COMBINED MOTION OF FUEL AND COOLANT DUE TO FUEL-COOLANT INTERACTIONS UNDER HIGH RAMP RATE REACTIVITY INSERTION

by

K. I. Chang and D. H. Cho

Reactor Analysis and Safety Division

July 1978
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOMENCLATURE</td>
<td>8</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>9</td>
</tr>
<tr>
<td>I. INTRODUCTION</td>
<td>10</td>
</tr>
<tr>
<td>II. FORMULATION OF THE MODEL</td>
<td>12</td>
</tr>
<tr>
<td>1. Physical Model and Assumptions</td>
<td>12</td>
</tr>
<tr>
<td>2. Mathematical Formulation</td>
<td>13</td>
</tr>
<tr>
<td>III. NUMERICAL PROCEDURE</td>
<td>20</td>
</tr>
<tr>
<td>IV. ILLUSTRATIVE CALCULATIONS</td>
<td>31</td>
</tr>
<tr>
<td>1. Uniform Fragmentation</td>
<td>32</td>
</tr>
<tr>
<td>2. Progressive Fragmentation</td>
<td>36</td>
</tr>
<tr>
<td>V. SUMMARY</td>
<td>41</td>
</tr>
<tr>
<td>APPENDIX - Thermodynamic Properties of Sodium, Fuel, and Fission-product Gas</td>
<td>43</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>46</td>
</tr>
<tr>
<td>REFERENCES</td>
<td>47</td>
</tr>
<tr>
<td>No.</td>
<td>Description</td>
</tr>
<tr>
<td>-----</td>
<td>------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>IV-1</td>
<td>Schematic Diagram of FCI Zone</td>
</tr>
<tr>
<td>IV-2</td>
<td>Distribution of Sodium-vapor and Fission-gas Void Fractions for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-3</td>
<td>Pressure Distribution for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-4</td>
<td>Fuel-particle and Sodium-mixture Velocity Distributions for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-5</td>
<td>Sodium-mixture Macroscopic Density Distribution for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-6</td>
<td>Fuel-temperature Distributions for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-7</td>
<td>Sodium-mixture Temperature Distributions for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-8</td>
<td>Dependence of Pressure History on the Fuel-particle Size for Uniform Fragmentation</td>
</tr>
<tr>
<td>IV-9</td>
<td>Distributions of Fuel Volume Fraction for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-10</td>
<td>Mass Effluxes of Fuel and Sodium-mixture for Uniform Fragmentation</td>
</tr>
<tr>
<td>IV-11</td>
<td>Expansion History of FCI Zone for Uniform Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-12</td>
<td>Distributions of Fragmented-fuel Volume Fractions for Bottom-initiated Progressive Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-13</td>
<td>Distribution of Fuel Volume Fraction for Bottom-initiated Progressive Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-14</td>
<td>Void-fraction Distributions of Sodium Vapor and Fission Gas for Bottom-initiated Progressive Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-15</td>
<td>Pressure Distributions for Bottom-initiated Progressive Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
<tr>
<td>IV-16</td>
<td>Volume-fraction Distributions of Fragmented Fuel for Top-initiated Progressive Fragmentation ( (d_p = 0.05 \text{ cm}) )</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES (Contd.)

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV-17</td>
<td>Distributions of Fuel Volume Fraction for Top-initiated Progressive Fragmentation (d_p = 0.05 \text{ cm})</td>
<td>39</td>
</tr>
<tr>
<td>IV-18</td>
<td>Void-fraction Distributions of Sodium Vapor and Fission Gas for Top-initiated Progressive Fragmentation (d_p = 0.05 \text{ cm})</td>
<td>39</td>
</tr>
<tr>
<td>IV-19</td>
<td>Pressure Distributions for TOP-initiated Progressive Fragmentation (d_p = 0.05 \text{ cm})</td>
<td>40</td>
</tr>
<tr>
<td>IV-20</td>
<td>Mass Effluxes of Fuel and Sodium-mixture for Progressive Fragmentation (d_p = 0.05 \text{ cm})</td>
<td>40</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>$C_D$</td>
<td>Drag coefficient</td>
<td></td>
</tr>
<tr>
<td>$C_{p,l}$</td>
<td>Specific heat of liquid sodium</td>
<td></td>
</tr>
<tr>
<td>$C_{p, fu}$</td>
<td>Specific heat of fuel</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>Hydraulic diameter of coolant channel</td>
<td></td>
</tr>
<tr>
<td>$d_p$</td>
<td>Diameter of fuel particle</td>
<td></td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Friction factor</td>
<td></td>
</tr>
<tr>
<td>$f_p$</td>
<td>Function defined in Eq. (II.10)</td>
<td></td>
</tr>
<tr>
<td>$g$</td>
<td>Acceleration due to gravity</td>
<td></td>
</tr>
<tr>
<td>$K$</td>
<td>Momentum exchange function defined in Eq. (II.5)</td>
<td></td>
</tr>
<tr>
<td>$k_p$</td>
<td>Thermal conductivity of fuel</td>
<td></td>
</tr>
<tr>
<td>$L$</td>
<td>Length of FCI zone</td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>Number of fuel particles per unit volume</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>Pressure</td>
<td></td>
</tr>
<tr>
<td>$q$</td>
<td>Function defined in Eq. (II.13)</td>
<td></td>
</tr>
<tr>
<td>$R_g$</td>
<td>Gas constant for fission gas</td>
<td></td>
</tr>
<tr>
<td>$R_v$</td>
<td>Gas constant for sodium vapor</td>
<td></td>
</tr>
<tr>
<td>$R$</td>
<td>Heat-exchange function defined in Eq. (II.15)</td>
<td></td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
<td></td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td></td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
<td></td>
</tr>
<tr>
<td>$U_1$</td>
<td>Lower sodium-slug velocity</td>
<td></td>
</tr>
<tr>
<td>$U_2$</td>
<td>Upper sodium-slug velocity</td>
<td></td>
</tr>
<tr>
<td>$U$</td>
<td>Velocity</td>
<td></td>
</tr>
<tr>
<td>$V$</td>
<td>Specific volume</td>
<td></td>
</tr>
<tr>
<td>$X$</td>
<td>Quality</td>
<td></td>
</tr>
<tr>
<td>$z_{ex}$</td>
<td>Position of subassembly exit</td>
<td></td>
</tr>
<tr>
<td>$z_c$</td>
<td>Axial position</td>
<td></td>
</tr>
<tr>
<td>$z_u$</td>
<td>Axial position of upper sodium slug</td>
<td></td>
</tr>
<tr>
<td>$z_l$</td>
<td>Axial position of lower sodium slug</td>
<td></td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Volume fraction of fuel</td>
<td></td>
</tr>
<tr>
<td>$\alpha_g$</td>
<td>Thermal-expansion coefficient of liquid sodium at constant pressure</td>
<td></td>
</tr>
<tr>
<td>$\beta_T$</td>
<td>Void fraction of sodium vapor and fission gas</td>
<td></td>
</tr>
<tr>
<td>$\rho'$</td>
<td>Isothermal compressibility of liquid sodium</td>
<td></td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td></td>
</tr>
<tr>
<td>$\eta$</td>
<td>Macroscopic density</td>
<td></td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Axial position in the normalized coordinate system</td>
<td></td>
</tr>
<tr>
<td>$\mu$</td>
<td>Time in the normalized coordinate system</td>
<td></td>
</tr>
<tr>
<td>$\mu$</td>
<td>Viscosity</td>
<td></td>
</tr>
<tr>
<td>$g$</td>
<td>Fission-product gas</td>
<td></td>
</tr>
<tr>
<td>$i$</td>
<td>Node number</td>
<td></td>
</tr>
<tr>
<td>$\ell$</td>
<td>Liquid sodium</td>
<td></td>
</tr>
<tr>
<td>$m$</td>
<td>Sodium/Fission-gas mixture</td>
<td></td>
</tr>
<tr>
<td>$Na$</td>
<td>Sodium</td>
<td></td>
</tr>
<tr>
<td>$p$</td>
<td>Fuel particle</td>
<td></td>
</tr>
<tr>
<td>$v$</td>
<td>Sodium vapor</td>
<td></td>
</tr>
</tbody>
</table>
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ABSTRACT

