NERGY LABORATORY

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

ADVANCED METHODS DEVELOPMENT FOR LWR TRANSIENT ANALYSIS, FINAL REPORT: 1981 - 1982 by

D. P. Griggs, M. S. Kazimi and A. F. Henry Energy Laboratory Report No. MIT-EL 82-021 May 1982





Room 14-0551 77 Massachusetts Avenue Cambridge, MA 02139 Ph: 617.253.5668 Fax: 617.253.1690 Email: docs@mit.edu http://libraries.mit.edu/docs

DISCLAIMER OF QUALITY

Due to the condition of the original material, there are unavoidable flaws in this reproduction. We have made every effort possible to provide you with the best copy available. If you are dissatisfied with this product and find it unusable, please contact Document Services as soon as possible.

Thank you.

Pages are missing from the original document.

Appendix pages A B & C ave missing from the original archival version. This is the most complete. copy available.

Energy Laboratory

and

Department of Nuclear Engineering

.

Massachusetts Institute of Technology Cambridge, Mass. 02139

ADVANCED METHODS DEVELOPMENT FOR LWR TRANSIENT

ANALYSIS, FINAL REPORT: 1981-1982

by

D. P. Griggs, A. F. Henry and M. S. Kazimi

May 1982

sponsored by

Boston Edison Company Long Island Lighting Company Northeast Utilities Service Company PSE & G Research Corporation Yankee Atomic Electric Company

under

M.I.T. Energy Laboratory Electric Utility Program Energy Laboratory Report No. MIT-EL 80-021

ADVANCED METHODS DEVELOPMENT FOR LWR TRANSIENT ANALYSIS, FINAL REPORT: 1981-1982

ABSTRACT

The initial development of TITAN, a three-dimensional coupled neutronics/thermal-hydraulics code for LWR safety analysis, has been completed. The transient neutronics code QUANDRY has been joined to the two-fluid thermal-hydraulics code THERMIT with the appropriate feedback mechanisms modeled. A detailed steady-state and transient coupling scheme based on the tandem technique was implemented in accordance with the important structural and operational characteristics of QUANDRY and THERMIT. A two channel sample problem formed the basis for steady-state and transient analyses performed with TITAN. TITAN steady-state results were compared with those obtained with MEKIN and showed good agreement. A fuel pin model sensitivity study was performed for steady-state problems. Null transients, simulated turbine trip transients, and a rod withdrawal transient were analyzed with TITAN and reasonable results were obtained.

| TAB | LE | 0F | CON | TE | N | ΤS |
|-----|----|----|-----|----|---|----|
| | | | | | | |

| | | <u>Pa</u> | age |
|----|-------|---|-----|
| 1. | INTRO | DUCTION | 4 |
| | 1.1 | Motivation | 4 |
| | 1.2 | Background | 8 |
| | | 1.2.1 TITAN | 8 |
| | | 1.2.2 QUANDRY | 9 |
| | | 1.2.3 THERMIT | 10 |
| | 1.3 | Preview 1 | 12 |
| 2. | PREVI | DUS WORK | 13 |
| | 2.1 | Literature Review 1 | 13 |
| | 2.2 | QUANDRY Conversion 1 | 13 |
| | 2.3 | Steady-State Coupling and Sample Problem | 14 |
| | 2.4 | Transient Coupling 1 | 14 |
| 3. | CODE | JEVELOPMENT | 15 |
| | 3.1 | Coupling of OUANDRY and THERMIT 1 | 15 |
| | 3.2 | Steady-State Coupling Methodology | 22 |
| | 3.3 | Transient Coupling Methodology | 24 |
| | 3.4 | Additional Code Features | 28 |
| | | 3.4.1 Steady-State Neutronic/Thermal-Hydraulic Iteration Variation | 28 |
| | | 3.4.2 Improved Inner (Pressure) Iteration Method | 30 |
| | | 3.4.3 Improvements to Heat Transfer Package | 31 |
| | | 3.4.4 Direct Moderator Heating | 31 |
| | | 3.4.5 Simple Boiling Thermal-Hydraulics Model | 33 |

.

•

**

.

•

| | | - | Page |
|-----|--------|--|------|
| 4. | CODE | APPLICATIONS | 34 |
| | 4.1 | Sample Problem | 34 |
| | 4.2 | Steady-State Results | 37 |
| | | 4.2.1 Investigation of Feedback Sensitivity | 37 |
| | | 4.2.2 TITAN Results, Non-Boiling Steady-State Case | 37 |
| | | 4.2.3 TITAN Results, Steady-State Boiling Case | 40 |
| | | 4.2.4 Fuel Pin Model Sensitivity Studies | 49 |
| | 4.3 | Transient Results | 56 |
| | | 4.3.1 TITAN Null Transient Analyses | 56 |
| | | 4.3.2 Simulated Turbine Trip Analyses | 58 |
| | | 4.3.3 Rod Withdrawal Transient | 66 |
| 5. | PROJE | CT STATUS AND FUTURE WORK | 69 |
| | 5.1 | Summary of Project Results | 69 |
| | 5.2 | Future Work | 70 |
| REF | ERENCE | S | 71 |
| APP | ENDIX | A. TITAN Fortan Listing (pre-release version) | |
| APP | ENDIX | B. Sample Input | |
| APP | ENDIX | C. Sample Output | |

.

1. INTRODUCTION

1.1 Motivation

The safe and reliable operation of nuclear power plants requires that the consequences of anticipated transients and postulated accidents be mitigated by conservative design and engineered safety features. Owing to the impracticality and undesirability of actually testing power plants under accident conditions, analytical simulations are used to investigate reactor transients. These analytical simulations are performed using computer programs of varying scope and size which attempt to simulate the important physical processes by solving complicated systems of mathematical equations, empirical correlations and tabular data.

The analysis of light water reactor transients requires computer codes capable of modeling diverse physical processes and their interactions. These processes include neutron physics, fluid dynamics, heat transfer, structural mechanics, materials behavior, chemical reactions and electron-Numerous computer codes of varying sophistication and having a wide ics. range of applications have been developed and applied in the design and licensing of nuclear power plants. A large number of these have involved simulating the generation and removal of fission energy within nuclear reactor cores. These codes are primarily concerned with modeling processes which may be separated into two categories called neutronics and thermal-hydraulics. Neutronics (equivalently neutron kinetics) refers to the processes by which neutrons are produced and interact with the materials in the reactor core. Thermal-hydraulics refers to the processes by which fission energy is transported from its source to the appropriate destination. Thermal-hydraulics codes may therefore model more than just the reactor core and indeed may be general enough to be used in non-nuclear applications.

-4-

The analysis of nuclear reactor cores often reflects the division of processes into the neutronics/thermal-hydraulics categories, resulting in the widespread use of computer codes which model the transport of neutrons or the transport of fission heat, but not both. In this approach, a thermal-hydraulics code requires that the space- and time-dependent heat source (fission rate) be supplied by some means. Similarly, the neutronics code requires some knowledge of the temperatures and densities of the important core materials in order to determine the nuclear cross sections. Thermal-hydraulics and neutronics codes are therefore not independent of each other even when it is assumed that the processes are independent. In reality, thermal-hydraulics and neutronics processes are dynamically linked by complicated forms of interaction of core materials with neutrons brought about by temperature and density variations. These dependencies, known collectively as feedback effects, are frequently neglected in reactor analyses with the assumption that this results in acceptably small and conservative errors. Nevertheless. for many transients of interest the feedback between neutronics and thermal-hydraulics can be significant enough to warrant the development of codes modeling neutronics, thermal-hydraulics and feedback mechanisms. Indeed, a number of coupled neutronics/thermal-hydraulics codes have been developed and used for reactor analyses. Several of these coupled codes have been summarized in Table 1. Some of these codes have relatively simple models for the neutronics or thermal-hydraulics or both. These simple models give only approximate results and are generally accurate for limited applications. Examples of such model limitations are the use of point kinetics approximations for neutronics calculations or homogeneous equilibrium models for two-phase flow.

