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WANL-TME-684
FEBRUARY, 1964

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VARI-QUIR II: SPACE-TIME NEUTRON DIFFUSION WITH FEEDBACK

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February 21, 1964

* Mr. R. W. Schroeder, Chief
Space Nuclear Propulsion Office
NASA Lewis Research Center
21000 Brookpark Road
Cleveland 35, Ohio

Subject: WANL-TME-684 dated February 1964, "Vari-Quir II: Space-Time
Neutron Diffusion with Feedback"

Dear Mr. Schroeder:

Transmitted herewith are three (3) copies of the subject report.

This report is transmitted for your information.

Respectfully,

H. F. Faught
Program Manager
NERVA Nuclear Subsystem

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cc: Mr. R. Wilke - SNPO-C Resident at WANL
Mr. M. Fleishman - SNPO-C - w/encl.

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INTRODUCTION

In WANL-TNR-133⁽¹⁾ (September, 1963), we reported the development of the reactor kinetics code VARI-QUIR. Starting from the well-known variational principle for the diffusion equation, a new type of trial function was introduced: the fluxes were allowed complete freedom in time, but their space dependence was restricted to being quadratic within each region and continuous over the entire interface between regions. Based on this theory, the code VARI-QUIR was written to solve the diffusion equation, in space and time, for up to 4 energy groups and 6 precursor groups. The spatial part of the code checked out extremely well in both accuracy and speed, against the only available criteria, namely, comparison with steady-state diffusion codes like CURE. The time-dependent part of the code also checked nicely on simple problems where analytic solutions were available for comparison.

In Chapter III of the above report, we listed as "Further Plans and Suggestions" a number of items which could be grouped broadly as follows: (1) improvements to, and refinements in, the neutronics code itself; (2) addition to the code of the non-neutronics equations describing the fluid flow in a NERVA reactor, and the "feedback" effects of temperature, hydrogen density, and solid density on the reactivity; and (3) application of our VARI-QUIR technique to other problem areas, as, for example, more efficient solution of the transport equation. This report describes work done to date on the first two of these three problems.

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In Chapter I, we list and describe the modifications in the neutronics code since the last report. These affect accuracy, convenience in use, and computer storage space available for addition of feedback.

The simplest but least satisfying approach to the use of VARI-QUIR on feedback problems is considered in Chapter II. An existing code like TNT,⁽²⁾ containing detailed fluid-flow but fairly simple neutronics, could be used to obtain an initial solution. The output density and temperature schedule (i.e., time-dependence) could be used to calculate a nuclear parameter (cross sections, etc.) schedule, which could be input into VARI-QUIR to obtain a power schedule. This more accurate power response could be used first to check the TNT power output. (One such possible check is demonstrated by a sample problem.) Second, if the two did not agree, one might iterate back and forth, carrying a power schedule from VARI-QUIR to the fluid-flow part of TNT, and a temperature and density (hence cross-section) schedule from TNT to VARI-QUIR, using the entire time-solution on each such iteration. Such a procedure might or might not converge.

In Chapter III we undertake the problem of writing the fluid flow and feedback equations directly into VARI-QUIR. This includes a consideration of the fluid-flow and heat transfer equations, to determine which time lags are always short enough to be negligible; generation of a grossly simplified (but still meaningful) fluid flow and heat transfer model suitable for a first run-through in VARI-QUIR; obtaining the feedback coefficients for the effects of density and temperature

upon the nuclear parameters; coding; and some sample problems, with resulting plots and discussion.

Finally, Chapter IV discusses future work, both within this project and in other applications.

I. IMPROVEMENTS IN THE NEUTRONICS CODE

Before getting into the non-neutronics (feedback) problem, several improvements and refinements were made in the neutronics code itself. Three of these, to be described below, are fulfillments of the "Further Plans and Suggestions", items #2, 3, and 4, anticipated in WANL-TNR-133⁽¹⁾

Note that, corresponding to these changes, there will be slight modifications of input and output from the format described in WANL-TNR-133⁽¹⁾

A. Iteration to Convergence

In the kinetics portion of the code (i.e., beyond the initializing steady-state section), there are two distinct places where iterations are involved. First, the equation for the time derivative of the flux (but not the precursor) density at any point involves derivatives at neighboring points, because of the closely-coupled nature of the variational solution. To use subroutine ICE (Integration with Controlled Error) to integrate these time derivatives, one must first be able to evaluate the derivative at each point separately, hence an iterative procedure is necessary to solve these simultaneous, coupled equations. True, not very many iterations will usually be required, because a good starting guess is available, namely the values of the derivatives at the preceding time point. Nevertheless, sudden changes may occur from time to time, hence the required number of iterations

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changes. Thus it has been found necessary to require iteration to some pre-specified accuracy, rather than a given number of iterations.

Secondly, for those fast flux groups where the time lag is neglected and the response treated as instantaneous (described as "out-of-ICE" in WANL-TNR-133), a small steady-state problem is solved at each time-step, the "source" being the lower energy flux groups and the precursors. In this case, the equation for the flux at each point involves not only the fluxes at neighboring space points, but the fluxes in all other energy groups at the same, and neighboring, space points. Precisely the same situation holds as in the preceding paragraph regarding the availability, usually, of a good starting guess, but the uncertainty as to the number of iterations.

In both of these cases, therefore, the code has been changed to allow input of an error criterion, rather than a specified number of iterations. Iteration continues until even the worst point meets the accuracy requirement.

B. Interpolation

Because of the pre-set "quadratic-in-region" spatial behavior of the solutions, sufficient information to completely specify the solution at any time is given by a knowledge of the value of three points per region (nine points in two-dimensional cases) for each energy and precursor group. However, it is not convenient for the user, e.g., when plotting the solution in space over a large region,

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to be forced to calculate by hand some intermediate values based on the known quadratic behavior. Provision has therefore been made to input to the code a requirement for any desired number of interpolated points to be printed out in the solution at each time.

This interpolation is done only at each printout time. Thus the code preserves the advantage of working with far fewer points during the bulk of its labor, i.e., the many time-steps between each printout.

C. Increased Computer Space for Feedback

As reported in WANL-TNR-133,⁽¹⁾ one of the major obstacles to the introduction of any very detailed feedback into this code was the amount of core storage taken up by just the neutronics - specifically, all but about 1,000 locations. This large storage requirement resulted from the detailed spatial analysis in this code, compared to most (space-independent) kinetics codes.

To write the feedback equations on a separate computer chain appeared highly undesirable from a standpoint of computing time; with the many time-steps involved in this program, reading a complete program tape in and out at each time-step seemed prohibitive. As an alternative, it was anticipated that the allowable problem size (number of spatial regions, or energy groups, or precursors) might have to be cut down.

However, this alternative has been avoided (or at least postponed, depending upon how detailed our feedback eventually becomes) by the following expedient. The entire steady-state part of the program

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has been deleted from the kinetics program and written as a separate chain. This frees several thousand extra core locations in the kinetics program for feedback equations and storage. At the same time, since the steady-state section is used only once in each problem, for initialization, the increase in computing time is quite negligible.