An analysis has been made of the combined motion of fuel and coolant due to fuel-coolant interactions following a massive fuel failure in a high-ramp overpower transient. The motion of fuel and coolant was described using a two-fluid model formulation in which the mixture of sodium liquid and vapor and of fission gas, on the one hand, and the fuel particles, on the other, were treated as two superimposed continua. The method of solution employed was a numerical procedure called the ACE method, a modified version of the IMF technique.

Illustrative calculations were made for a fuel rupture length of 60 cm in the FFTF geometry. Three different modes of fragmentation were considered. First, upon pin failure, molten fuel is completely fragmented and uniformly distributed in the coolant (uniform fragmentation). Second, fragmentation is initiated at the bottom of the mixing zone and propagates upward (bottom-initiated progressive fragmentation). Third, fragmentation is initiated at the top of the mixing zone and propagates downward (top-initiated progressive fragmentation).
I. INTRODUCTION

For a large LMFBR with a strong positive sodium-void coefficient, localized voiding in a loss-of-flow accident without scram may bring the reactor near prompt-critical with a large fraction of the core still full of liquid sodium. In such a situation, high reactivity ramp rates may be produced, resulting in massive fuel failures and the penetration of molten fuel into unvoided coolant channels. Experiments and analyses thus far seem to indicate that the possibility of an energetic thermal interaction between molten fuel and coolant is extremely remote, at least in the oxide-fueled system. Even if the fuel-coolant interaction (FCI) should be nonenergetic, however, there exists a problem of concern that is related to accident energetics. If reactivity gains due to sodium voiding override reactivity losses due to fuel dispersal, autocatalytic effects leading to a violent disassembly may arise. To assess the potential for such autocatalytic effects, the combined motion of fuel and coolant associated with the interaction needs to be investigated.

A number of computer codes have been developed to describe sodium voiding and fuel motion due to FCIs under mild transient overpower conditions. These codes consider molten fuel being ejected continuously into the coolant channel through a relatively small rupture area. The fuel motion inside the pin is explicitly taken into account and is coupled with the FCI process in the coolant channel.

For a high-ramp transient, however, a massive failure of fuel pin along the pin length would be expected. In this case, molten fuel would be ejected en masse into the coolant channel and fuel motion inside the pin would be minimal. The FCI process would then be governed by the mode of mixing and breakup of molten fuel and coolant immediately following the pin burst, details of fuel motion inside the pin being relatively unimportant.

A large amount of uncertainty exists regarding the mode of cladding failure and material intermixing under high-ramp transient overpower conditions. This report describes a computational tool that should be useful investigating some of the key uncertainties involved. It is a computer program which operates on a stand-alone mode, so that the effects of various physical processes (such as mixing, fragmentation, and heat transfer) on the combined motion of fuel
and coolant may be examined separately. The formulation of the model is given in Sect. II, and the numerical technique is described in Sect. III. Section IV presents illustrative calculations made for a fuel-rupture length of 60 cm in the FFTF geometry. In these calculations, three different modes of fragmentation were considered: 1) upon pin failure the molten fuel is completely fragmented and uniformly distributed in the coolant (uniform fragmentation); 2) fragmentation is initiated at the bottom of the mixing zone and propagates upward (bottom-initiated progressive fragmentation); 3) fragmentation is initiated at the top of the mixing zone and propagates downward (top-initiated progressive fragmentation). The calculations seem to indicate that reactivity losses due to fuel dispersal are likely to offset reactivity gains due to sodium ejection, minimizing the potential for autocatalytic effects. However, it would be very difficult to make a conclusive argument until the physical processes that characterize the FCI zone, including cladding failure, mixing, and heat transfer, are better understood. This would require an experimental data base which is statistically meaningful.
II. FORMULATION OF THE MODEL

1. Physical Model and Assumptions

The numerical model described in this report analyze the motion of fuel and coolant due to FCIs following a massive fuel failure in a high-ramp overpower transient. It is assumed that upon pin failure, molten fuel along with fission-product gas is ejected en masse into the coolant channel through a long cladding rupture. An FCI zone is formed as the ejected fuel fragments and mixes with the sodium in the coolant channel. The FCI is considered to take place in an intact coolant channel, and the FCI zone is bounded by the sodium columns above and below it. The fuel motion inside the pin subsequent to the initial ejection is ignored. It is assumed that the fuel remaining inside the pin is effectively isolated and does not participate in the FCI process, so the fuel mass in the FCI zone remains constant.

The present model does not treat mechanistically the mode of cladding failure or the mixing and fragmentation process during the fuel ejection. The starting point of the analysis is a distinct FCI zone that is formed following the fuel ejection; a given amount of molten fuel is assumed to be mixed with sodium liquid and vapor and fission-product gas. (Some sodium vaporization is considered to have taken place during the ejection and mixing process.) The sodium columns above and below the FCI zone are simply treated as incompressible liquid slugs. Other major assumptions are as follows:

(1) The sodium liquid and/or vapor and fission-product gas in the FCI zone are considered to form a homogeneous mixture in thermal equilibrium.*

(2) When the molten fuel mass becomes fragmented, it fragments into particles of the same size.

(3) The mixture and fuel-particle flows in the FCI zone are one-dimensional.

(4) No heat transfer occurs between the FCI zone and the surroundings.

*Throughout this report, the mixture of sodium liquid and vapor and fission gas will simply be referred to as "mixture".
The pressure of the FCI zone is the sum of the partial pressures of the sodium vapor and fission-product gas.