-5-

TABLE 1

SUMMARY OF NEUTRONIC/THERMAL-HYDRAULIC CODES

| | Thermal-Hydraulics | Neutronics |
|---------------------|---|--|
| CHIC-KIN [5] | 1-D, single channel model | point kinetics |
| PARET [6] | four channel model | point kinetics |
| TWIGL [7] | lumped parameter model, no boiling allowed | 2-D, 2-group finite difference diffusion theory model |
| WIGL3 [8] | lumped parameter model, no boiling allowed | 1-D, 2-group finite difference diffusion theory model |
| BNL-TWIGL [9] | time-dependent two-phase model | 2-D, 2-group finite difference diffusion theory model |
| SAS2A (LMFBR) [10] | 1-D with sodium bubble model | point kinetics |
| FX2-TH (LMFBR) [11] | 1-D with no boiling | 3-D, multi-group diffusion theory, quasistatic method |
| HERMITE [12] | 2-D homogeneous equilibrium model | 3-D finite element diffusion theory, 1 to 4 groups |
| MEKIN [13] | 2-D homogeneous equilibrium . | 3-D finite difference 2-group diffusion theory |
| RAMONA3B [14] | 1-D nonequilibrium model with BWR loop | 3-D, $1\frac{1}{2}$ -group nodal method |
| THIOD [15] | 1-D, two-fluid model, nonequilibrium | point kinetics |
| THERMIT-3 [15] | 3-D two-fluid model, nonequilibrium | point kinetics |

/

.

Table 1 (continued)

.

.

Thermal-Hydraulics

QUANDRY [2] lumped parameter model, no boiling TITAN 3-D two fluid, nonequilibrium model for LWR

Neutronics

.

.

3-D, 2 group nodal diffusion theory model

3-D, 2-group nodal diffusion theory model

.

.

In order to maximize the potential accuracy and generality of application of a coupled code, it is necessary to model all the relevant processes as completely and rigorously as possible. To this end, a research project has been sponsored under the M.I.T. Energy Laboratory Utilities Program to develop a state-of-the-art code to calculate three-dimensional steady-state and transient neutronics and thermalhydraulics with feedback. 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 was to be accomplished by uniting THERMIT with QUANDRY [2], an advanced three-dimensional transient neutronics code. During the initial phase of work, the coupling strategy was devised, the two codes were merged, and the coding for steady-state operation was implemented. A report summarizing that phase was published [3]. Subsequently, a second 12-month period of work was begun in March 1981 to continue development of the combined code. This report presents the work performed during that time.

1.2 <u>Background</u>

1.2.1 <u>TITAN</u>

The coupling of QUANDRY and THERMIT has resulted in the computer code TITAN, as shown in Table 1. TITAN is an acronym for <u>Three-dimensional</u> <u>Integrated Thermal-hydraulics And Neutronics</u>. In order to understand the details of TITAN and the results of TITAN analyses, it is useful to review the two codes from which TITAN was developed.

-8-

1.2.2 QUANDRY

QUANDRY [2] is a neutronics code developed at M.I.T. based on an analytic 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 homogenized regions (or nodes), for which equivalent diffusion theory parameters 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. OUANDRY has a built-in thermal-hydraulic feedback capability, based on a simple lumped heat capacity model with a linear cross section model. The thermalhydraulic 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 calculational volume (i, j, k) is determined by an equation of the form:

-9-

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

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.

1.2.3 THERMIT

THERMIT [1] is an advanced two-fluid thermal-hydraulics 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 nonequilibrium 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 than other models.

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 [4]. 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:

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

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. 1.3 Preview

٩,

This introductory chapter has provided the motivation and background for the current work. Chapter 2 contains a review of the previous work performed on this project. Chapter 3 contains a detailed discussion of the development of the TITAN code. Chapter 4 presents the results of the application of TITAN to steady-state and transient sample problems. Chapter 5 summarizes the progress made and briefly presents future work. The report concludes with references and appendices.

2. PREVIOUS WORK

2.1 Literature Review

In the initial year of development, a number of preparatory steps were performed. The open literature on coupled codes was reviewed and the features and coupling strategies of these codes were assessed. It was found that essentially all of the codes reviewed used some form of the tandem coupling method, in which the neutronics and thermal-hydraulics calculations are performed alternately, with feedback information passed between each segment as required. The feedback loops were either for reactivities or cross sections, depending on the neutronics model used. The details of the coupling strategies varied among the codes investigated, particularly in the method for determining steady-state convergence. The primary conclusion drawn from this survey was that tandem coupling strategies were almost universal and seemed to work well for the codes reviewed.

2.2 QUANDRY Conversion

The QUANDRY code was developed on an IBM 370/168 computer, while essentially all of the THERMIT developmental work was performed on the M.I.T. MULTICS computer system. MULTICS is an interactive computer system incorporating a Honeywell computer and an extensive complement of software features. In addition, the MULTICS system has considerable cost advantages over the IBM system, an important consideration for developmental work. It was therefore decided to convert QUANDRY to the MULTICS system prior to beginning the actual coupling. This conversion was accomplished and several sample problems were run to verify the proper operation of the code.

2.3 <u>Steady-State Coupling and Sample Problem</u>

The major task in the previous work was the development and implementation of the steady-state coupling methodology. The details of this coupling methodology are discussed in full in Chapter 3. The implementation of this coupling methodology required numerous changes to both original codes, resulting in one unified code which performs the functions of both original codes in the context of the coupling methodology. The input handling functions were unified and all variable arrays were consolidated into one container array. The control of program flow and the interfacing between neutronics and thermal-hydraulics required the elimination of several existing subroutines and the addition of new subroutines as well as numerous changes and additions to existing subroutines. A subroutine was added to calculate the average nodal properties needed for the feedback calculation. Certain input variables, such as axial and transverse power shapes, were eliminated, since these are calculated internally by the coupled code. Though these changes had all been implemented, successful demonstration of a coupled steady-state calculation had not been attained at the end of the first year. A simple two channel BWR problem was selected and modeled for the purpose of debugging and verifying the coupled code. This problem is described in detail in Chapter 4.

2.4 Transient Coupling

The principles of the transient coupling had been defined, but were not implemented pending successful demonstration of the steady-state coupling methodology. A rod withdrawal problem based upon the simple two channel BWR geometry was selected for the purpose of debugging and verifying the transient mode.

3. CODE DEVELOPMENT

3.1 Coupling of QUANDRY and THERMIT

The coupling methodology used in TITAN was devised after reviewing other coupled codes and after considering many of the important characteristics of QUANDRY and THERMIT. A number of these characteristics will be discussed prior to presenting the coupling methodology.

Both THERMIT and QUANDRY can model a nuclear reactor core as a collection of large homogenized volumes or nodes. In addition, THERMIT can also be used for rod bundle analyses using coolant-centered subchannels. However, THERMIT does not allow both types of control volumes in the same model. Therefore, it was determined that only the rod-centered channel modeling capability of THERMIT would be utilized in TITAN. In order to simplify the coupling logic, it was assumed that the same geometric model would be used for both neutronics and thermal hydraulics calculations. This was thought to be appropriate for most applications. The ability to have more flexibility in modeling reactor cores could be added later if desired.