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II. USE OF VARI-QUIR NEUTRONICS AS A CHECK ON OTHER CODES

A. Suggested Procedure

In this chapter we wish to point out ways in which the code VARI-QUIR might be used effectively in its September, 1963 form (i.e., neutronics only, with no feedback equations added in), referred to below as VQ-1. In problems where feedback is unimportant, such use is obvious. But worthwhile information can be extracted from the code even in feedback problems, as follows.

Code VQ-1 solves the space-time kinetics problem for any input cross-section schedule; i.e., given the values of the nuclear parameters (cross-sections, diffusion coefficients, etc.) in each spatial region as functions of time, the code solves for the power distribution, flux magnitude and shape in each group, and precursor density distribution, as functions of time. Suppose, then, that an existing code like TNT, containing detailed fluid flow but relatively simple neutronics, is used to solve a feedback problem. In addition to yielding total power vs. time, TNT would output a schedule including temperature and fluid density as functions of time. One could therefore calculate the nuclear parameters as functions of time, and input this information to VQ-1. The resulting solution for total power vs. time could be compared to the TNT power schedule as a check upon the latter. One would thus be at least aware of what sort of inaccuracies were involved in a separable kinetics treatment.

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Secondly, the VQ-1 solution would provide further information not available from the TNT solution, such as the spatial shapes of the power and fluxes at any time.

Finally, if the comparison of total powers disclosed an unacceptable error, some sort of iteration procedure between the two codes might be devised to yield improved accuracy. One might, for example, carry the VQ-1 power schedule to TNT, use only the non-neutronic portion of the latter to obtain a new temperature and density schedule, input the resultant cross-section schedule into VQ-1 to obtain an improved power schedule, etc. While there is no guarantee, one feels that such a procedure might converge fairly rapidly, for negative temperature feedback.

B. Sample Problem

We demonstrate here the use of VQ-1 in the first mentioned capacity, as a check on space-independent neutronics. We consider a sample startup problem, taken from an internal memorandum. The problem (solved using TNT) in that memorandum was to obtain a ramp rise in power. Given that desired power rise, one could (in the space-independent, or separable, approximation) deduce a required reactivity schedule. Further, from the given power rise, one could compute temperatures, densities, etc., and hence an (uncontrollable) feedback reactivity. The control vanes were then given a compensating schedule such that the total required reactivity schedule was met.

A basic assumption (and the one we wish to check here with VARI-QUIR) was that the addition of reactivity had the same effect, regardless of where added. For purposes of this check, let us idealize* the desired reactivity schedule to the sequence of ramps shown in the top curve of Figure 1. Let us further consider two extreme cases, one in which all of this reactivity is obtained by varying ρ in the core, the other in which all of the reactivity is obtained by varying $\Sigma_{\text{absorption}}$ in the control vanes.

In this problem VARI-QUIR was used with 7 radial regions: core, core, core, reflector, reflector, absorbing annulus (to simulate the control vanes), and more reflector. Four flux energy groups and six precursor groups were used. Reactivity was defined as static reactivity i.e., difference between the multiplication factor and unity. Thus, for the case in which ρ in core was varied, the ρ - schedule was obtainable by definition from the reactivity schedule. For the case in which $\Sigma_{\text{absorption}}$ in the absorbing annulus was varied, several steady-state VARI-QUIR runs had to be made, to calibrate $\Sigma_{\text{absorption}}$ vs. reactivity.

*The roughness of this idealization makes no difference, since we will be comparing two different curves following this same schedule.

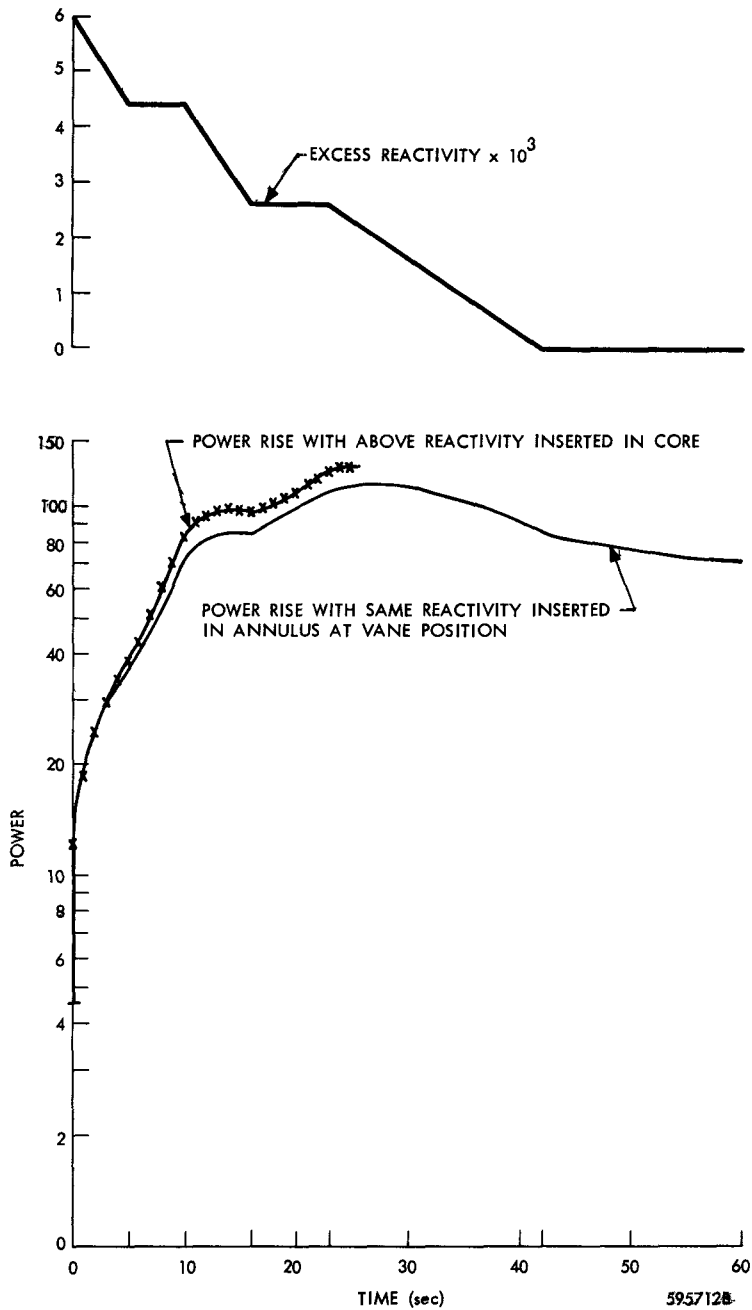


FIGURE 1

CHANGE IN POWER RISE DUE TO CHANGE IN
LOCATION OF REACTIVITY INSERTION

C. Discussion of Results

The resultant power schedules are shown in Figure 1, bottom curves. Their difference, under identical static reactivity schedules, must be due to the spatial dependence of where the reactivity is added, in core or reflector. Since the plots are only of total power (integrated over space), one can be sure that the difference in spatial shapes between the two curves is much greater.

For both cases, the great departure of our power output from a ramp is due to the difference between our reactivity schedule (a jump, followed by a series of ramps) and the smooth reactivity variation theoretically required. Of particular interest are the occasional downward dips in power, occurring at the "corners" of our reactivity schedule - i.e., where our reactivity departs farthest from the required smooth curve. Such decreases in power, even momentarily, at positive reactivity, would seem at first glance to be unreal - and, indeed, led us to look first for an error in the code. We soon discovered, however, that they are quite real and rather simple to explain, as follows.