2. Mathematical Formulation

A two-fluid model formulation was employed to describe the combined motion of fuel and sodium in the FCI zone. In this formulation, the mixture (two-phase sodium and fission-product gas) and the fuel particles are treated as two superimposed continua, and a set of conservation equations for mass, momentum, and energy is needed for each component. The mixture component was treated as a compressible fluid, while the fuel-particle component was treated as an incompressible fluid. In addition, the equation of state for the mixture is required for the complete analysis. In the following equations the subscripts \( m \) and \( p \) denote the mixture and the fuel-particle component, respectively.

(1) Mass-conservation equations

Fuel particle:

\[
\frac{\partial a}{\partial t} + \frac{\partial}{\partial z} \left( a U_p \right) = 0 .
\]  

(II.1)

Mixture:

\[
\frac{\partial}{\partial t} \rho_m^* + \frac{\partial}{\partial z} \left( \rho_m^* U_m \right) = 0 ,
\]  

(II.2)

where \( \rho_m^* = (1-a)\rho_m \).

In the above equations, \( a \) is the volume fraction of fuel particles, \( U_p \) and \( U_m \) are the fuel-particle and mixture velocities, respectively, and \( \rho_m \) is the true (microscopic) density of the mixture, defined as

\[
\frac{1}{\rho_m} = \frac{1-X_v-X_g}{\rho_{Na,f}} + \frac{X_g}{\rho_{Na,v}} + \frac{X_v}{\rho_g},
\]  

(II.2a)
where $X_v$ = mass fraction of the sodium vapor in the mixture; $X_g$ = mass fraction of the fission-product gas in the mixture; $\rho_{Na,l}$ = density of liquid sodium; $\rho_{Na,v}$ = density of sodium vapor; $\rho_g$ = density of fission-product gas.

As will be seen later in this section, $\rho_{Na,v}$ and $\rho_g$ are determined from the equation of state for sodium vapor and for fission-product gas, respectively. The density $\rho_{Na,l}$ is given as a function of temperature in the Appendix. In Eq. (II.1) the fuel-particle density $\rho_p$ has been taken to be constant.

(2) Momentum-conservation equations

Fuel particle:

$$\frac{3U_p}{2t} + U_p \frac{3U_p}{3z} - \frac{1}{\rho_p} \frac{3\rho}{3z} + \frac{K}{\alpha p} (U_m - U_p)$$

$$- \frac{2f}{D} (1-\alpha)^2 \rho_p |U_m| U_m - \frac{f_p}{\rho_p} - g .$$

Mixture:

$$\frac{3}{3t} (\rho_m U_m) + \frac{3}{3z} (\rho_m U_m U_m) = -(1-\alpha) \frac{3\rho}{3z} - K(U_m - U_p)$$

$$- \frac{2f}{D} (1-\alpha)^2 \rho_m |U_m| U_m - (1-\alpha)f_p - (1-\alpha) \rho_m g .$$

For the momentum exchange function $K$ the following form is used:

$$K = \frac{3C_D}{4d_p} \alpha \rho_m |U_m - U_p| (1-\alpha)^{-2.7}$$

(II.5)

where $d_p$ is the fuel-particle diameter and $C_D$ is the drag coefficient for a single sphere given by $^6$
\[ C_D = \begin{cases} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) & \text{when } Re_p < 1000 \\
0.44 & \text{when } Re_p > 1000. 
\end{cases} \]  \hspace{1cm} \text{II.6}

Here \( Re_p \) is the particle Reynolds number defined by

\[ Re_p = \frac{\rho m d_p |U_m - U_p|}{\mu_m} , \]  \hspace{1cm} \text{II.7}

where \( \mu_m \) is the volume-averaged viscosity of the mixture. Notice that the momentum-exchange term is simply the drag force for single particle multiplied by the number of particles per unit volume and by the factor \((1-\alpha)^{2.7}\) which is an experimentally determined factor to account for the effect of the particle concentration on the drag force.\(^7\) In the momentum equations, \( f \) is the Fanning friction factor given by \(^8\)

\[ f = \begin{cases} 16/Re & \text{when } Re < 2,300 \\
0.079 Re^{-0.25} & \text{when } 2,300 < Re < 30,000 \\
0.046 Re^{-0.2} & \text{when } Re > 30,000 , 
\end{cases} \]  \hspace{1cm} \text{II.8}

where \( Re \) is the coolant-channel Reynolds number

\[ Re = \frac{\rho m U D}{\mu_m} \]  \hspace{1cm} \text{II.9}

and \( D \) is the coolant-channel hydraulic diameter. The quantity \( f_p \) represents an extra wall friction due to the presence of fuel particles:\(^9\)

\[ f_p = \frac{\pi \rho_p \sqrt{\rho_p}}{4D} \sqrt{\frac{\rho_p}{\rho_m}} \alpha (1-\alpha) U_p |U_m|. \]  \hspace{1cm} \text{II.10}

In the present analysis a constant value of \( 1.5 \times 10^{-5} \) was used for \( \psi \).

It should be noted that the nonconservative form of the particle-momentum equation has been employed. This is done because in the conservative form \((\alpha U_p)\) may become unsuitable as a primary variable for very small values of the particle volume fraction \( \alpha \).
(3) **Energy-conservation equations**

**Fuel particle:**

\[
\frac{\partial T_p}{\partial t} + \frac{\partial U_m T_p}{\partial z} = \frac{\partial P}{\partial z} \frac{\partial U_m}{\partial z} = \frac{R}{\alpha_p C_{p, fu}} (T_m - T_p),
\]

**Mixture:**

\[
\frac{Dh_m}{Dt} = \frac{1}{\rho_m} \frac{DP}{Dt} + \frac{q}{\rho_m},
\]

where

\[
q = \frac{R}{(1-\alpha)} (T_p - T_m) + \frac{2f}{D} (1-\alpha) \rho_m |U_m| U_m^2
\]

and

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + U_m \frac{\partial}{\partial z}.
\]

In the above energy equations, \(T_p\) and \(T_m\) are the fuel-particle and mixture temperatures, respectively, \(h_m\) is the enthalpy of the mixture, and \(C_{p, fu}\) is the specific heat of the fuel particle.

The heat-exchange function \(R\) is defined by

\[
R = nhA_p = \frac{6ah}{d_p},
\]

where \(n\) is the number of particles per unit volume and \(A_p\) is the particle surface area. The heat-transfer coefficient \(h\) is given by

\[
h = \frac{2k_p}{d_p} (1-\alpha_g),
\]

where

- \(k_p\) = thermal conductivity of fuel particle;
- \(\alpha_g\) = void fraction of sodium vapor and fission gas in the mixture.
This form of the heat-transfer coefficient has been used in the PLUTO code\(^3\) and is similar to the formulation of Cho et al.\(^9\) The nonconservative form of the energy equation for the mixture enables us to combine the energy equation with the mixture equation of state for pressure iterations, as will be seen later.