The QUANDRY code was written with a feedback capability supplied by a simple thermal-hydraulics model and the linear cross section model described earlier. The simple thermal-hydraulics model is used to supply the average fuel temperatures, average moderator temperatures, and average moderator densities needed for the cross section calculation. The simple thermal-hydraulics model assumes no boiling, neglects the gap between fuel and cladding, assumes no pressure drop, and assumes no reverse flow. Feedback calculations are performed for steady-state and transient calculations.

-15-

The solution of the thermal-hydraulics equations in THERMIT requires that the local power be specified. The initial total reactor power is an input parameter. The local power is determined by an axial and a transverse power shape which are also given as input. During a transient, the total reactor power may be given as an exponential function of time or in tabular form. The power shapes are assumed to remain constant during a transient. The use of two power shape functions does not allow an arbitrary distribution of nodal powers to be modeled, since each channel is assumed to have the same axial power profile. This type of nodal power specification was therefore unsatisfactory for a three-dimensional coupled code. The two power shapes were replaced by an array containing the local nodal powers as calculated by the neutronics package. This constitutes the feedback from neutronics to thermal-hydraulics.

The contribution of the thermal-hydraulics calculation to the feedback is temperatures and densities for the fuel and moderator. Since there was an existing feedback model in QUANDRY, it was decided to retain it for the initial coupling of QUANDRY and THERMIT. This model requires the calculation of the average fuel temperature and the average moderator temperature and density for each node. Since THERMIT is a two fluid code, temperatures and densities are calculated for the fluid and the vapor in each node. The fuel pin model allows for the calculation of a temperature distribution, with a user-specified number of radial locations calculated. Thus, it was necessary to add some averaging logic in order to obtain the correct nodal values to use in the linear cross section model. The average parameters are calculated as follows:

-16-

$$\overline{T}_{f} = \frac{\sum_{i=1}^{N} \pi (0.5) (T_{i+1} + T_{i}) (r_{i+1}^{2} - r_{i}^{2})}{\pi r_{N+1}^{2}}$$

where \overline{T}_{f} = node averaged fuel temperature T_{i} = calculated temperature at point "i" in the fuel r_{i} = radial location of point "i" in the fuel N = number of calculational cells in the fuel

and

$$\overline{\rho}_{m} = \alpha \rho_{V} + (1 - \alpha) \rho_{\ell}$$

where $\overline{\rho_{m}}$ = node averaged moderator density, α = node void fraction ρ_{v} = vapor density ρ_{g} = liquid density

and,
$$\overline{T}_{m} = \frac{\alpha \rho_{v} T_{v} + (1 - \alpha) \rho_{\ell} T_{\ell}}{\overline{\rho}_{m}}$$

 \overline{T}_{m}

T_v

where

 T_{q} = liquid temperature.

The calculation of these average parameters, together with the linear cross section model, constitutes the thermal-hydraulics to neutronics feedback.

The solution method of THERMIT requires that a set of initial conditions be supplied as input to the code. These initial conditions include the pressure, void fraction, vapor temperature, and vapor axial velocity for each node. If a heat transfer calculation is being performed, the initial clad surface temperature for each node is also required. The initial fuel temperatures are set equal to the clad surface temperature in the code. The user must determine appropriate initial conditions from some auxiliary calculation or simply make a reasonable guess. Experience with THERMIT has not shown that there is much sensitivity of running time or steady-state solution to these initial conditions. However, it seemed likely that the convergence of TITAN might be more sensitive to the initial conditions, since the fuel temperatures, moderator temperatures, and moderator densities are also feedback parameters. Therefore, it was decided to replace the input initial conditions with the simple thermal-hydraulics model already included in QUANDRY. This model is capable of supplying reasonable values for the average fuel temperature and the average coolant temperature in each node. Since the model cannot calculate either boiling

conditions or pressure drop, the initial pressures and void fractions were still required to be supplied. In addition, the use of this simple model precludes the analysis of problems having boiling at steady-state. This limitation was acceptable for the initial development of TITAN and has been subsequently removed (see Section 3.4.5).

Considerations of code structures and operational characteristics were important in devising the TITAN coupling methodology. The most important consideration involved the numerical technique used in THERMIT. The semi-implicit Newton-Raphson method does not allow for the solution of the steady-state conservation equations. As a result, there is no convenient way to generate a steady-state solution with THERMIT. Steadystate solutions are obtained by running an unperturbed transient from an initial guess of thermal-hydraulic conditions, which eventually converges to a solution which changes little from time step to time step. This limitation cannot be removed without devising a fully implicit solution method for the three-dimensional, two fluid equations. As a result, THERMIT has been programmed to operate as a two-step, interactive process. When a steady-state solution has been obtained, the calculation is terminated by the user and the steady-state conditions are stored on a disk file.

The transient calculation is a separate problem, beginning with reading the initial conditions from the disk file. This two step method allows the user to monitor the steady-state convergence and ensure that an appropriate set of initial conditions are used in the transient calculation. In addition, a number of transient calculations can be done using the same steady-state solution. Despite its merits,

-19-

the two step operation of THERMIT is only convenient for interactive computer systems such as MULTICS. It is possible to program the code to perform steady-state and transient calculations within one continuous operation. However, for the initial development of TITAN, the two step operational strategy was retained and incorporated into the coupling methodology.

The QUANDRY solution method provides for direct calculation of the static and transient nodal neutron diffusion equations. The static (steady-state) solution procedure is very fast and convenient to use. A transient calculation follows immediately after the completion of the static calculation, continuing until the specified transient time has elapsed. It was therefore necessary to split up the "one-step" structure of QUANDRY in order to couple it to the "two-step" structure of THERMIT. The coupling methodology also had to coordinate the two solution methods of QUANDRY with the single solution method of THERMIT.

Both QUANDRY and THERMIT require the specification of "time steps" for transient calculations. The time steps specify the discrete points in time for which the solutions are obtained. For THERMIT, steady-state calculations also require the specification of time steps. In order to couple the codes together, it was necessary to coordinate the time steps used for the neutronics and thermal-hydraulics calculations. There can be a large difference in time scales between the response on the neutronic component and the thermal-hydraulic component during a transient. Therefore, it is likely that the appropriate neutronic and thermalhydraulic time steps will be different during a transient calculation. For TITAN, this is further complicated by the "Courant" stability limit inherent in the THERMIT numerical method. The maximum acceptable time

-20-

time step is determined by the geometric model and by the maximum fluid velocity. THERMIT was written to determine the appropriate time step size (within user-supplied upper and lower limits) during the calculation of a transient. Therefore, it is not possible to know exactly what thermal-hydraulic time step sizes will be used prior to running the actual problem. The coupling methodology had to be designed to accommodate these characteristics.

The successful development of TITAN required that all of the important characteristics of the two parent codes be considered. None of these characteristics precluded a tandem scheme similar to those used by most of the coupled codes reviewed. Indeed, a tandem approach seemed particularly appropriate since QUANDRY and THERMIT were complete and wholly independent codes having rather different solution schemes. The basic philosophy behind the development of the coupling strategy was that the common support functions, such as input, initialization and editing, would be integrated while the dissimilar computational functions would be linked only by the two sets of feedback information, as described previously. Because of the decision to retain the two step operational characteristic of THERMIT, the coupling process regards THERMIT as the "host" code with the essential parts of QUANDRY installed in it. Within this framework, a coupling strategy was devised which would allow the two codes to function well as a unified code, TITAN. This was accomplished in two parts. First, the coupling necessary to give steady-state analysis capability was implemented and tested. Secondly, this coupling was extended to provide transient analysis capability.