To demonstrate the effect requires only one flux group and one delayed neutron (precursor) group - no spatial dependence need be postulated. The necessary equations are therefore:

$$\frac{1}{V} \frac{d\phi}{dt} = [k(1-\beta) - 1] \frac{\phi}{\Lambda} + \lambda C \quad (1)$$

$$\frac{dC}{dt} = -\lambda C + k\beta \phi \Lambda^{-1} \quad (2)$$

where now k is assumed to be some function of time, $k(t)$. We can even strip the system down a little further: assume a fast reactor, so that V is very large, and the left-hand side of (1) may be replaced by 0; i.e., the fluxes adjust instantaneously* to the precursor source C and reactivity k . For this assumption to be valid requires further that we stay below prompt critical, i.e., $k-1-\beta k < 0$, otherwise the fluxes would "adjust instantaneously" to infinity. With equation (1) now an algebraic (not differential) equation, it may be solved at once for ϕ in terms of C and k , and the result substituted into (2), to yield:

$$\frac{dC}{dt} = -\left[\frac{k-1}{k-1-\beta k}\right] \lambda C$$

The solution, for arbitrary $k(t)$, may be written at once as

$$C = C_0 \exp \left\{ + \int_0^t \left[\frac{k-1}{1-k+\beta k} \right] \lambda dt' \right\}$$

Therefore, from equation (1),

$$\phi = \phi_0 \cdot \left[\frac{1-k_0+\beta k_0}{1-k+\beta k} \right] \cdot \exp \left\{ \int_0^t \left[\frac{k-1}{1-k+\beta k} \right] \lambda dt' \right\} \quad (3)$$

where the denominators are always positive, because of our assumption of staying below prompt critical. Therefore the exponential will always be increasing as long as $k > 1$. In equation (3), for the flux or power, this exponential factor corresponds to one's intuitive feeling

*This assumption, particularly good for the present reactor, is equivalent to our taking the fluxes "out-of-ICE" in our code, as our option allows. It is, however, only convenient, not necessary, for the above explanation.

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that the flux will always be rising for positive reactivity. The precursors, in fact, contain only this factor, and do indeed always rise for $k > 1$.

However, equation (3) has another factor, $\frac{1-k_0 + \beta k_0}{1-k + \beta k}$, corresponding to the equilibrium ratio between the flux, or power, and its precursor source. On any sudden drop in k , to a lower but still > 1 value (positive reactivity), the denominator of this factor will rise suddenly, hence the overall factor will drop suddenly. This drop can be as fast as we wish, hence easily can be greater than the rise in the exponential factor.

To be a little more quantitative, the logarithmic time derivative of (3) is

$$\frac{1}{\phi} \frac{d\phi}{dt} = \left[\frac{1-\beta}{1-k+\beta k} \right] \frac{dk}{dt} + \lambda \left[\frac{k-1}{1-k+\beta k} \right]$$

Therefore, if the power is never to drop ($\frac{d\phi}{dt} \geq 0$), the fastest allowable rate of reactivity drop from positive values toward zero is given by

$$-\frac{dk}{dt} \leq \frac{\lambda(k-1)}{(1-\beta)} \quad (4)$$

The curve of dropping k vs. time which would just keep the power constant is given by integrating (6) with the equality holding, to yield:

$$k(t) - 1 = (k_0 - 1) \exp \left\{ \frac{-\lambda t}{1-\beta} \right\} \quad (5)$$

Any reactivity ($k-1$) fall-off faster than the exponential in (5) leads to power drops at still positive reactivities.

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As we stated earlier, the dropping of the $\frac{1}{V} \frac{d\phi}{dt}$ term in our treatment is merely convenient, and not necessary for the final result. If we retain the full equations (1) and (2), we can no longer obtain a simple closed form like (3) for the power in terms of arbitrary $k(t)$; but we can still obtain equation (5) for the limiting rate of reactivity fall-off if the power is to hold steady, not drop. If we substitute into (1) the condition that $\phi = \phi_0 = \text{constant}$, solve for k , substitute into (2) to eliminate k (the presence of ϕ does not prevent integration because it is now a constant ϕ_0), integrate to find $C(t)$, and again substitute into (1) to obtain $k(t)$, we finally arrive at precisely the same equation as (5). For a reactivity fall-off more rapid than (5), we must again obtain an actual drop in power.

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III. INTRODUCTION OF FEEDBACK EQUATIONS DIRECTLY INTO VARI-QUIR

The most desirable treatment of feedback effects would be to have the appropriate heat transfer, fluid flow, and feedback equations incorporated into VARI-QUIR. It would be obviously more efficient than any iteration between codes, requiring only one pass per problem, and the question of convergence would never arise. A direct approach would be to combine the already written codes VARI-QUIR and TNT. The first problem here is one of storage - each code by itself occupies almost the entire computer core. To run each program in and out of the computer on tapes, at every time-step, would increase the computer running time drastically, and is therefore to be avoided if possible. For this reason, it seemed worthwhile to investigate the possibility of writing some simpler, less detailed fluid flow equations directly into VARI-QUIR as subroutines.* Progress and results in this area are reported in this chapter.

Since our work up to the last milestone (TNR-133, September, 1963) was predominantly concerned with the neutronics, a good deal of time has been spent just getting familiar with the fluid flow equations. This is essential in order to set up a simplified model, decide which

*Even if combination of TNT and VARI-QUIR does turn out ultimately to be required for accuracy, this joining of the two codes requires a good deal of knowledge of the fluid flow; thus the experience gained in the present approach would still be highly useful.

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effects are to be omitted on a first trial, and which are controlling and essential to the problem. Particularly helpful in this phase of the work has been WANL-TME-103, "NERVA Power Range Analysis",⁽³⁾ which presents a good overall view of the system without excessive detail.

It was decided to consider only fluid flow through the core in our first model, for two reasons: The bulk of the heat transfer occurs there, hence it is the main temperature control; and the reactivity feedback from changes in coolant density is concentrated mainly in fluid flowing through the core.

A. Fluid Flow and Heat Transfer Time Constants

One of the more important concepts developed in WANL-TNR-133 was that of treating differently the various time differentials involved in the neutron diffusion equations. A similar analysis must now be applied to the fluid-flow and heat-transfer time constants, to determine which are fast enough to be taken as instantaneous (i.e., the time derivative dropped from the equation), which are slow enough to be done as a simple forward time-step at the end of each ICE step, and which are of such intermediate speed as to require calculation within the ICE subroutine.

The mass, momentum, and energy (including heat) conservation equations for one-dimensional flow down a core channel may be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0 \quad (6)$$

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$$\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x} + \frac{\partial P}{\partial x} = f \rho v^2 \quad (7)$$

$$\frac{\partial}{\partial t} \left[\rho \left(U + \frac{v^2}{2} \right) \right] + \frac{\partial}{\partial x} \left[\rho v \left(H + \frac{v^2}{2} \right) \right] = Q_v \quad (8)$$

where f is the friction factor, U and H the internal energy and enthalpy per unit mass, respectively, Q_v the heat source (from the sides of the channel) per unit volume of channel, and the remaining symbols have obvious meanings. Axial heat conduction within the fluid has been ignored, being small compared to the heat transported by the fluid motion itself.