(4) Equations of state

For the present study it is assumed that the fission-gas temperature is the same as the sodium-vapor temperature at all times. Therefore, the mixture temperature corresponds to the sodium saturation temperature when sodium vapor exits at a given location. When the sodium is in a single-phase liquid state, however, the mixture temperature is calculated from the equation of state for liquid sodium.

It should be noted here that whether sodium is in a liquid state or in a two-phase state in a given node depends solely on the local sodium density. When the sodium density is lower than the saturation liquid density corresponding to the local temperature, the sodium is regarded as a saturated two-phase mixture.

It is assumed that the fission-product gas is noncondensable and that no more fission gas is added after the initial ejection of the molten fuel. Therefore, the quality of the fission gas remains constant everywhere in the FCI zone.

When the sodium is in a saturated two-phase state, the pressure is determined by

\[
p_m(z,t) = p_{Na,v}(z,t) + p_g(z,t), \tag{II.17}
\]

where \(p_{Na,v}\) and \(p_g\) are the partial pressures due to the sodium vapor and the fission-product gas, respectively. These partial pressures are related to the system pressure \(p_m\) by

\[
p_{Na,v} = \frac{X_{R'} p_m}{X_{R'} + X_{R_g}}, \tag{II.18}
\]
and

\[ p_g = \frac{X R_p m}{\frac{X R_p}{v} + \frac{X R_g}{g}} \]  \hspace{1cm} (II.19)

where

\[ R_g = \text{gas constant for the fission gas}; \]
\[ R_v = Z_{c v} R_v; \]
\[ R_v = \text{gas constant for the sodium vapor}; \]
\[ Z_c = \text{compressibility factor}. \]

The sodium-vapor and fission-gas densities are given by

\[ \rho_{Na,v} = \frac{p_m}{R_v T} \]  \hspace{1cm} (II.20)

and

\[ \rho_{g} = \frac{p_m}{R T_g}. \]  \hspace{1cm} (II.21)

When the sodium is in a single-phase liquid state, we have

\[ p_m = p_g \]  \hspace{1cm} (II.22)

and

\[ dV_{Na,L} = -\beta_T V_{Na,L} \frac{dp_m}{p} + \alpha_p V_{Na,L} \frac{dT}{T}, \]  \hspace{1cm} (II.23)

where

\[ V_{Na,L} = \text{specific volume of liquid sodium}; \]
\[ \beta_T = \text{isothermal compressibility of liquid sodium}; \]
\[ \alpha_p = \text{thermal-expansion coefficient of liquid sodium at constant pressure}. \]

(5) Inertial constraint

The liquid-sodium columns above and below the FCI zone are treated as incompressible liquid slugs. No heat transfer is assumed to take place.
between the FCI zone and the sodium columns. The heated sodium in the FCI zone then expands against the inertia of the unheated liquid-sodium columns.

A macroscopic momentum balance gives the equations of motion of the liquid-sodium columns:

\[ \frac{dU_2}{dt} = -g + \frac{p - p_{\text{ex}}}{\rho_0 (z_{\text{ex}} - z_u)} - 2 U_2 |U_2| f/D \]  \hspace{1cm} (II.24)

and

\[ \frac{dU_1}{dt} = -g - \frac{p - p_{\text{in}}}{\rho_0 z_l} - 2 U_1 |U_1| f/D , \]  \hspace{1cm} (II.25)

where \( U_2 \) and \( U_1 \) are the upper and lower slug velocities, respectively, \( p_{\text{ex}} \) is the exit plenum pressure, \( p_{\text{in}} \) is the inlet plenum pressure, \( \rho_0 \) is the density of liquid sodium at 950 K, \( z_u \) and \( z_l \) are the interfacial positions between the FCI zone and the upper and lower sodium columns, respectively, and \( z_{\text{ex}} \) is the subassembly exit position.

(6) **Thermodynamic properties**

The thermodynamic properties of sodium, fission-product gas, and fuel used in the present analysis are given in the Appendix.
III. NUMERICAL PROCEDURE

At first, the implicit multifield [IMF] technique\(^{10,11}\) was successfully used to analyze the adiabatic expansion of a pressurized mixture of fuel particles and two-phase sodium against the inertia of a liquid-sodium column.\(^{12}\) However, the addition of energy equations revealed that the IMF technique could lead to severe computational difficulties. This may be due to the fact that there exists a large density difference between sodium liquid and vapor, and that convection, rather than compression, is the primary cause of density change in the IMF technique.

Therefore, a modified version of the IMF technique, which is called the ACE method,\(^{13}\) was employed to solve the system of equations given in the previous section. Although the ACE method was originally developed for a one-component, two-phase flow, this technique seems to work fairly well also for a two-component flow such as is considered in the present analysis.

The ACE method employed here utilizes a completely Eulerian mesh of finite-difference cells in which field variables, such as fuel volume fraction, pressure, and density, are cell-centered quantities, whereas velocities are calculated at the cell boundaries, as shown below.

\[
\begin{array}{c|c|c}
& \alpha, p, p_m^*, T & \\
\hline
\bullet & \bullet & \bullet \\
i-1 & i & i+1 \\
\hline
U_p & U_p & \\
i-1/2 & i+1/2 & \\
U_m & U_m & \\
i-1/2 & i+1/2 & \\
\end{array}
\]

A complete donor-cell differencing is used for the calculation of the convective flux of a field variable. This differencing scheme eliminates the necessity for an explicit artificial diffusion term since it mitigates truncation-error effects automatically.\(^{14}\) Angular brackets will be used to
denote such donor-cell fluxes, and two examples for some quantity Q follow:

\[
<QU_m>_{i+1/2} = \begin{cases} 
Q_i U_m i+1/2 & \text{if } U_{i+1/2} > 0 \\
Q_{i+1} U_m i+1/2 & \text{if } U_{i+1/2} < 0 
\end{cases} \tag{III.1}
\]

and

\[
<QU^2_m>_{i} = \begin{cases} 
Q_i U_m^2 i-1/2 & \text{if } (U_{i-1/2} + U_{i+1/2}) > 0 \\
Q_{i+1} U_m^2 i+1/2 & \text{if } (U_{i-1/2} + U_{i+1/2}) < 0 
\end{cases} \tag{III.2}
\]

In addition, the \((z,t)\) coordinate system was transformed into the \((n,\zeta)\) coordinate system in such a way that the number of nodes remained constant at all times, i.e.,

\[
\eta = \frac{z - z_u}{L(t)} = \frac{z - z_{\hat{u}}}{z_u(t) - z_{\hat{u}}(t)} \tag{III.3}
\]

and

\[
\zeta = t \tag{III.4}
\]

where \(z_u(t)\) and \(z_{\hat{u}}(t)\) are the positions of the upper and lower ends of the FCI region, respectively, and \(L(t)\) is the total length of the FCI zone at time \(t\). To accommodate this coordinate transformation, the time and space derivatives are replaced by

