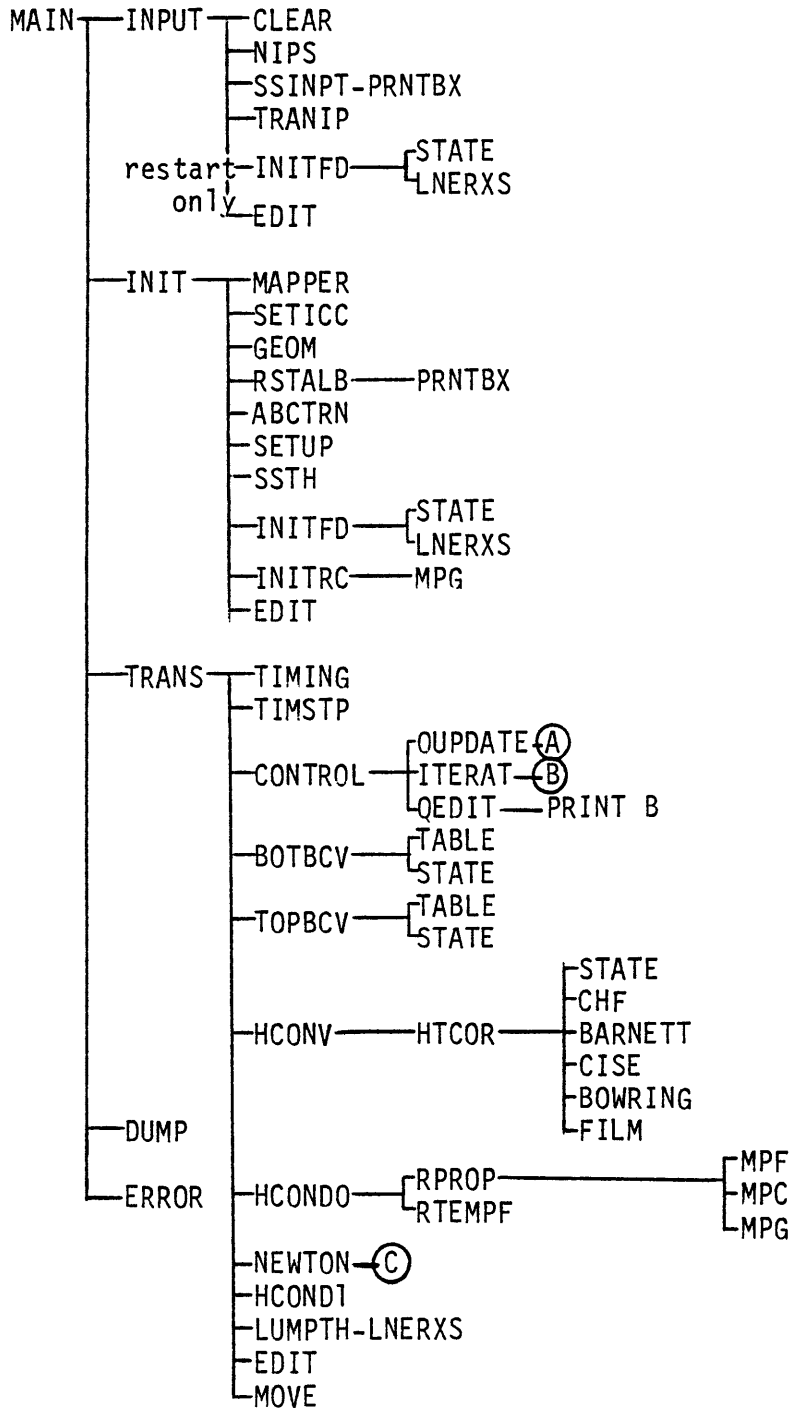
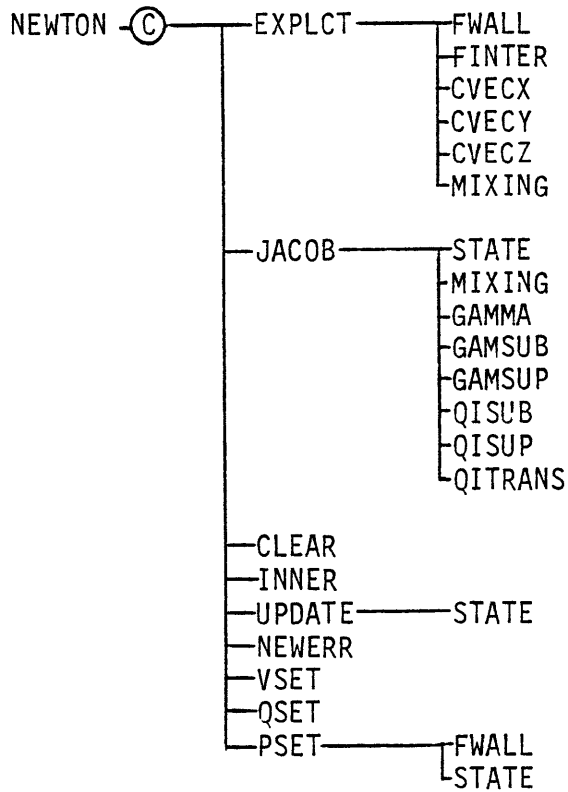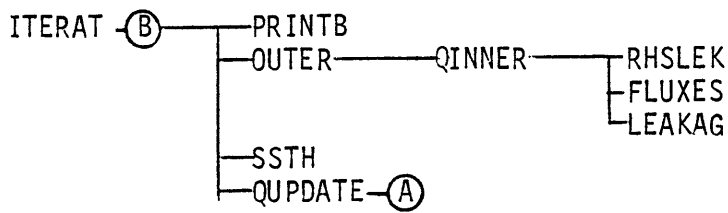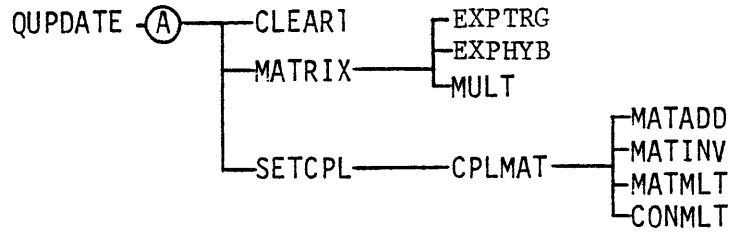FIGURE 5: QUANDRY/THERMIT FLOW CHART

FIGURE 5 (cont.): QUANDRY/THERMIT FLOW CHART

CHAPTER 5. SUMMARY OF PROJECT STATUS

5.1 Review

An investigation of the existing coupled neutronics/thermal-hy-draulics codes has been performed and reported. It was found that all of the known codes have limitations in their neutronic and/or thermal-hydraulic models which limit their generality of application and accuracy. It was also found that a tandem coupling scheme was most often employed and generally performed well. A detailed steady-state and transient coupling scheme based on the tandem technique was devised, taking into account the important operational characteristics of QUANDRY and THERMIT. The two codes were combined and the necessary programming modifications were performed to allow steady-state calculations with feedback. A simple steady-state sample problem was produced for the purpose of testing and debugging the coupled code.

5.2 Project Status

The coupled steady-state code has been successfully compiled on the MULTICS computer. The code has been debugged through all the input processing. However, some errors in the initialization process have prevented the completion of the calculation. Hence, no calculational results are available currently.

5.3 Future Work

The debugging process must be completed so that the sample problem

can be analyzed and results checked for accuracy. The additional pro-
gramming needed for transient calculations must be performed and the
steady-state/transient version must be compiled and debugged. The
first transient analyzed will be a null based on the steady-state
sample problem.

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