We wish now to demonstrate that, for all three of these equations, the time derivative terms may be omitted for normal startup or shutdown problems.* This is equivalent to saying that the fluid flow in the channel adjusts instantaneously, for all practical purposes, to changes in inlet temperature, inlet pressure, and heat source from the sides of the channel.† Thus equations (6)-(8) need merely be solved in steady-state at each new time-step. This is the procedure already built into the TNT code. (2)

*I.e., exclusive of fast excursion or accident calculations.

†But this heat source still lags the fission power because of heat transfer through, and accumulation in, the solid. The relevant delay will be treated later in this section.

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The physical basis for our development will be roughly as follows. Any deviations of the fluid density (equation 6) or enthalpy (equation 8) from being in equilibrium with source and inlet conditions can last no longer than the time it takes for these deviations to be carried through the reactor by the fluid itself. Thus the appropriate time constant here is average fluid velocity divided by total channel length, i.e., v/L . On the other hand, for the pressure drop equation (7), the flow rate will turn out to be largely friction - rather than inertia-controlled, so the relevant parameter here is the ratio of frictional to inertial forces. In the "overdamped" mechanical analogue,

$$m \dot{v} + a v = 0,$$

the solution $e^{-t/\tau}$ has a time constant $\frac{1}{\tau} = \frac{a}{m}$, which is just the ratio of the slope of the force vs. velocity curve to the mass. In equation (7), where these quantities are on a volume basis, the corresponding time constant will be simply $\frac{2f \rho}{\rho} v$, or $2fv$.

To formally obtain these time constants, in their recognizable physical form, from equations (6)-(8), one needs an analytic rather than numerical solution. Understandably enough, to accomplish this will require some drastic simplification of the above equations. This is quite justified by the fact that we seek only orders of magnitude, not precise values, for these time constants.

We begin by replacing equation (8) with the simpler approximate form

$$\frac{\partial}{\partial t} (\rho H) + \frac{\partial}{\partial x} (\rho v H) = Q_v \quad (8-a)$$

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This involves two approximation. The first is that the kinetic energy of the fluid, $\frac{\rho v^2}{2}$, is negligible compared to the heat energy ρH . Some rough numbers derived from the full-power conditions of reference #3 are

$$\frac{\rho v^2}{2} \approx 7 \text{ lbs./in.}^2 \tag{9}$$

$$\rho H \approx 7600 \text{ lbs./in.}^2 \tag{10}$$

in the core, which certainly satisfies our approximation. The second assumption in (8-a) is that ρH is also large enough to mask the P term which differentiates ρH from ρU , in the thermodynamic identity

$\rho H = \rho U + P$. A typical figure here is

$$P \approx 600 \text{ lbs./in.}^2 \tag{11}$$

which is down from (10) by a factor of about 1/13, hence again our approximation is adequate.

We next decide to simplify the right-hand side of (7) to $f'v$ where

$$f' = f \rho v \tag{12}$$

is taken as constant during the transient problem. This merely approximates the friction vs. velocity curve by a straight line in the vicinity of our average conditions, with slope wrong by a factor of 2. It does not change any of the qualitative features of our model.

Finally, the spatial dependence of equation (6)-(8-a) is replaced by the simplest possible difference equations, namely a two-point mesh. This will of course completely hide any spatially complicated

(and hence high-frequency) solutions, but will preserve the lowest-frequency, or slowest, solutions that we seek, with roughly correct values. The difference equations which finally replace (6), (7), and (8-a) are given by (13)-(15):

$$\frac{d\rho}{dt} = \frac{\rho}{L} (v_1 - v_2) \quad (13)$$

$$\rho \frac{d}{dt} (v_1 + v_2) + \frac{\rho}{L} (v_2^2 - v_1^2) - \frac{2\Delta P}{L} = -f'(v_1 + v_2) \quad (14)$$

$$\frac{1}{2} \frac{d}{dt} [\rho (H_1 + H_2)] = Q_v + \frac{\rho}{L} (v_1 H_1 - v_2 H_2) \quad (15)$$

$$\rho = \rho_1 - \frac{\Delta P}{2} \left(\frac{\partial \rho}{\partial P} \right)_H + \frac{1}{2} \left(\frac{\partial \rho}{\partial H} \right)_P (H_2 - H_1) \quad (16)$$

$$\left. \begin{array}{l} \text{Given: } H_1, \rho_1, \Delta P \\ \text{To Find: } H_2, \rho, v_1, v_2 \end{array} \right\} \quad (17)$$

Equation (16) follows from applying the equation of state in the center of our region. In the boundary conditions (17), the usual specification of inlet pressure P_1 and outlet pressure P_2 is replaced for convenience by the quantities ρ_1 and ΔP . This is completely equivalent since, given P_1 and H_1 , ρ_1 could certainly be computed from the equation of state at the inlet.

The steady-state solution of (13)-(17) can be obtained by straight-forward algebra. We shall need only the following parts of this solution:

$$\begin{aligned} v_2 &= v_1 \\ H_2 &= H_1 + \frac{L Q_v}{\rho v} \end{aligned} \tag{18}$$

We now wish to superimpose on this steady-state solution a small-amplitude transient, and observe how it settles out in time. Preservation of only first-order terms in this perturbation linearizes the equations. Assuming that the perturbed quantities have the time-dependence e^{wt} , and equating to zero the determinant of the coefficients, one proceeds directly to the following equation for the time constant w :

$$\begin{aligned} w^2 + w \left[f' + \frac{2\rho v}{L} + \frac{2v}{L}(H_2 - H_1) \left(\frac{\partial \rho}{\partial H} \right)_P \right] + \\ \frac{f'v}{L} \left[2 + \frac{1}{\rho}(H_2 - H_1) \left(\frac{\partial \rho}{\partial H} \right)_P \right] = 0 \end{aligned} \tag{19}$$

where the variables ρ , v , etc., are the unperturbed (steady-state) values. To make the time constants $\frac{v}{L}$ and $2fv$ fall out, we simplify to the case where the heat source $Q_v = 0$, whence, from equation (18), $H_2 = H_1$. The solutions of (19) are then

$$\frac{1}{\tau} \equiv -w = \begin{cases} \frac{2v}{L} \\ \frac{f'}{\rho} \end{cases} \tag{19-a}$$

where, from (12), f'/ρ is just another form for fv .

Instead of setting $Q_v = 0$, a more realistic approximation would be that so much heat is added in the channel that the outlet density is negligible compared to the inlet density, i.e.,

$$(H_2 - H_1) \left(\frac{\partial \rho}{\partial H} \right)_P \approx \Delta \rho \approx -\rho$$

in which case the solutions of (19) reduce to

$$\frac{1}{\tau} \equiv -w = \frac{1}{2} \left\{ \frac{f'}{\rho} \pm \sqrt{\left(\frac{f'}{\rho} \right)^2 - 4 \left(\frac{f'}{\rho} \right) \left(\frac{v}{L} \right)} \right\} \quad (19-b)$$

From reference #3, we calculate rough values for $\frac{f'}{\rho} = fv \approx 1000/\text{sec.}$, $\frac{v}{L} \approx 375/\text{sec.}$ for the time constants in (19-a). If the solution is taken as (19-b), the quantity under the square root becomes slightly negative, giving the solution a slightly oscillatory character; but its real part still yields a decay constant $\frac{1}{\tau} \approx 500/\text{sec.}$

We conclude that the fluid flow time constants are of the order of a few milliseconds. Therefore, in a startup problem, where we will generally not be interested in anything shorter than ~ 0.1 sec., these time lags may be neglected. This in turn means that steady-state solution of equations (6)-(8), omitting the time derivatives, will be adequate.