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial \zeta} + \frac{1}{L(t)} \left[ \frac{dz_{\hat{u}}}{dt} (\eta - 1) - \eta \frac{dz_u}{dt} \right] \frac{\partial}{\partial \eta} \tag{III.5}
\]

and

\[
\frac{\partial}{\partial z} = \frac{1}{L(t)} \frac{\partial}{\partial \eta} \tag{III.6}
\]

In Eq. (III.5) \(dz_u/dt\) and \(dz_{\hat{u}}/dt\) represent the velocities \(U_2\) and \(U_1\) of the upper and lower slugs, respectively. The normalization eliminates uncertainties involved in assigning new field variables after the rezoning that is otherwise required for the Eulerian mesh with moving boundaries.
It was found, however, that the calculations of $\alpha$ and $\rho_m^-$ from the normalized continuity equations introduced, at each time step, errors in the total masses of fuel and mixture in the FCI zone. These errors eventually reached a few percent of the total masses. To remove these errors, $\alpha$ and $\rho_m^-$ were calculated explicitly in the physical coordinate system in the following manner:

$$a_i^{n+1} = a_i^n + \frac{\Delta t}{\Delta z} \left[ <aU_p>_{i-1/2} - <aU_p>_{i+1/2} \right]$$  \hspace{1cm} (III.7)

and

$$\rho_m^i \bigg|_{n+1} = \rho_m^i \bigg|_{n} + \frac{\Delta t}{\Delta z} \left\{ \left[ \rho_m^i \bigg|_{n+1} \right]_{i-1/2} - \left[ \rho_m^i \bigg|_{n+1} \right]_{i+1/2} \right\}$$  \hspace{1cm} (III.8)

where the superscripts $n$ and $n+1$ count the time steps; wherever the superscript is omitted, the time step is considered to be $n$. The quantities in the last bracket in Eq. (III.8) are not donor-cell fluxes. These quantities are calculated directly from the mixture momentum equation and are linearly dependent on the total pressure $\rho_m^i$, as will be discussed later. In other words, the change in the macroscopic density of the mixture is determined by the compression due to pressure rather than to the convective flux. This is one of the major differences between the IMF and the ACE techniques, which seems to make the ACE method numerically stable.

The interfaces between the sodium columns and the FCI zone at both ends move either upward or downward, depending on the pressures of the nodes next to the interfaces and on the inlet and exit pressures, as shown in Equations (II.24) and (II.25). To take these movements into account, the continuity equations (III.7) and (III.8) were applied to the boundaries as follows: Suppose the upper and lower ends of the FCI region have moved upward by $\Delta z_u$ and $\Delta z_l$, respectively, as depicted below.
The macroscopic density of the mixture for the newly generated (N+1)th node, which is much smaller than the regular node, can be calculated by

$$\rho_{m, N+1}^* = \frac{\Delta t}{\Delta z} \left[ \rho_{m, N}^* U \right]^{N+1/2}.$$  \hspace{1cm} (III.9)

Then, the (N+1)th node is combined with the Nth node. For the first node, we have

$$\rho_{m, 1}^* = \rho_{m, 1}^* - \frac{\Delta t}{\Delta z} \left[ \rho_{m, m}^* U \right]^{3/2}.$$  \hspace{1cm} (III.10)

When the lower slug moves upward, the first node becomes smaller than the regular one. This shrinkage of the node may be taken into account by multiplying $$\rho_{m, 1}^*$$ in Eq. (III.10) by $$\Delta z/(\Delta z - \Delta z_1)$$. Finally, assuming a step-function distribution of the macroscopic density of the mixture, the mixture density of every node is readjusted in such a way that all the nodes are of equal length. The calculation then proceeds to the next step. A similar procedure is followed for the calculation of $$a_{N+1}^*$$ in Eq. (III.7).

After the two continuity equations (III.7) and (III.8) have been solved, the fuel-particle energy equation is also solved explicitly. The difference equation for the fuel temperature in the normalized coordinate system can be written as

$$- \frac{\Delta t}{2L^{n+1} \Delta n} \left[ U_1(n_1'-1) - n_1 U_2 \right] T_{p1-1}^{n+1} + \frac{\Delta t}{2L^{n+1} \Delta n} \left[ U_1(n_1'-1) - n_1 U_2 \right] T_{p1+1}^{n+1}$$

$$= T_{p1}^{n} + \frac{\rho_{m, 1} \Delta t}{\Delta n} \left( U_{p1+1/2}^{n} - U_{p1-1/2}^{n} \right) + \frac{\Delta t}{L \Delta n} \left[ <T_p U_p>_{i-1/2} - <T_p U_p>_{i+1/2} \right]$$

$$+ \frac{\Delta t}{\sigma_i \rho P_{c, p}} \left( T_{m, i}^{n} - T_{p, i}^{n} \right).$$  \hspace{1cm} (III.11)

When the fuel temperature of each node reached the melting point, the fuel temperature was kept constant at that temperature until the total heat loss from the fuel particles in the node surpassed the heat of fusion of the fuel. In this way, the effect of the heat of fusion was taken into account rather accurately.
The fuel-temperature calculation concludes the first explicit part of the solution scheme. The second part consists of implicit calculations of the total pressure, mixture temperature, and the velocities of the mixture and fuel-particle components.

At first, the iterative equation necessary for the pressure calculation is generated by combining the mixture continuity equation with the mixture energy equation, the mixture equation of state, and the two momentum equations. For simplicity, this procedure will be described in the physical coordinate system.

The mixture continuity equation (II.2) can be rewritten as

\[
\frac{1}{\rho_m} \frac{D\rho_m}{Dt} + \frac{\partial U_m}{\partial z} - \frac{1}{(1-\alpha)} \left[ \frac{\partial \alpha}{\partial t} + U_m \frac{\partial \alpha}{\partial z} \right] = 0 ,
\]  

Assume that the mixture equation of state can be expressed by

\[
\rho_m = \rho_m(h_m, p_m) .
\]  

Then we have

\[
\frac{1}{\rho_m} \frac{D\rho_m}{Dt} = \left[ \frac{\partial \rho_m}{\partial h_m} \right]_{p_m} \frac{Dh_m}{Dt} + \left[ \frac{\partial \rho_m}{\partial p_m} \right]_{h_m} \frac{Dp_m}{Dt} .
\]  

Substituting the mixture energy equation (II.14) into Eq. (III.14) and combining with Eq. (III.12), we have

\[
\frac{\partial U_m}{\partial z} + \frac{1}{\rho_m} \left( \frac{\partial \rho_m}{\partial h_m} \right)_{p_m} \frac{\partial h_m}{\partial z} + \frac{1}{\rho_m} \left( \frac{\partial \rho_m}{\partial p_m} \right)_{h_m} \frac{\partial p_m}{\partial z} \right] \frac{Dp_m}{Dt} 
\]

\[
- \frac{1}{(1-\alpha)} \left[ \frac{\partial \alpha}{\partial t} + U_m \frac{\partial \alpha}{\partial z} \right] = 0 .
\]  