-21-

3.2 Steady-State Coupling Methodology

The major task of the TITAN steady-state coupling methodology is to provide a mechanism for generating a set of neutronic and thermal-hydraulic parameters which correspond to a steady-state condition for the reactor modeled. This could have been accomplished in one of two ways. Average fuel temperatures, coolant temperatures, and coolant densities could be supplied periodically and the appropriate matrix updates performed during a single static neutronics calculation. This is analogous to the procedure followed in QUANDRY for feedback calculations. Another approach is to perform periodic static neutronics calculations while the thermalhydraulics solution is converging. Each static neutronics calculation uses the latest thermal-hydraulic data (and corresponding cross sections) as its starting point and converges to a steady-state solution with no feedback updates.

The latter approach was selected for TITAN. This approach takes advantage of the speed and economy of the QUANDRY static solution method and recognizes that convergence of the thermal-hydraulics solution is the more difficult and time-consuming process. In the former approach, the cross section updates are based on thermal-hydraulic solutions which themselves are not converged and, hence, introduce some error into the static neutronics convergence procedure. The powers supplied to the thermal-hydraulics package are also obtained at some point during the neutronic convergence, again contributing some error to the process. In short, an approach in which both thermal-hydraulics and neutronics solutions are attempting to converge "simultaneously" seemed problematical with respect to even obtaining a unified steady-state solution. It may well be that this procedure could be made to work, but the second

-22-

procedure posed no obvious problems and is consistent with the concept of THERMIT as "host" code.

The steady-state mode of TITAN involves most of the input and initialization functions required for the code. The code is designed to be used interactively, with the user controlling the operation remotely at a terminal. The steady-state coupling procedure takes advantage of this fact, allowing the user to monitor and alter the convergence procedure. An outline of this procedure is as follows:

- Read in input data from an on-line data file. Free format is used; data arrays are placed in a large container array and a pointer system is used to locate individual subscripted variables. This permits object-time dimensioning, if desired.
- Perform initializations. The initial thermal-hydraulic conditions are calculated with a simple model and the initial cross-sections are calculated.
- An entire static neutronics calculation is calculated with the current cross sections. No feedback updates are performed during the static convergence.
- The nodal powers are calculated and these are passed to the thermal-hydraulics segment.
- 5) A thermal-hydarulics calculation is performed for one or more unperturbed time steps (time step size determined by the code). The average nodal thermal-hydraulic feedback parameters and the new cross sections are calculated.
- 6) The current transient time is checked to see if the end of the current time domain has been reached. If the time domain end has not been reached, return to 3) and continue until the end of the time domain. If the end of the last time domain has been reached, the code will do one of two things, depending on the

input option selected. One option is for the calculation to end, writing the steady-state conditions on a disk file if desired. The other option is for the user to be prompted at the terminal for additional time domain information to continue the convergence procedure. If the energy and flow errors displayed at the terminal indicate satisfactory convergence, the user can end the calculation, saving the steady-state conditions on a disk file for a transient calculation. If not, the specification of new time domain information will continue the procedure, returning to 3).

This procedure is summarized in Figure 1. The necessary programming to implement this process has been completed, the code has been compiled, and sample problems have been successfully analyzed. It has been demonstrated that this tandem method converges to a good steady-state solution with a reasonable amount of computational effort for the problems analyzed. The steady-state results are discussed in Chapter 4.

3.3 Transient Coupling Methodology

The primary task of the transient coupling logic in TITAN is to provide the necessary structure to permit the neutronic and thermalhydraulic analysis of a variety of types of transients. The transients of interest may be initiated by changes in reactivity, core flow rate, inlet temperature, reactor pressure or combinations of these. Proper coordination of thermal-hydraulic and neutronic time steps is also required.

The tandem coupling scheme developed for TITAN uses a staggered approach in which it is assumed that the transient is initiated by either neutronics or thermal-hydraulics. The first transient time step is calculated for that segment of the code, subject to the user-supplied forcing functions

-24-

·~ ,



Figure 1: Steady-State Coupling Strategy

and with no feedback contribution included. Following this initial time-step (or time-steps), the relevant feedback information is calculated and, together with any applied forcing functions, constitutes the perturbation which is applied in advancing the other segment to the same transient time. This is illustrated in Figure 2. As is shown in the figure, the segment on the "leading edge" of the feedback loop does not receive the contribution of the feedback until the loop has been closed. This is an inherent limitation of the tandem method which could only be eliminated by either a simultaneous solution of all the governing equations or an iterative solution for each feedback loop. For time steps of the order of tens of milliseconds, the feedback lag of the simple tandem method should not be a significant factor in the results.

As in the steady-state mode, transients are designed to be run interactively. Steady-state conditions must have been previously generated and stored on an on-line disk file in order to do a transient analysis. Additional input data required includes time-dependent pressure and flow boundary conditions and/or cross section perturbations. Cross section perturbations may be applied instantaneously or over a continuous time interval. Only one cross section perturbation per node is allowed during a transient. For the initial coupling, it was assumed that the neutronic and thermal-hydraulic time steps were identical. The transient procedure is as follows:

- 1) Read common blocks and container array from steady-state disk file,
- 2) Read transient input from data file,
- 3) Perform any needed initializations,
- 4) Calculate the time steps, subject to Courant numerical stability

-26-



Thermal-Hydraulically Initiated Transient



Figure 2. Transient Feedback Loops

-27-

Neutronically Initiated Transient

limitations and user-supplied upper and lower bounds,

- Determine whether the transient is initiated in the neutronics segment or in the thermal-hydraulics segment. If neutronics, go to 6). If thermal-hydraulics, go to 7),
- 6) Perform one complete feedback loop, beginning with the transient neutronics calculation. Calculate the new nodal powers and update these in the thermal-hydraulics calculation for the same time period. Calculate the average feedback parameters and the new cross sections. Go to 8),
- 7) Perform one complete feedback loop, beginning with the thermalhydraulics calculation. Calculate the average feedback parameters and the new cross sections. Perform the transient neutronics calculations for the same time period. Calculate the new nodal powers and update them in the thermal-hydraulics segment.
- 8) Check for the end of the current time domain. If the end has not been reached, return to step 4). If the time domain has ended, the calculation ends or the user is prompted for new time domain information.

This procedure is shown in Figure 3.

The transient coupling methodology has been devised and the necessary programming changes and additions have been made. The code has been compiled on the MULTICS computer and sample problems have been devised and successfully executed. The transient results are presented in Chapter 4.

3.4 Additional Code Features

3.4.1 Steady-State Neutronic/Thermal-Hydraulic Iteration Variation

The initial steady-state coupling logic provided for feedback loops consisting of one static neutronic calculation and one thermal-hydraulic time step. During a steady-state convergence, many time steps may be required to converge the flow and heat transfer solutions. The changes in local feedback parameters during the latter part of this convergence are



Figure 3: Transient Coupling Strategy

small from time step to time step. As a result, many of the static neutronic calculations are close to repetitions of previous neutronic iterations. This led to the implementation of a mechanism to vary the ratio of thermal-hydraulic time steps to static neutronic calculations. For each time domain, the user specifies the number of thermal-hydraulic time-steps to be performed in each feedback loop. Thus, when the thermal-hydraulics calculations are not changing significantly with each time step, the neutronic calculation may be performed after several time steps, saving a significant amount of computer time with no impact on the results obtained. In practice, it has been found that up to a 50% reduction in running time can be realized through judicious use of this feature of TITAN.