There is, however, a non-negligible time lag involved in transfer of heat through the solid to the channels. Any changes in power must first begin to heat up the solid before being felt in the channel. Again picking representative values of $.005 \text{ Btu/sec.} \cdot \text{in.}^2 \cdot ^\circ\text{R}$ for the heat transfer coefficient, $0.5 \text{ Btu/lb.} \cdot ^\circ\text{R}$ for the specific heat of

graphite, 0.1 in. for a typical solid thickness between channels, and 0.083 lbs./in.³ for the graphite density, one obtains for the heat transfer time constant

$$\tau \approx 0.8 \text{ sec.},$$

certainly not a short enough time lag to be neglected. It is, in fact, probably a sufficiently slow process (τ is sufficiently large) to be integrated as a simple forward time-step at the end of each ICE step-integration of the neutronics.

B. Simplified Model for a First Trial in VARI-QUIR

The foregoing section discusses approximations which will generally be valid in any model of the reactor. In the present section we wish to set up a grossly simplified model suitable for a first incorporation of fluid flow, heat transfer, and reactivity feedback into VARI-QUIR. This model should contain just the barest essentials necessary to represent the working of the reactor. Its primary functions will be to check out our technique for tying feedback into the code, and to establish a starting point for further, more refined models.

In the discussion that follows, we shall use three subscripts: G to refer to the solid (graphite) core, C to refer to properties of the coolant in the core channels, and P to refer to properties of the coolant in the outlet plenum.

As stated earlier, we shall consider only flow through the core. We now lump the core into a single element, at some uniform (but time-dependent) temperature T_G . This temperature is determined by a

balance of heat input from fission, minus heat loss to the coolant:

$$\frac{dT_G}{dt} = \frac{1}{C_G} (Q_{\text{fission}} - Q_{\text{loss}}) \quad (20)$$

where C_G is the total heat capacity of the graphite core, Q_{fission} is the power (proportional to $\int dV \sum_f \cdot \phi$), and Q_{loss} is the total heat energy per unit time going into the coolant. As stated in Section A, this differential equation is to be solved by a simple time-step at the end of each ICE integration of the neutronics.

Calling T_C some average coolant temperature in the channel, we may determine Q_{loss} from

$$Q_{\text{loss}} = h(T_G - T_C) \quad (21)$$

where h is a heat transfer coefficient for passage of heat through the solid and into the coolant in the channel. Equations (20) and (21) thus replace the thermal diffusion equation in the core.

The coolant pressure drop across the core, while not negligible in any detailed treatment, is nevertheless small compared with the pressure drop across the nozzle, from the outlet plenum (pressure ≈ 550 psi at full power) to atmosphere or vacuum. We shall therefore neglect all pressure differences between inlet plenum, core, and outlet plenum, and simply set

$$P_C = P(t) \quad (22)$$

$$P_P = P(t) \quad (23)$$

where $P(t)$, the pressure entering the core, is controlled externally, and is therefore an input variable to our program.

By the same taken, the flow rate is controlled mainly by the nozzle, according to the nozzle equation

$$W = K_P P_P / \sqrt{T_P} \quad (24)$$

where W is the weight flow rate through the core. Equations (22)-(24) thus replace the momentum equation (7) in our present model. The mass conservation equation (6) is implicitly present by the fact that W , the mass flow rate, has no subscript, and has therefore been assumed constant everywhere.

Finally, instead of the energy equation (8), we have simply that the total energy loss to the fluid is carried out through the outlet plenum; i.e.,

$$H_P W = Q_{\text{loss}} \quad (25)$$

where we have neglected other contributions to the enthalpy (e.g., viscous heating, which is trivial compared to the heat input from the core power.) At some average position down the channel, we assume that the fluid enthalpy has risen half-way from its entrance value (small enough to be negligible) to its exit value (H_P); i.e.,

$$H_C = H_P / 2. \quad (26)$$

A better averaging method could undoubtedly be found, based on the actual power distribution in the core.

With Q_{fission} determined by the neutronics part of the code, and the inlet pressure $P(t)$ controllable externally, we have 7 equations (20)-(26) for the 9 variables T_G , T_C , T_P , Q_{loss} , P_C , P_P , W , H_P , and H_C .

The two extra equations which are required to determine the system will, of course, come from the fluid enthalpy equation of state (to be discussed in the next section). This relation, $H = H(P,T)$, will be used once in the channel and once in the plenum, furnishing two more equations.

The other fluid equation of state, for $\rho(P,T)$, has not yet entered because we have not needed the fluid density ρ . This need will arise when we come to determine the reactivity feedback effect of core hydrogen density.

As an estimate suitable for our first problem, the fluid flow constants h (equation 21) and K_p (equation 24) were determined by requiring equations (21) and (24) to be satisfied in steady-state by the 100% values (listed in TME-103) for the variables Q_{loss} , T_g , T_C , W , P_p , and T_p . The heat capacity of the graphite core, C_G , needed for equation (20), was computed from the core weight and a handbook value for the specific heat of graphite at a temperature appropriate to full power.

C. Hydrogen Equations of State

The properties of hydrogen over a wide range of conditions have been compiled in WANL-TNR-043, "Hydrogen Properties for Project NERVA".⁽⁴⁾ According to that report, the hydrogen below 700°R is mostly para, and above 700°R the properties of ortho and para are essentially the same. Hence we shall use the parahydrogen properties described there.

From a study of these tables and graphs, it was concluded that the density of hydrogen could be represented quite well by

$$\rho = \frac{1 \text{ lb.}}{55 \text{ ft.}^3} \times \frac{P}{600 \text{ psi.}} \times \frac{6000^\circ\text{R}}{T} \quad (27)$$

for $\left\{ \begin{array}{l} 60^\circ\text{R} < T < 6000^\circ\text{R} \\ 100 \text{ psi.} < P < 1500 \text{ psi.} \end{array} \right\}$

Similarly, a less accurate (but adequate for our first model) representation of the enthalpy equation was found to be

$$H = 0.383 \frac{\text{Btu}}{\text{lb.}} \times \left(\frac{T}{1^\circ\text{R}}\right)^{1.44} \quad (28)$$

for $\left\{ \begin{array}{l} 200^\circ\text{R} < T < 5000^\circ\text{R} \\ 14.7 \text{ psi.} < P < 1500 \text{ psi.} \end{array} \right\}$

Both of these equations may, of course, be improved in accuracy when required and/or justified by refinements in the rest of our model.

D. Reactivity Feedback

The feedback subroutine accounts for changes in the nuclear constants as a result of changes in temperature and hydrogen density in the core.*

*Solid density changes due to thermal expansion would appear to affect the reactivity only in second order, for two reasons. First, the highly reflected nature of the reactor makes buckling small to begin with, so that changes in buckling should be negligible. Second, because of the structure of the reactor, fuel element expansion will be largely into the voids, over which these fuel elements have already been homogenized in our treatment.