The finite-difference equation for Eq. (III.15) becomes in the normalized coordinate system.
\[
\frac{1}{L^{n+1} \Delta n} \left( U_{m}^{n+1} i +1/2 - U_{m}^{n+1} i-1/2 \right) + \frac{A_{i}}{\Delta t} p_{m}^{n+1} i + \frac{A_{i}}{2L^{n+1} \Delta n} \left[ U_{1}(\eta_{i}-1) - \eta_{i} U_{2} + U_{m}^{n+1} i +1/2 \right] \times \left( p_{m}^{n+1} i +1 - p_{m}^{n+1} i-1 \right) + B_{i} = E_{i+1}^{n+1},
\] (III.16)

where

\[
A_{i} = \frac{1}{p_{mi}} \left( \frac{\partial \rho_{mi}}{\partial h_{mi}} \right) p_{mi} + \frac{1}{p_{mi}} \left( \frac{\partial \rho_{mi}}{\partial \rho_{mi}} \right) h_{mi}
\] (III.17)

and

\[
B_{i} = \frac{1}{p_{mi}} \left( \frac{\partial \rho_{mi}}{\partial h_{mi}} \right) p_{mi} q_{i} - \frac{A_{i} p_{mi}^{n}}{\Delta t} - \frac{1}{(1-\alpha_{i+1})} \left\{ \alpha_{i+1}^{n+1} - \alpha_{i-1}^{n+1} \right\} + \frac{1}{2L^{n+1} \Delta n} \left[ U_{1}(\eta_{i}-1) - \eta_{i} U_{2} + U_{m}^{n+1} i +1/2 \right] \left( \alpha_{i+1}^{n+1} - \alpha_{i-1}^{n+1} \right).
\] (III.18)

Note that \( A_{i} \) and \( B_{i} \) can be calculated explicitly, so that these quantities need not be updated during pressure iterations.

The two partial derivatives of \( p_{mi} \) shown above can be calculated from the appropriate equation of state for the mixture. When the sodium is in a saturated two-phase state, we have

\[
\frac{1}{\rho_{m}} = V_{m} = (1-X) V_{Na, l} + X V_{Na, v} \Delta V_{h, v} + X V_{g, g}
\] (III.19)

and

\[
h_{m} = h_{Na, l} + X \Delta h_{Na, v} + \Delta h_{Na, v} \]
(III.20)

where

\[
V_{m} = \text{specific volume of the mixture};
\]

\[
V_{Na, v} = \text{specific volume of the sodium vapor};
\]

\( E_{i+1}^{n+1} \) represents an error term that is used in the iteration scheme to be discussed later.
\[ v_g = \text{specific volume of the fission gas}; \]
\[ \Delta V_{l,v} = v_{Na,v} - v_{Na,\ell}; \]
\[ h_{Na,\ell} = \text{specific enthalpy of the liquid sodium}; \]
\[ h_{Na,v} = \text{specific enthalpy of the sodium vapor}; \]
\[ \Delta h_{l,v} = h_{Na,v} - h_{Na,\ell}. \]

Thus, the first derivative in Eq. (III.17) becomes

\[ \frac{1}{\rho_m} \left( \frac{\partial h_m}{\partial \rho_m} \right) p_m = -\frac{\Delta V_{l,v}}{\Delta h_{l,v}}. \]  

Substitution of Eqs. (II.20) and (II.21) into Eq. (III.19) yields

\[ \rho_m = \frac{\rho_{Na,\ell} p_m}{(1-X_v-X_g) p_m + (X_{R'}+X_{R}) \rho_{Na,\ell} T}. \]  

The second derivative, \( \frac{\partial^2 h_m}{\partial \rho_m} \), may be calculated from Eqs. (III.22) and (III.20) using expressions for \( h_m \) in terms of temperature, as well as the vapor-pressure equation of sodium.

When the sodium is in a liquid phase, the derivatives can be calculated from Eq. (II.23) using the following expression:

\[ h_m = C_{p,\ell} T_m, \]  

where \( C_{p,\ell} \) is the specific heat of the liquid sodium.

The advanced-time velocities in Eq. (III.16) should be obtained from the momentum equations in terms of the advanced-time pressures. Therefore, the iteration scheme for Eq. (III.16) will be discussed after the momentum equations have been considered.

In order to calculate the velocities of the fuel particle and the mixture, the momentum equations for the two components, Eqs. (II.3) and (II.4), should be solved simultaneously. Equation (II.3) can be written, in the finite-difference form, as
\[ U_{i+1/2}^{n+1} = \frac{\Delta t}{\rho_p^{N+1/2}} \left( p_{m, i+1}^{n+1} - p_{m, i}^{n+1} \right) + \frac{K_{i+1/2}^{N+1/2}}{\alpha_{i+1/2}} \left( U_{m, i+1/2}^{n+1} - U_{p, i+1/2}^{n+1} \right) + G_{i+1/2} \] (III.24)

where \( G_{i+1/2} \) is an explicit term, i.e.,

\[ G_{i+1/2} = U_{p, i+1/2}^{n+1} - \Delta t \left[ U_{i}^{n} \left( \eta_{i+1/2} - 1 \right) - \eta_{i+1/2}^{n+1} U_{m}^{2} \right] \]

\[ \left( U_{p, i-1/2}^{n} - U_{p, i+3/2}^{n} - \frac{2f_{i}^{t}}{\rho_{p}^{D}} \left( 1 - \alpha_{i+1/2}^{n+1} \right)^{2} \rho_{m} \right) \right] U_{m, i+1/2}^{n} + \]

\[ - \frac{f_{p}^{2}}{\rho_{p}^{t+1/2} \Delta t} \]

(III.25)*

For the mixture momentum equation we write

\[ \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} = \frac{(1 - \alpha_{i+1/2}^{n+1})^{2} \Delta t}{\Delta t \eta_{i+1/2}^{n+1} \Delta n} \left( p_{m, i+1/2}^{n+1} - p_{m, i+1}^{n+1} \right) - K_{i+1/2}^{N+1/2} \left( U_{m, i+1/2}^{n+1} \right) \]

\[ - U_{p, i+1/2}^{n+1} \right) + H_{i+1/2} \] (III.26)

where

\[ H_{i+1/2} = \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n} + \frac{\Delta t}{\Delta t \eta_{i+1/2}^{n+1} \Delta n} \left\{ \rho_{m}^{2} - \rho_{m}^{2} \right\} + \frac{\Delta t}{2 \Delta t \eta_{i+1/2}^{n+1} \Delta n} \left\{ \frac{\rho_{m}}{U_{m}} \right\}_{i+1/2}^{n+1} \]

\[ \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n} \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} \left[ \rho_{m} U_{m} \right]_{i+1/2}^{n+1} \right] \]

\[ - \frac{2f_{i}^{t}}{D} \left( 1 - \alpha_{i+1/2}^{n+1} \right)^{2} \rho_{m} \left[ U_{m, i+1/2}^{n+1} \right] - \left( 1 - \alpha_{i+1/2}^{n+1} \right) f_{p}^{i+1/2} \Delta t \right) \]