3.4.2 Improved Inner (Pressure) Iteration Method

The solution method for the inner iterations (or pressure iterations) in the fluid dynamics portion of TITAN has been modified to improve computational efficiency. No acceleration techniques were incorporated into the original THERMIT pressure solution, since it was assumed the number of pressure iterations would have a negligible effect on the execution time [16]. However, experience has shown that a large number of pressure iterations may be required for large problems. Therefore, an acceleration scheme developed by Schor [17] was incorporated into TITAN which applies an over-relaxation to the block Gauss-Seidell solution method. The solution method is only applicable to problems having interconnected flow channels. In addition, a regular rectangular geometry is assumed in the current version. This constraint can be relaxed without creating a major change in the code.

-30-

3.4.3 Improvements to Heat Transfer Package

A number of improvements and updates to the heat transfer package have been made. These changes involve improvements in the modeling of critical heat flux and post-CHF heat transfer which had been incorporated into THERMIT concurrently with the current work. The TITAN heat transfer models are now consistent with those in the latest versions of THERMIT. In particular, a new film boiling point heat transfer coefficient has replaced the two correlations originally in THERMIT. Figure 4 summarizes these changes.

3.4.4 Direct Moderator Heating

The energy released by nuclear fission occurs in several forms. The largest part is contained in the kinetic energy of the fission products, which is converted to heat energy within the fuel. A portion of the energy is contained in the gamma rays and neutrons produced in the fission reaction. Some of this energy escapes the fuel and is deposited directly into the coolant by gamma ray absorption and neutron moderation. This direct heating of the moderator has been shown to be an important contributor for some reactor transients of interest [19]. The QUANDRY code was written to account for this effect by allowing the power to be partitioned into a portion which is deposited in the fuel and a portion which is deposited directly into the coolant. The fraction deposited directly in the coolant is a constant supplied by the user. The THERMIT code did not allow for this effect, assuming that all the reactor power is produced and deposited in the fuel. A model similar to that used in QUANDRY has been built into TITAN, except that the absorption of gamma and neutron energy has been assumed to depend linearly on the void fraction in the nodes. The fraction of the fission energy which is deposited directly in the coolant is deter-

-31-

| | Regime | Correlation |
|-----|---|---|
| 1. | Forced convection to single-phase liquid | Sieder-Tate |
| 2. | Natural convection to single-phase liquid | McAdams |
| 3. | Subcooled boiling | Chen |
| 4. | Nucleate boiling | Chen , |
| 5. | Transition boiling | Interpolation between ^q CHF ^{and q} msfb |
| 6. | High P, high G film boiling | Groeneveld 5.7* |
| 7. | Low P, high G film boiling | Modified Dittus-Boelter* |
| 8. | Low x film boiling | Modified Bromley ** |
| 9. | Forced convection to single-phase vapor | Sieder-Tate |
| 10. | Natural convection to single phase vapor | McAdams |
| | | |
| | Regime Checkpoints | Correlation |
| 1. | Critical Heat Flux | Biasi, W-3**, CISE-4** Bowring**, Barnett**, Hench-Levy** |
| 2. | Minimum Stable Film Boiling Temperature | Henry |
| 3. | Slug-Annular Transition | Wallis** |

* Correlation deleted in this research ** Correlation added in this research

Figure 4. Changes to Heat Transfer Package [17]

•

mined for each node by the following relation:

$$E_{d}^{i,j,k} = \theta(1 - \alpha_{i,j,k})$$

where θ is a user-supplied constant and $\alpha_{i,j,k}$ is the local void fraction. The addition of this model should enable TITAN to model transients more accurately.

3.4.5 Simple Boiling Thermal-Hydraulic Model

The steady-state coupling methodology relies on an internal model to supply an appropriate initial guess for the fluid and fuel temperatures needed by the thermal-hydraulics solution method. The first version of TITAN utilized the simple model included in QUANDRY to perform this function. This model assumed no boiling and therefore imposed this limit on the initial conditions to which TITAN could be applied. An extended model which could calculate steady-state boiling conditions was developed by Khalil [20] and implemented into QUANDRY. This model has been placed into TITAN, replacing the original simple model. As a result, problems which have boiling present in the steady-state can now be analyzed with TITAN. Several boiling cases have been successfully analyzed, using the simple boiling model to initialize the code. These results are presented in Chapter 4.
4. CODE APPLICATIONS

4.1 Sample Problem

A sample problem was selected for testing, debugging and verification of the TITAN code. The problem consists of two adjacent part-length boiling water reactor fuel assemblies, as shown in Figure 5. The problem was devised by Rodriquez-Vera [21] to serve as the basis for a transient benchmark problem to check the numerical accuracy of codes which model threedimensional neutronics with feedback. The problem has been analyzed using QUANDRY and MEKIN, providing reference solutions to which TITAN results can be compared. The problem was designed to have geometrical characteristics typical of a BWR (in particular, Brown's Ferry). Table 2 summarizes the important characteristics of the sample problem. The model was limited to two partial assemblies in order to keep computational costs low. However, the problem was designed to present a challenge to a coupled code by using control rod positions to induce large horizontal power gradients and by having substantial boiling at steady-state to strengthen the feedback effects. All of these considerations made this an ideal problem for the current work, so the MEKIN benchmark problem was selected as the basis for all the initial TITAN analysis.

The sample problem consists of 20 nodes, 10 in each channel, with seven different neutronic compositions. The neutronic boundary conditions are specified albedos on three vertical sides and on the top, with a zero flux boundary condition on the bottom and the fourth vertical side. The thermal-hydraulic boundary conditions specified are inlet coolant velocity and exit pressure. Both channels have control rods modeled at steady-state. For channel 1, the control rod is inserted 76 cm, half-way up the channel.

-34-



Figure 5: Sample Problem.

TABLE 2

Sample Problem Characteristics

| Total power | 6077.6 | kw |
|-------------------------------------|--------|-------------------|
| Number of fuel assemblies | 2 | |
| Assembly length | 152.4 | cm |
| Number of fuel rods per assembly | 64 | |
| Average fuel power density | 366.38 | w/cm ³ |
| Average linear heat generation rate | 9.496 | kw/ft |
| Fuel rod diameter | 1.226 | cm |
| Clad thickness | .0813 | cm |
| Gap thickness | .0114 | cm |
| Inlet temperature | 548 | °K |
| Total flow rate | 31.703 | kg/s |
| Channel 1 flow velocity | 1.946 | m/s |
| Channel 2 flow velocity | 2.511 | m/s |
| Outlet pressure | 7.136 | MPa |
| Channel flow area | 93.5 | cm^2 |

.

•

The control rod in channel 2 is inserted four-fifths of the length of the channel, a distance of 121.6 cm. This model was used for all the analyses presented in this report.

4.2 Steady-State Results

4.2.1 Investigation of Feedback Sensitivity

Three steady-state QUANDRY cases were run to assess the sensitivity of the sample problem to the feedback function. One case was run with no feedback (constant temperature), and a non-boiling and a boiling case with feedback were modeled. Figure 6 shows the axial power shape calculated for channel 1, while Figure 7 shows the axial power shape calculated for channel 2. The results show that the inclusion of feedback reduces the power peaking in the upper nodes, particularly when boiling is present. This effect is more pronounced in channel 1 than in channel 2. Changes in fuel temperatures, moderator temperatures, and moderator densities are therefore more pronounced in channel 1. With no boiling present, the power shapes are similar to those obtained with no feedback included. The moderator density contributor to the feedback is quite strong when boiling occurs, as Figures 6 and 7 demonstrate. This effect may be exaggerated for QUANDRY calculations, since thermal equilibrium and equal phase velocities are assumed in the simple thermal-hydraulics model.