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The temperature effects are those of spectral shift and doppler broadening. Spectral shift means the "hardening" of the neutron spectrum as a result of increased core temperature. The core temperature affects only the low energy neutron spectrum. Since the scheme used in these calculations was a four energy group system, the result of spectral shift is a change in the nuclear cross sections in the fourth group (up to 1.86 ev) only. The increase in the absorption of neutrons as a result of the broadening of absorption resonances by the doppler effect must be taken into account. Since all resonances occur in group three, only group three cross sections are affected by this phenomenon.

The change in hydrogen density does indeed change all cross sections in all groups. Except for the transfer cross sections, however, most changes are almost negligibly small in the range of hydrogen content of interest. The transfer cross sections are those that give the probability of a neutron's being transferred from one group to another, as a result of a scattering collision.

The standard design method used at WANL for finding cross sections is to determine the doppler effects from a code, QUERY, input these data into MUFT, which finds the fast groups constants, and finally, find the thermal group cross sections from TNS. It is obvious that it would be far too time consuming to use each of these three codes, or even a single subroutine to replace all three, every time the temperature or the hydrogen density changed. Furthermore, for any given core composition,

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it seems quite likely that the variation of the cross sections with temperature and hydrogen concentration may be represented by a relatively simple function or functions.

In view of these considerations, a "typical" NRX-A material composition was chosen to investigate these variations of cross sections. The main constituent, other than hydrogen, that varies greatly in amount in different regions of an NRX-A type core is uranium. Therefore the cross sections for this typical composition with uranium loadings of 200, 300, 400, and 500 mg/cc were found at temperatures of 293, 500, 800, 1500, and 2000°C. For one case, that of 400 mg/cc loading and one temperature, the cross sections were determined with hydrogen densities varying from the full power value to one-tenth that of the full power case.

The number densities used in those calculations were:

Nb	0.00060
Fe	0.00009
Ni	0.00020
Cr	0.00006
H	0.00012 - 0.000012
C	0.064582 - 0.066004
U-238	0.00005371 - 0.00002149
U-235	0.00072276 - 0.00028911

It should be noted that no Ta was included so that only uranium resonance broadening was considered.

The results of the QUERY's, MUFT's, and TNS's were then used to determine an analytic expression that would give a reasonable fit to the points. It was found that in every case the cross-sections

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could be represented by an expression of the form

$$\Sigma = \Sigma_0 (1 + A_1 T)$$

or

$$\Sigma = \Sigma_0 (1 + A_2 C)$$

where the A_1 and A_2 are the constants determined and the T and C are temperature and hydrogen concentrations respectively.

The accuracy of these expressions is quite good, typical root mean square errors being about 0.02%, and the worst case used being about 0.2%.

In future work, where more accurate feedback is desired, it may be necessary to expand the functions given above. Furthermore, it would be desirable to be able to determine the feedback coefficients without running all the other codes first. Therefore the determination of the variation of cross-sections with temperature or hydrogen density, and including other slightly different compositions, will be continued to determine if a simple method of calculating the feedback coefficients can be found. Whatever method is found will be included as part of the VARI-QUIR input formulation.

E. Communication Between Feedback Subroutines

The fluid flow, heat transfer, and reactivity feedback equations are written into VARI-QUIR as three subroutines to the main (neutronics) program. The first of these subroutines is used to read in all the non-neutronics constants, and the initial values (either power and inlet

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pressure or power and mass flow rate) for the problem; it can also be used to prescribe various ramps in time for the pressure or flow rate. The second subroutine, at the end of each (neutronics) time-step in ICE, first integrates the flow and temperature variables, depending on the length of the last ICE time-step; secondly, it adjusts the nuclear constants (cross-sections, diffusion coefficients, etc.) to new values appropriate to the temperature and hydrogen density. The third subroutine allows printout of any desired fluid-flow variables, at whatever times the neutronics variables are printed out by the main program.

The principal reasons for having the feedback located in subroutines is that any changes in or additions to the feedback (such as introducing the particular model described in the preceding sections of this chapter) require a recompiling only of these FORTRAN subroutines. The rather lengthy main program need not be recompiled. Now, communication between each of these subroutines and the main program is accomplished by having an identical COMMON statement (for all the neutronics variables) in the main program and all three subroutines.

With the introduction of non-trivial fluid flow, the problem now arises as to how to communicate these new variables between subroutines. They are not needed in the main program, but the feedback time-step subroutine needs to know, for example, what starting pressure was read into the feedback initializing subroutine. To add to the COMMON of the main program, each time the feedback model is changed, would require

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recompiling of this main program, and defeat the purpose of having the feedback in subroutines; while to put an additional dummy section in the COMMON of the main program is rather restrictive, because one has no idea ahead of time how many variables might be required in various feedback models. Making this dummy section too large, for example, might uselessly tie up space needed for subroutine instructions.

To handle this problem, we added to the COMMON of all three subroutines, after their COMMON which is identical to the main program, a COMMON section for the new fluid flow variables. Being below the main program COMMON, it does not upset the location of the neutronics variables. At the same time, the fluid flow variables are stored in a unique place, available to each subroutine independently.

F. A Sample Problem

To test the code and demonstrate our model, the following problem was constructed. The reactor was assumed to be operating on a power plateau (i.e., in steady state) at 2.5×10^5 Btu/sec. (about 25% of full power), with a hydrogen flow rate of 30 lbs./sec. Then, at time $t = 0$, the control vanes were suddenly rotated to give the equivalent of $k = +.006$. (In our R-Z code, this was accomplished by an appropriate step-reduction in absorption cross-section, and increase of diffusion coefficient, in our absorbing-annulus region). On the other hand, the inlet pressure to the core was maintained constant at its steady-state value. The physical idea, roughly, was that the vanes were accidentally

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rotated; however, through some failure, the pump never got the message, but continued to operate at constant pressure. We have no wish to imply that such a combination of occurrences is a plausible accident; it is assumed merely as a test problem for the code.

The neutronics model was about the same as that described in Chapter II, Section B: 4 flux energy groups, 6 precursor groups, 7 radial regions, etc. In addition, we assumed that our steady-state cross-sections were correct for the starting conditions of temperature and hydrogen density. Feedback changed the cross-sections only as a result of changes in the flow variables from their initial conditions.

Some of the overall (integrated over space) results for this problem are plotted in Figures 2-4. The four curves on each figure demonstrate what happens, respectively, with no feedback at all (nuclear parameters such as microscopic cross-section remain constant), with feedback only through the temperature spectral shift, with full temperature feedback including doppler broadening, and, finally, with the complete temperature and hydrogen density effects.

To further clarify, in all four cases the full fluid flow model was present, responding to the power rise. But the feedback effects, through which the flow variables caused effects on the power, were "plugged in" one at a time as described in the preceding paragraph.