(III.27)*

The advanced-time mixture velocity \( U_{m, i+1/2}^{n+1} \) in the momentum-exchange terms

*The gravity term is neglected in Eqs. (III.25) and (III.27).
was replaced by \( \rho_m^{i+1/2} \), where \( \rho_m^{i+1/2} \) is the donor density, and Eqs. (III.24) and (III.26) were solved simultaneously to give

\[
\left[ \rho_m^{i+1/2} \right]^{n+1} = \left\{ C_{i+1/2} \left( p_i^n - p_{i+1}^n \right) + \frac{a_{i+1/2}^{n+1}}{a_{i+1/2}^{n+1} + \rho_p K_{i+1/2} \Delta t} G_{i+1/2} \right\} / (1 + \frac{K_{i+1/2} \Delta t}{a_{i+1/2}^{n+1} + \rho_p K_{i+1/2} \Delta t}), \tag{III.28}
\]

where

\[
C_{i+1/2} = \frac{(1 - \alpha)}{L_{n+1} \Delta n} + \frac{K_{i+1/2}^{2}(\Delta t)}{L_{n+1} \Delta n \left( \alpha_{i+1/2}^{n+1} + \rho_p K_{i+1/2} \Delta t \right)}, \tag{III.29}
\]

\[
D_{i+1/2} = 1.0 + \frac{K_{i+1/2}^{2} \Delta t}{\rho_m^{i+1/2} - \rho_m^{i+1/2} \left( \alpha_{i+1/2}^{n+1} + \rho_p K_{i+1/2} \Delta t \right)} \tag{III.30}
\]

and

\[
U_p^{n+1} = \left\{ \frac{K_{i+1/2} \Delta t}{\alpha_{i+1/2}^{n+1} + \rho_p \rho_m^{i+1/2}} \left[ \rho_m^{i+1/2} U_m^{n+1} \right] + \frac{\Delta t}{\rho_p L_{n+1} \Delta n} (p_i^n - p_{i+1}^n \right\} / (1 + \frac{K_{i+1/2} \Delta t}{\alpha_{i+1/2}^{n+1} + \rho_p K_{i+1/2} \Delta t}). \tag{III.31}
\]

As can be seen in Eq. (III.28), \( \rho_m^{i+1/2} \) is linearly related to the pressure, since nonlinear terms are linearized using the initial values at each time step. The linearity of Eqs. (III.16) and (III.28) with respect to the pressure was used to construct an iteration scheme. First, the updated mixture velocities are expressed in terms of the updated pressure \( \rho_m^{n+1} \) by dividing the right-hand side of Eq. (III.28) by the donor density \( \rho_m^{i+1/2} \). This expression is then substituted into Eq. (III.16) to generate a set of algebraic equations for \( \rho_m^{n+1} \). By use of a set of assumed values for \( \rho_m^{n+1} \), error terms \( E_{1}^{n+1} \) in Eq. (III.16) are calculated. At first the initial pressure \( \rho_m^{n} \) is used for \( \rho_m^{i} \). When the average value of \( E_{1}^{n+1} \) is larger than a specified error criterion, the pressure calculation is iterated to force the errors \( E_{1}^{n+1} \) to zero on a point relaxation basis. The incremental changes \( \delta p_m^{i} \) necessary for getting \( \rho_m^{n+1} \) can be obtained from.
\[
\frac{1}{L^{n+1}} \Delta n \left( \frac{C_{i+1/2}}{D_{i+1/2} \rho^*_{m} i+1/2} (\delta p_{m i} - \delta p_{m i+1}) - \frac{C_{i-1/2}}{D_{i-1/2} \rho^*_{m} i-1/2} (\delta p_{m i-1} - \delta p_{m i}) \right) \\
+ \frac{A_i}{\Delta t} \delta p_{m i} + \frac{A_i}{2L^{n+1} \Delta n} \left[ u_{m}^{n+1} (\eta_i - 1) - \eta_1 u_{m}^{n+1} + u_{m}^{n+1} (\delta p_{m i+1} - \delta p_{m i-1}) \right] \\
= - E_{n+1}^{i},
\]

where 

\[\delta p_{m i} = \text{Newly updated values for} \ p_{m i}^{n+1} - \text{Assumed values for} \ p_{m i}^{n+1}.\]

The set of algebraic equations as given by Eq. (III.32), along with appropriate equations for the boundary nodes, can be solved using the Gaussian elimination technique for a tridiagonal matrix.\(^{16}\)

Given \(\delta p_{m i}^{n+1}\), the incremental change in the mixture momentum can be obtained from Eq. (III.28):

\[
\delta [\rho^* u_m]_{i+1/2} = \frac{C_{i+1/2}}{D_{i+1/2}} (\delta p_{m i} - \delta p_{m i+1}),
\]

and the incremental change in the fuel-particle momentum is obtained from Eq. (III.31):

\[
\delta u_{p i+1/2} = \frac{K_{i+1/2} \Delta t}{\alpha_{i+1/2} \rho p^* i+1/2} \delta [\rho^* u_m]_{i+1/2} + \frac{\Delta t}{\rho p^{n+1} \Delta n} (\delta p_{m i} - \delta p_{m i+1})
\]

\[
/(1 + \frac{K_{i+1/2} \Delta t}{\alpha_{i+1/2} \rho p}) .
\]

The above calculational procedures were repeated until the average value of \(E_{n+1}^{i}\) became smaller than an error criterion of \(10^{-5}\). Less than five iterations were required for most of the illustrative calculations reported in the next section.
After the pressure $p_{m}^{n+1}$ had been determined, the quality of the sodium was obtained from Eq. (III.19) along with Eqs. (II.20) and (II.21). The positive quality of the sodium vapor indicates that the sodium is in a saturated two-phase state. In this case, the sodium vapor pressure was obtained from Eq. (II.18), and the mixture temperature was taken to be equal to the sodium saturation temperature, viz.,

$$T_m = \frac{12016.6}{10.40861 - \ln p_{Na,v}},$$  \hspace{1cm} (III.35)

where $p_{Na,v}$ is the sodium vapor pressure in atm. When the quality becomes less than zero, however, the mixture temperature was calculated from Eq. (II.23), the equation of state for liquid sodium, viz.,

$$T_{m1}^{n+1} = T_{m1}^{n} + [\beta_T(p_{m1}^{n+1} - p_{m1}^{n})/\alpha_p].$$ \hspace{1cm} (III.36)
As mentioned in Sect. II, the model assumes a distinct FCI zone formed in the coolant channel, where a given amount of molten fuel is mixed with the sodium. Illustrative calculations have been performed considering three different modes of fragmentation in the mixing zone. First, upon pin failure, molten fuel is ejected into the coolant channel and completely fragmented. The fragmented fuel particles are uniformly distributed in the FCI zone (uniform fragmentation). Second, fragmentation is initiated at the bottom of the mixing zone and propagates upward (bottom-initiated progressive fragmentation). Third, fragmentation is initiated at the top of the mixing zone and propagates downward (top-initiated progressive fragmentation). It was assumed that the heat transfer from the unfragmented fuel to the coolant was negligible and that the unfragmented fuel mass remained stationary. The progressive fragmentation modes might also be applicable to the case in which the pin rupture occurs progressively along the fuel-pin length.