4.2.2 TITAN Results, Non-Boiling Steady-State Case

The sample problem was analyzed with TITAN for an inlet temperature of 500°K, resulting in a converged steady-state solution with no boiling present. The results obtained compared well with those obtained with QUANDRY. Figures 8 and 9 show a comparison of the axial power shapes calculated



Figure 6. QUANDRY Steady-State Axial Power Shapes, Channel 1, with and without Feedback

-38-



Figure 7. QUANDRY Steady-State Axial Power Shapes, Channel 2, with and without Feedback

by TITAN and QUANDRY for channels 1 and 2, respectively. The power shapes show very good agreement, indicating that the feedback in TITAN is operating properly. TITAN calculated somewhat lower power in the top two nodes of channel 1 than did QUANDRY. This was the result of higher average fuel temperatures calculated by the TITAN model, giving stronger negative feedback than in QUANDRY.

4.2.3 TITAN Results, Steady-State Boiling Case

Several steady-state boiling cases were calculated with TITAN and good results were obtained. The boiling cases were identical to the non-boiling case except that the inlet temperatures were assumed to be 548 °K. Constant fuel and clad thermal conductivities and gap heat transfer coefficients were used for a base case analysis. The results of this analysis compare well to those obtained by Rodriquez-Vera with MEKIN [21]. Figures 10 and 11 show the axial power shapes as calculated by QUANDRY, MEKIN, and TITAN for channels 1 and 2, respectively. Figure 10 shows that TITAN and MEKIN produced very similar results for the channel 1 power shape. TITAN calculated slightly lower power levels in the top two nodes of channel 1 than did MEKIN. The nodal powers calculated by QUANDRY were significantly lower in the upper nodes than calculated by MEKIN or TITAN. This is attributable to the simple boiling model used in QUANDRY. The small differences between TITAN and MEKIN are attributable to differences in the fuel temperature calculations. Figures 12 and 13 show the fuel centerline temperatures as calculated by MEKIN and TITAN for channels 1 and 2, respectively. These figures show that TITAN predicted significantly higher centerline temperatures than did MEKIN, particularly for channel 1. This discrepancy is attributable to the different fuel thermal conductivities. used in the two codes. The MEKIN code permits the user to specify the

-40-



Figure 8. TITAN and QUANDRY Steady-State Axial Power Shapes, Channel 1, Non-Boiling



Figure 9. TITAN and QUANDRY Steady-State Axial Power Shape, Channel 2, Non-Boiling

-42-



,

Figure 10. TITAN, MEKIN, and QUANDRY Steady-State Axial Power Shapes, Channel 1, Boiling

.



Figure 11. TITAN, MEKIN, and QUANDRY Steady-State Axial Power Shapes, Channel 2, Boiling

fuel thermal properties, but the TITAN code has built-in properties. The MEKIN analysis used a value of 3.4615 watts/meter-°K for the fuel thermal conductivity, while the TITAN code uses 2.4 watts/meter-°K (More elaborate models for the fuel are available in TITAN, as discussed in section 4.2.4). Thus, the TITAN code calculates higher fuel temperatures than did MEKIN for the sample problem. The very high fuel centerline temperatures shown in Figure 12 reflect the very high power output of the upper nodes of channel 1. The peak linear heat generation rate for this problem is approximately 23 kw/ft, a value well above that allowed for actual BWR operation. The MEKIN analysis apparently underpredicts the fuel centerline temperatures in these high power nodes. Despite the disagreement in fuel temperatures, the results indicate that TITAN is capable of generating an accurate steady-state solution for a boiling problem.

The boiling problems required about four times as much computational effort as the comparable non-boiling problems. The presence of vapor necessitated the use of smaller time steps in order to satisfy the Courant stability limit. In addition, the convergence of the boiling cases required more time steps to achieve energy and flow errors comparable to those obtained for non-boiling cases. The power shape convergence demonstrated a damped oscillatory behavior which probably contributed to the increased "transient time" required. Figure 14 shows the variation of nodal power with a number of iterations for a representative node. This oscillatory behavior is thought to be a result of the tandem method employed in TITAN. The MEKIN code also demonstrated oscillatory behavior during its early development [22].

-45-



Figure 12. TITAN and MEKIN Steady-State Fuel Centerline Temperatures, Channel 1



Figure 13. TITAN and MEKIN Steady-State Fuel Centerline Temperatures, Channel 2



Figure 14. Nodal Power Oscillations During Steady-State Convergence, Boiling Problem

4.2.4 Fuel Pin Model Sensitivity Studies

The TITAN code allows three different options for modeling the fuel rods. The fuel and clad can be assumed to have temperature-independent thermal conductivities and heat capacities with a constant gap heat transfer coefficient. The fuel properties are built in the code while the gap coefficient is an input parameter. This option is referred to as the simple fuel pin calculation. An intermediate fuel pin calculation option uses temperature-dependent fuel properties with a user-supplied constant gap coefficient. The temperature-dependent fuel properties are supplied by TITAN subroutines containing correlations for the fuel and cladding materials. These correlations were taken or adapted from the MATPRO [23] models for fuel material properties. The full fuel pin calculation option combines temperature-dependent fuel properties with a model to calculate the local gap heat transfer coefficient. The gap coefficient model is also based on MATPRO, with the addition of a radiation heat transfer model. Since the average fuel temperature is one of the three feedback parameters, the sensitivity of the steady-state results to the choice of fuel pin options was assessed. Two cases were examined, the base case plus a reduced power case. The fuel was modeled with six nodes in the fuel and three nodes in the clad in each case.

One steady-state analysis of the base case two channel problem was performed for each of the three fuel pin model options. The analyses were converged to approximately the same flow and energy errors. Figures 15 and 16 show the fuel centerline temperatures calculated by TITAN with all three fuel pin options for channels 1 and 2, respectively. The results indicate that the fuel centerline temperatures were rather sensitive to the model employed. The simple model yielded the highest

-49-



Figure 15. TITAN Steady-State Fuel Centerline Temperatures, Channel 1, Three Fuel Pin Models



Figure 16. TITAN Steady-State Fuel Centerline Temperatures, Channel 2, Three Fuel Pin Models

fuel temperatures calculated by TITAN. The maximum fuel temperature for channel 1 calculated with the simple model exceeded the maximum temperatures calculated with the intermediate and full fuel pin models by 447 °K and 672 °K, respectively. The intermediate model resulted in lower temperatures than did the simple model for all nodes in the sample The full fuel pin model produced the lowest fuel centerline problem. temperatures for all nodes calculated. All three TITAN analyses resulted in higher maximum fuel temperatures than that calculated with MEKIN. This result supports the view that the MEKIN results underpredict the fuel centerline temperatures in the high power nodes. This illustrates one of the problems with fuel pin models which use a single constant value for the material properties. In order to select an appropriate value for the fuel thermal conductivity, it is necessary to estimate the average temperature of the fuel in the high power node. The results obtained are rather sensitive to the fuel thermal conductivity, since the difference in the fuel centerline and surface temperatures is inversely proportional to the thermal conductivity. When the average fuel temperature varies significantly in the problem, any constant value model must produce fuel temperatures that are in error, since one value of thermal conductivity cannot be appropriate everywhere. These deficiencies are usually compensated for by selecting properties which will give conservative results for the maximum fuel temperatures (i.e., which will over-predict the maximum fuel temperatures). It is not clear that this approach is acceptable for a coupled code where the fuel temperatures are important as feedback parameters.

-52-

The combination of a high average linear heat generation rate with a severely skewed axial power shape yields very high fuel temperatures for the sample problem. In order to perform a fuel pin model sensitivity study for a "realistic" problem, the power and flow rates of the sample problem were reduced and three steady-state cases were run. The total power for these cases was 4000 kw and the flow velocities for channels 1 and 2 were 1.28 and 1.65 m/s, respectively. This combination of power and flow results in a power shape similar to that of the base case. However, the peak linear heat generation rate for the reduced power problem was 15.88 kw/ft. As a result, the calculated fuel centerline temperatures are more "reasonable" than those shown in Figures 15 and 16.