Consider first the features common to all four cases. Following the step in reactivity, the power (Fig. 2) jumps immediately from 25% to about 68%, coming into a new equilibrium (based on the new reactivity)

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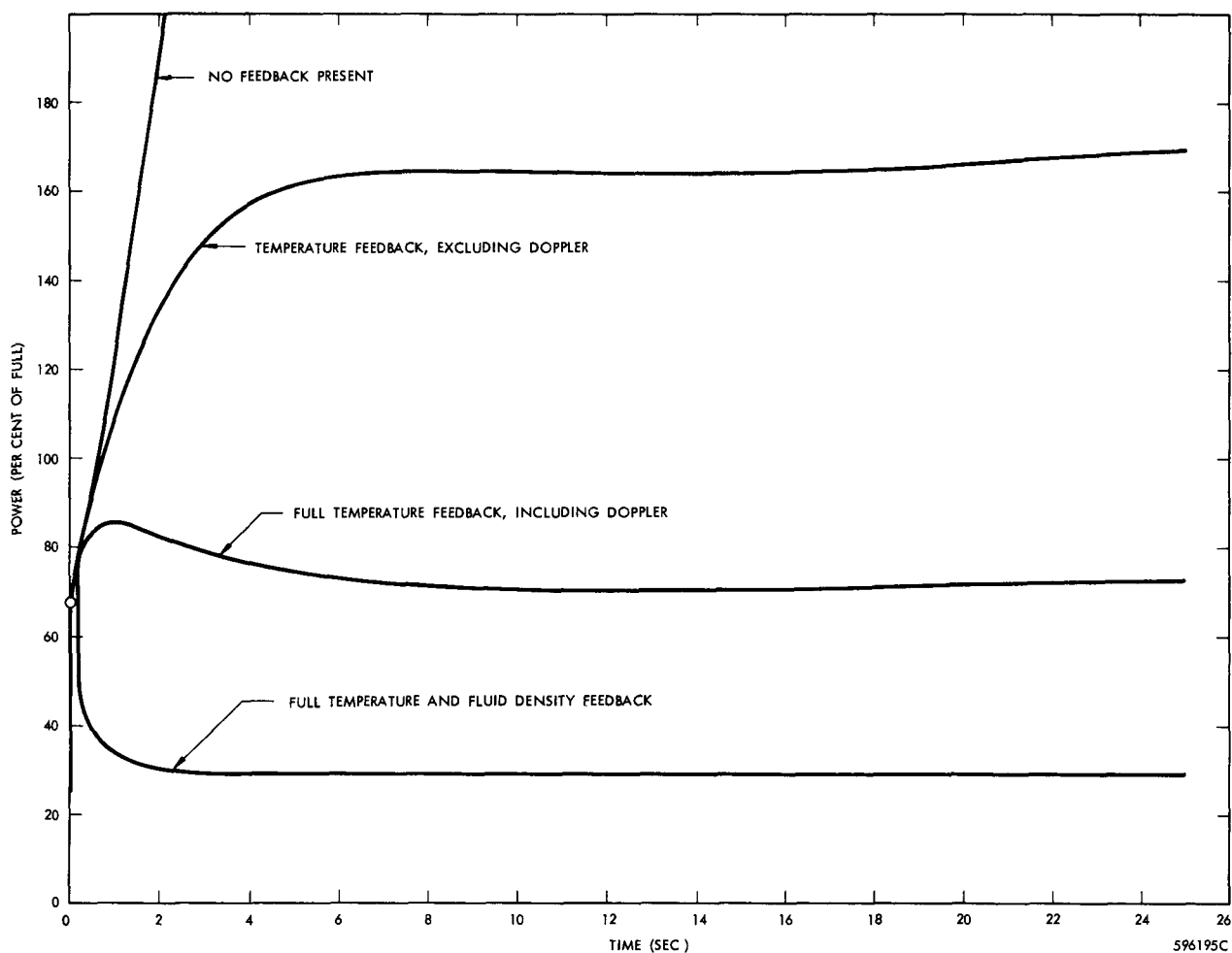


FIGURE 2

POWER RISE FOLLOWING REACTIVITY STEP
(CONTROL VANE TURNED SUDDENLY, FLUID
PRESSURE HELD CONSTANT)

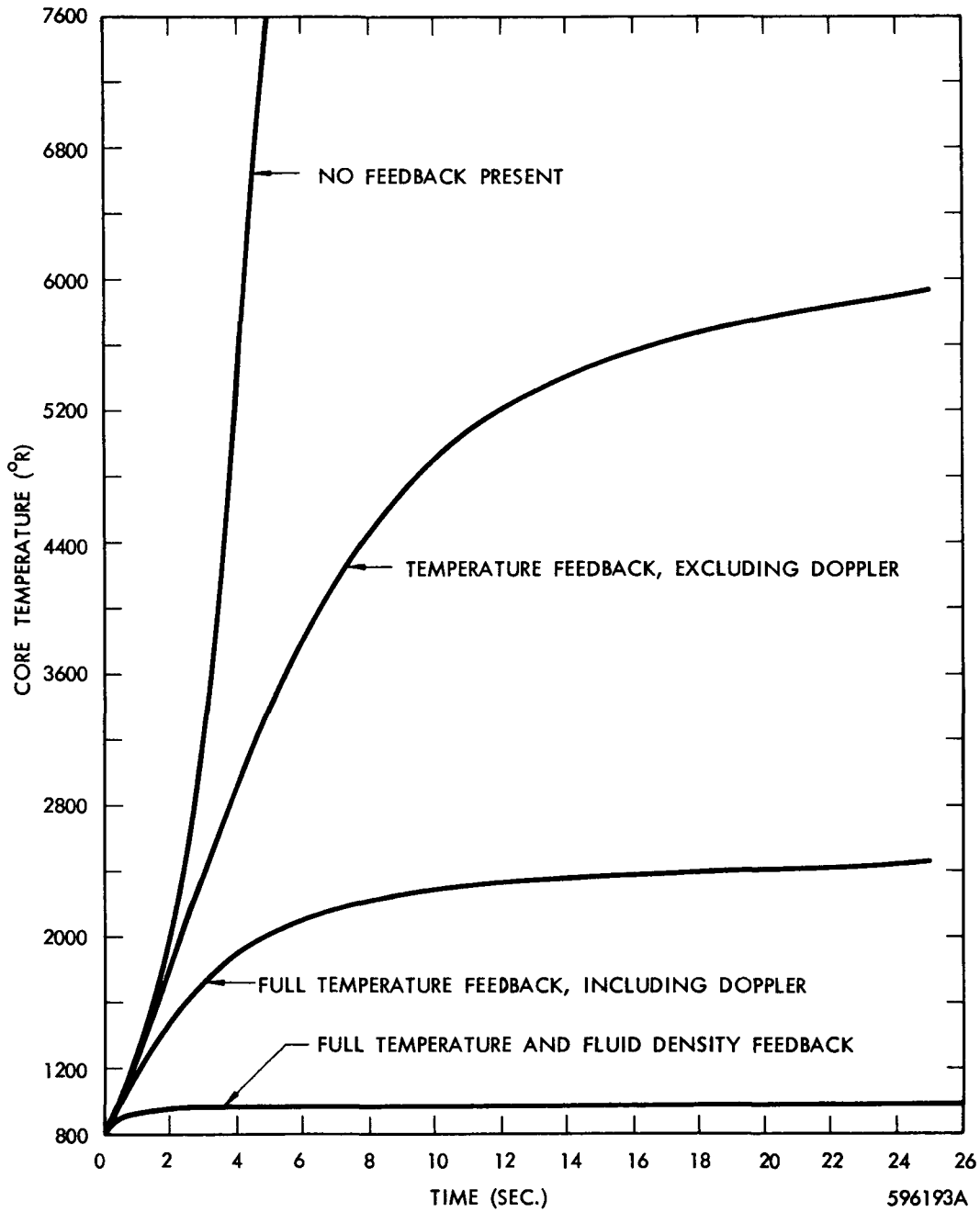


FIGURE 3

CORE TEMPERATURE RISE FOLLOWING REACTIVITY STEP
(CONTROL VANE TURNED SUDDENLY, FLUID PRESSURE
HELD CONSTANT)