Figures 17 and 18 ahow the calculated fuel centerline temperatures as a function of axial position for channels 1 and 2, respectively. The three fuel pin options were used so that the impact of selecting a simple, intermediate or full fuel pin model could be assessed. Figures 17 and 18 show that the results obtained with the three models are somewhat different. The simple model consistently produced the highest centerline temperatures, while the full fuel pin model consistently produced the lowest centerline temperatures. The centerline temperatures calculated with the intermediate model always fell between those of the other two models. When the fuel temperatures are relatively low (as in nodes 1-5, of channel 1 and all of channel 2), the intermediate model is closer to the full model than to the simple model. In the high temperature regions (such as nodes 6-10 in channel 1), the reverse is true. This indicates that the gap conductance model has a greater impact when the linear heat generation rate (and thus the fuel temperatures) is high. In the peak power node, the centerline temperature calculated with the simple model exceeded that calculated with

-53-







Figure 18. TITAN Steady-State Fuel Centerline Temperatures, Channel 2, Three Fuel Pin Models, Reduced Power

the intermediate and full fuel pin models by 83 °K and 436.9 °K, respectively.

These results indicate that the selection of a fuel pin model can be significant if fuel temperatures are expected to be limiting. However, the steady-state power shape was insensitive to the fuel pin option selected. The maximum difference in corresponding nodal powers among the three cases was approximately 3%. This indicates that the feedback contribution of the average fuel temperatures was not significant. This is not a general conclusion, since a different problem might well show a high fuel temperature feedback sensitivity. The computational time required to converge was relatively insensitive to the fuel pin option selected.

4.3 TITAN Null Transient Analyses

The first transient cases analyzed with TITAN were so-called "null" transients in which the transient solution method is applied in the absence of any applied forcing functions or perturbations. The purpose of this type of problem is to demonstrate that the transient solution method is working properly for the least demanding scenario. A null transient analysis will reveal if the transient solution method itself introduces any changes to the converged steady-state. Two null transients were calculated: a non-boiling problem with an inlet temperature forcing function of unity and a boiling problem with an outlet pressure forcing function of unity. Figure 19 shows the reactor power as a function of time for the non-boiling case. This shows that there was a very slight variation in total reactor power during the one second of transient time calculated. The maximum change in reactor power during the 20 time

-56-



Figure 19. Reactor Power During Null Transient, Non-Boiling

steps calculated was .0043% of the original steady-state power. This indicates that the steady-state solution was well converged. The normalized nodal powers remained equally steady during the transient. Figure 20 shows the reactor power as a function of time for a boiling case ($T_{in} = 548$ °K). This shows that the reactor power changed very little during the 56 time steps calculated. As in the non-boiling case, the local nodal powers remained essentially constant during the transient calculation. Thus, it has been demonstrated that the transient coupling of TITAN produces good results in the absence of external forcing functions or perturbations.

4.3.2 Simulated Turbine Trip Analyses

A pair of flow/pressure transients simulating turbine trip events have been analyzed with the TITAN code. These transients were simulated with time dependent inlet flow rate and outlet pressure boundary conditions. The first transient was based on one of the Peach Bottom turbine trips [15]. Figure 21 shows the forcing functions used for this analysis. The two channel sample problem with boiling was used for the analysis. This sample problem does not match the actual operational conditions of the Peach Bottom reactor, so the results should not be compared to measurements taken during the actual turbine trip event. In particular, the actual turbine trips were performed with the reactor at reduced power, while the initial conditions of the sample problem represent full power conditions. The purpose of this analysis was to perform a reasonable transient with thermal-hydraulic forcing functions to show that TITAN could produce results that were consistent with the observed or expected response of a boiling water reactor. Figure 22 shows the calculated reactor power as a

-58-



Figure 20. Reactor Power During Null Transient, Boiling



Figure 21: Forcing Functions for Simulated Turbine Trip (Peach Bottom)

function of time during the turbine trip transient. These results appear to be reasonable. However, no independent solution exists to which the TITAN results could be compared. The power rise seems to follow closely the inlet flow boundary condition. The magnitude and duration of the power rise is quite similar to that calculated for a turbine trip at full power at other BWR's [24], as is shown in Figure 23. No difficulties were encountered during the analysis and the computational time required was quite reasonable (275 cpu seconds).

A second turbine trip simulation was performed with TITAN in order to supplement the Peach Bottom analysis just described. As in the previous case, flow and pressure forcing functions were applied to a steady-state solution for the base case sample problem. The forcing functions were taken from the PSAR of the Duane Arnold Energy Center [24], as shown in Figure 23. The forcing functions correspond to a turbine trip from high power without bypass and with 60% relief flow. This transient is somewhat more severe than the previous example and is of longer duration. The actual forcing functions used in the TITAN analysis are depicted in Figure 24. As in the first turbine trip simulation, the TITAN model does not necessarily correspond to actual reactor conditions, nor can the results obtained be compared directly to those shown in Figure 23.

The transient response of the reactor power to the forcing functions of Figure 24 is shown in Figure 25. The reactor power shows three large peaks of relatively short duration. The first peak is of a duration similar to that of the previous analysis. The magnitude of the power peak was approximately 3.21 times the steady-state value (as opposed to a maximum power rise of 2.07 times the steady-state value for the

-61-



Figure 22. Reactor Power During Simulated Turbine Trip (Peach Bottom)



Figure 23. Duane Arnold Turbine Trip, PSAR [24]

.



Figure 24. Forcing Functions for Duane Arnold Turbine Trip



.

.

Figure 25. Reactor Power During Simulated Turbine Trip (Duane Arnold)

.

previous analysis). A second power peak of similar duration but slightly smaller magnitude (2.97 times steady-state) follows immediately after the first. This second peak occurs in response to a second peak in the flow forcing function (see Figure 24). A third power peak of lesser magnitude (1.73 times steady-state) and longer duration follows immediately after the second peak. The power peaks end at approximately 2.0 seconds into the transient, after which the reactor power decreases until the transient analysis ends at 4.0 seconds. By this time, the reactor power has dropped to a value below the original steady-state power. The reactor power begins to decline when the inlet flow begins to decline and the outlet pressure ceases to rise. The behavior of the flux in Figure 23 does not show the second and third peaks observed in the TITAN results. This is primarily due to the fact that no scram was modeled in the TITAN analysis. When this fact is considered, the general response of the two channel model to the forcing functions seems reasonable.

4.3.3 Rod Withdrawal Transient

A rod withdrawal transient has been analyzed with TITAN and some preliminary results have been obtained. The transient consists of a continuous withdrawal of the channel 2 control rod (see Figure 5) at a rate of 1.276 m/s. This withdrawal rate removes the rod entirely in 1.0 seconds. Figure 26 shows the calculated reactor power as a function of time during the transient. A rapid power rise produces a peak power of nearly 100 times the steady-state value. This dramatic power increase occurs in only 0.13 seconds and is immediately followed by an equally abrupt decrease in power. Between 0.13 seconds and 0.33 seconds the power

-66-



Figure 26. Reactor Power During Rod Withdrawal Transient

due to a large increase in the fuel temperature and an increase in the void fraction in many of the nodes. The minimum power level reached is approximately 25% of the initial power level. The power level subsequently begins a steady rise, reaching a second maximum of 3.5 times the initial value at 0.90 seconds. Thereafter the power decreases until the problem ends at 1.05 seconds. These results are considered preliminary, since no reference solution for this problem exists to date. A MEKIN solution for this problem is being prepared by Rodriquez-Vera [21] which should enable a better assessment of the TITAN result. The results should not be compared to those obtained for an entire reactor, since only two assemblies were modeled. The code performed this analysis with no difficulty and only required 317.7 cpu seconds for the 110 time steps calculated.