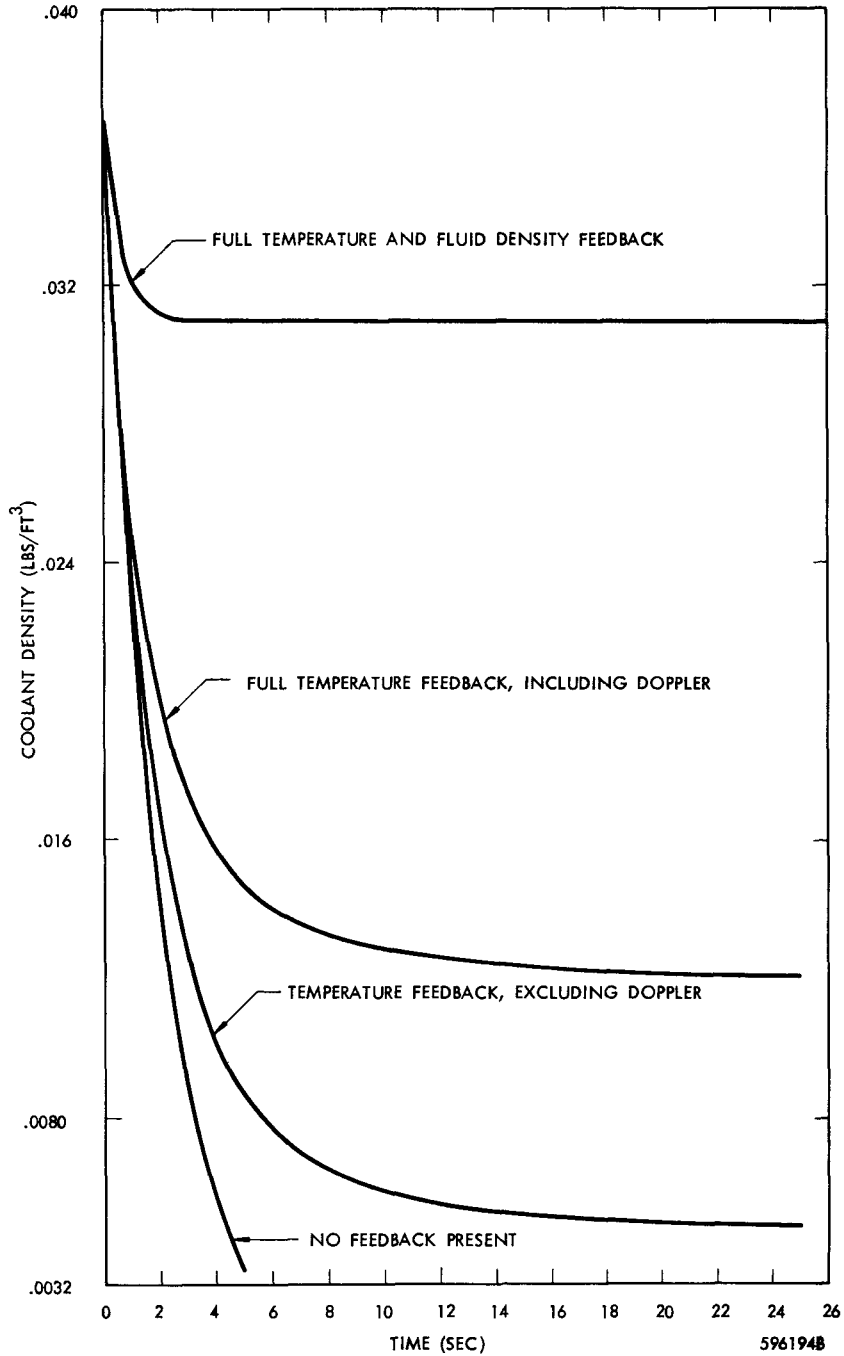


FIGURE 4

FLUID DENSITY IN CHANNELS FOLLOWING REACTIVITY STEP
(CONTROL VANE TURNED SUDDENLY, FLUID PRESSURE HELD
CONSTANT)

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with the old precursor density. Then, as the faster precursors begin to climb, so does the power, at a slower rate, of course.

Meanwhile, because of the higher power, the core temperature (Fig. 3) begins to climb - much more slowly, of course, varying only as the time-integral of the power (see equation 20). As the core temperature increases, so does the temperature of the hydrogen in the channels. Since its pressure is maintained constant, its density (Fig. 4) drops off inversely as its temperature, following equation (27). With this decreased density, the mass flow rate also drops off, although not as fast because the higher temperature means increased gas velocity. In fact, from equation (24), we see that the flow rate will fall off inversely with the square root of plenum temperature.

Returning now to Fig. 2, we see that, with no feedback, the reactor is soon off on a fast period ($\sim 80\%$ reactivity was added). With just the negative temperature effect of spectral shift plugged in, however, the power levels off at about 164%. With the doppler and doppler plus hydrogen, effects included, the power actually overshoots: by the time the temperature has risen enough to begin turning back the power, that power has reached a level higher than its eventual equilibrium.

Finally, after about 16 sec., the power in both intermediate-feedback cases begins another slow rise. This is apparently due to the slower precursors beginning to rise to come into balance with the higher power level. After a time of several half-lives of the slowest precursor group, a new equilibrium will ultimately be reached.

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The curve with hydrogen feedback shows no such effect, because the final power level is not much higher than the initial, hence the slow precursors have very little adjustment to make. They need increase only about 20% above their initial level, compared to about 200% and 600% for the two intermediate-feedback cases.

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IV. FURTHER PLANS

Attention is still to be given to items #5, 6, 7 and 8 listed as "Further Plans and Suggestions" in WANL-TNR-133.⁽¹⁾ Item #1, introduction of linear extrapolation distance, has at present a very low priority.

In addition to the above tasks, the following areas of interest have developed since September:

- A. A direct continuation of the work reported herein would be to refine our feedback model and insert more detailed fluid flow. It may also be desirable to introduce a delayed power calculation into the code, rather than to merely calculate power from $\int dV \Sigma_{\text{fission}} \phi$.
- B. It appears both feasible and desirable to combine VARI-QUIR with an excursion code like RAC for more detailed accident calculations. Prospects look good since RAC occupies only a small portion of the computer core. VARI-QUIR can also be compressed by a large factor in this application, since delayed neutron changes are probably negligible in the short times of interest here. Work has already begun on this problem under project #NE2710.
- C. The VARI-QUIR code might be extremely useful in the calculation of space-time transfer functions, of the type studied in reference #5. It appears that running problems on a space-time code like VARI-QUIR might be the ideal way to obtain

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input for a frequency-analysis code, whose output would be the desired transfer function. This area is being presently investigated but no results are yet available.

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