5. PROJECT STATUS AND FUTURE WORK

5.1 Summary of Project Results

The computer codes THERMIT and QUANDRY have been utilized to develop the three-dimensional coupled neutronics/thermal-hydraulics code TITAN. The TITAN code has been successfully operated in both steady-state and transient modes for a sample problem. Steady-state convergence for both boiling and non-boiling problems has been attained with good results. These steady-state results compare well with those obtained with MEKIN for the same problem.

A number of transient problems have been analyzed with TITAN to date. These include null transients, pressure/flow transients, and a control rod withdrawal transient. The results of these analyses appear reasonable, though no other solutions are available for comparison.

A number of refinements or additions to the models in TITAN have been accomplished. A single boiling thermal-hydraulics model was added to permit initialization of the steady-state problem. A term was added to the liquid energy equation to allow direct deposition of gamma and neutron heat into the moderator. Improvements were made to the constitutive relations for post-CHF heat transfer. An improved algorithm for solving the inner (pressure) iteration problem was installed. Finally, the capability was added to vary the alternation between thermal-hydraulic and neutronic calculations during the steady-state convergence process. This made it possible to significantly reduce the computational effort required to generate a converged solution.

-69-
5.2 Future Work

A number of additional tasks need to be performed in order to complete the development of TITAN. Some validation of the transient results obtained to date would be desirable (it is hoped that a MEKIN solution for the rod withdrawal problem will soon be available). Application of the code to larger, more realistic problems is necessary to determine the accuracy and economy of TITAN for practical analyses. Some minor modifications to the code may be required to enable such analyses to be performed. In particular, the time step selection logic currently used in the transient mode is not adequate for problems in which neutronic and thermal-hydraulic time scales are quite different. The performance of large TITAN analyses may motivate improvements designed to enhance the steady-state convergence and thereby reduce computational costs.

A major task will be to provide adequate documentation for TITAN. A thesis [25] is being prepared which will provide detailed documentation of the development and preliminary applications of TITAN.

REFERENCES

- 1. J. E. Kelly, S. P. Kao and M. S. Kazimi, "THERMIT-2: A Two-Fluid Model for Light Water Reactor Subchannel Transient Analysis," MIT-EL-81-014, (1981).
- K. S. Smith, "An Analytic Nodal Method for Solving the Two-Group, Multidimensional, Static and Transient Neutron Diffusion Equations," Nuclear Engineer Thesis, Massachusetts Institute of Technology (1979).
- 3. D. P. Griggs, A. F. Henry and M. S. Kazimi, "Development of a Three-Dimensional Two-Fluid Code with Transient Neutronic Feedback for LWR Applications," MIT-EL-81-013, (1981).
- 4. F. H. Harlow and A. A. Amsden, "A Numerical Fluid Dynamics Calculation Method for All Flow Speeds," Journal of Computational Physics, 8, 197, (1971).
- 5. J. A. Redfield, "CHIC-KIN-A FORTRAN Program for Intermediate and Fast Transients in a Water Moderated Reactor," WAPD-TM-479, Bettis Atomic Power Laboratory (1965).
- 6. C. F. Oben chain, et al., "PARET A Program for the Analysis of Reactor Transients," in "Proceedings of the International Conference on Research Reactor Utilization and Reactor Mathematics," Mexico City, (1967).
- 7. J. Yasinsky, M. Natelson, L. Hageman, "TWIGL A Program to Solve the Two-Dimensional, Two-Group, Space-Time Neutron Diffusion Equations with Temperature Feedback," WAPD-TM-743, Bettis Atomic Power Laboratory, (1968).
- 8. A. V. Vota, N. J. Curlee and A. F. Henry, "WIGL3 A Program for the Steady-State and Transient Solution of the One-Dimensional, Two-Group, Space-Time Diffusion Equations Accounting for Temperature, Xenon, and Control Feedback," WAPD-TM-788, Bettis Atomic Power Laboratory (1969).
- 9. D. J. Diamond, "BNL-TWIGL, A Program for Calculating Rapid LWR Core Transients," BNL-NUREG-21925, Brookhaven National Laboratory (1976).
- 10. F. E. Dunn, G. J. Fischer and T. J. Heames, "SAS2A LMFBR Accident-Analysis Computer Code," ANL-8138, Argonne National Laboratory (1974).
- R. A. Shober, T. A. Daly and D. R. Ferguson, "FX2-TH: A Two-Dimensional Nuclear Reactor Kinetics Code with Thermal-Hydraulic Feedback," ANL-78-97, Argonne National Laboratory (1978).
- 12. "HERMITE A 3-D Space-Time Neutronics Code with Thermal Feedback," CENPD-188, Combustion Engineering Company.

- R. Bowring, J. Stewart, R. Shoper, R. Sims, "MEKIN: MIT-EPRI Nuclear Reactor Core Kinetics Code," CCM-1, EPRI Report RP228 (1975).
- 14. D. J. Diamond, C. J. Ruger, D. I. Garber and S. V. Lekach, "RAMONA-3B: A Code for BWR Plant Transient Analysis," BNL-NUREG to published, Brookhaven National Laboratory (1982).
- 15. D. A. Dube, "Development of a Fully Implicit Two-Fluid, Thermal-Hydraulic Model for Boiling Water Reactor Transient Analysis," Ph.D. Thesis, Massachusetts Institute of Technology (1980).
- W. H. Reed and H. B. Stewart, "THERMIT: A Computer Program for Three-Dimensional Thermal-Hydraulic Analysis of Light Water Reactor Cores," M.I.T. Report (1978).
- 17. A. L. Schor, "Sodium Boiling in LMFBR Assemblies," Ph.D. Thesis (to be published), M.I.T. (1982).
- 18. S. P. Kao, "Dispersed Flow Heat Transfer and Prediction of Critical Heat Flux in Light Water Reactors," S.M. Thesis, M.I.T. (1981).
- H. S. Cheng, et al., "The Use of MEKIN-B for Light Water Reactor Transient Calculations," BNL-NUREG-28785, Brookhaven National Laboratory (1980).
- H. Khalil, "A Static, Two-Phase, Thermal Hydraulic Feedback Model for the Nodal Code QUANDRY," MITNE-235, Massachusetts Institute of Technology (1980).
- 21. F. J. Rodriguez-Vera, "Some Benchmark Calculations by Using the Computer Code MEKIN," M.S. and Nuclear Engineering Thesis Prospectus, M.I.T., Dept. of Nuclear Engineering (1981).
- 22. A. G. Cook, "Light Water Reactor Kinetics Analysis with Feedback: An Investigation of the Computer Code MEKIN," Ph.D. Thesis, M.I.T. (1978).
- 23. P. E. MacDonald and L. B. Thompson, "MATPRO: VERSION 09, A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior," TREE-NUREG-1005, E.G. and G. Idaho, Inc. (1976).
- 24. "Preliminary Safety Analysis Report, Duane Arnold Energy Energy Center," Iowa Electric Light and Power Company (1968).
- 25. D. P. Griggs, "An Advanced Three-Dimensional Coupled Neutronics/ Thermal-Hydraulics Code for Light Water Reactor Safety Analysis," Sc.D. Thesis to be published, M.I.T. (1982).

• <u>APPENDIX A</u>:

•

٠

.

TITAN FORTRAN LISTING (PRE-RELEASE VERSION)