Figure IV-1 shows a schematic diagram of the FCI zone considered in the illustrative calculations. The fuel-pin rupture length was taken to be 60 cm, which is two-thirds of the full fuel-pin length. All the geometrical dimensions used correspond to those for the Fast Flux Test Facility. The axial dimensions shown in the figure are the heights measured from the inlet. The hydraulic diameter of the coolant channel associated with a single pin is 0.3253 cm. The nominal inlet and outlet pressures are 0.83 and 0.137 MPa (8.2 and 1.35 atm), respectively. The volume fraction of fuel in the FCI zone was assumed to be 0.1. The initial velocities of the sodium and fuel particles were taken to be 0.1. The initial velocities of the sodium and fuel particles were taken to

*The FFTF dimensions were used for illustrative purposes only. For a small reactor like FFTF, a prompt-burst reactivity accident is highly improbable, so the fuel failure modes considered in the present report would not be applicable.
to be zero. Initially, the FCI-zone pressure was 0.66 MPa (6.5 atm), and the sodium and fuel temperatures were 1350 and 3500 K, respectively. The mass ratio of the fission product gas to the molten fuel was 0.0005. The ratio of the sodium-vapor and fission-gas volume to the liquid sodium volume was 0.25, which corresponds to a mixture void-fraction of 0.2. The fuel-particle sizes studied were 0.02, 0.05, and 0.1 cm in diameter. Most of the calculations, however, were made for a particle diameter of 0.05 cm. This particle size has previously been used in analysis of the TREAT tests, such as the H-2 experiment.  

The time step used for the numerical calculations was 0.05 ms. The computer time required for 750 calculations was approximately 70 s.

The initial node length was 2 cm, so the total number of nodes was 30. For the progressive fragmentation, both bottom- and top-initiated, the propagation speed was assumed to be one initial node length per millisecond, i.e., 2 cm/ms.

The results of the illustrative calculations are discussed below.

1. Uniform Fragmentation

Figure IV-2 shows the void-fraction distributions* of the sodium vapor and fission gas in the mixture at different times. It is seen that at 5 ms the void fraction in the FCI zone has decreased somewhat from the initial value, except near the ends. This is due to the fact that during the 5-ms period the pressure increased because of heat transfer, while the mixture density remained almost constant, as shown in Fig. IV-3. Note that the liquid sodium was not completely vaporized even after 30 ms. The shape of the void-fraction distribution at 15 ms in Fig. IV-2 resembles the letter "M." It appears that the expansion at the ends of the FCI zone has not fully propagated to the center nodes. The low void fractions near the ends of the FCI zone arise as a result of the mixture velocities there being larger than the liquid-sodium slug velocities, as can be seen in Fig. IV-4. (The slug

* Void fraction = \( \frac{\text{sodium vapor/fission-gas volume}}{\text{mixture volume}} \)
Fig. IV-2. Distribution of Sodium-vapor and Fission-gas Void Fractions for Uniform Fragmentation. 

d_p = 0.05 cm.

Fig. IV-3. Pressure Distribution for Uniform Fragmentation 

d_p = 0.05 cm. 
(10^7 dyne/cm^2 = 1 MPa).

Fig. IV-4. Fuel-particle and Sodium-Mixture Velocity Distributions for Uniform Fragmentation 

d_p = 0.05 cm.

Fig. IV-5. Sodium-Mixture Macroscopic Density Distribution for Uniform Fragmentation 

d_p = 0.05 cm.
velocities are indicated by $U_1$ and $U_2$.) In the nodes near the sodium slugs, the mass influxes exceed the mass effluxes due to the expansion of the FCI zone. Consequently, in those nodes, the void fraction decreases and the mixture density increases, as is shown in Fig. IV-5.

Figure IV-3 shows that the pressure distribution in the FCI zone is rather uniform. This suggests that various one-node models\textsuperscript{9,17-20} would predict the pressure history reasonably well.

In the present calculations the fuel-particle velocities at the ends of the FCI zone were assumed to be equal to the liquid-sodium slug velocities as given in Eqs. (II.24) and (II.25). This boundary condition may not be correct physically, because there should exist a velocity slip between the sodium mixture and the fuel particles. It is, however, consistent within the framework of the present formulation in which the fuel particles are treated as a continuum. To check the assumption, calculations were made allowing for a slip between the fuel particles and the sodium mixture at the slug interface. The calculational results were found to be little affected by the slip condition.

The fuel and mixture temperatures are presented in Figs. IV-6 and IV-7, respectively. It is seen that even after 30 ms the fuel temperatures in most of the interior nodes remain constant at the fuel melting point, because of the heat of fusion. In most nodes, the mixture temperature corresponds to the saturation temperature of sodium at the node pressure.

Figure IV-8 shows the effect of the fuel-particle diameter on the pressure history in the center nodes of the FCI zone. In view of the dependence of the heat-transfer coefficient on the particle size as given by Eq. (II.16), the results are not surprising.

Figure IV-9 shows the distributions of the fuel-particle volume fraction at various times. As seen in the figure, the volume fractions are not zero in the boundary nodes next to the sodium slugs. This may be due, in part, to the boundary condition that the fuel-particle velocities at the slug interfaces are equal to the slug velocities. Furthermore, in the present analysis, a completely Eulerian differencing scheme is used. Therefore, the volume
Fig. IV-6. Fuel-temperature Distribution for Uniform Fragmentation ($d_p = 0.05 \text{ cm}$).

Fig. IV-7. Sodium-mixture Temperature Distributions for Uniform Fragmentation ($d_p = 0.05 \text{ cm}$).

Fig. IV-8. Dependence of Pressure History on the Fuel-particle Size for Uniform Fragmentation.

Fig. IV-9. Distributions for Fuel Volume Fraction for Uniform Fragmentation. ($d_p = 0.05 \text{ cm}$).
fraction in a node is an average value smeared over the node. Because of this so-called arbitrary diffusion, no nodes are empty of fuel particles. The arbitrary diffusion may be eliminated by using a marker-particle approach which explicitly keeps track of the fuel-particle front. However, the diffusion is believed to have insignificant effect upon the overall mass effluxes of the fuel and sodium, which are of interest in the present study.

The mass effluxes from the initial FCI zone (i.e., the fuel failure zone) are presented in Fig. IV-10. For the fuel-particle sizes studied, the mass efflux of fuel was found to exceed that of sodium at all times. This indicates that the reactivity losses due to fuel removal would more than offset the reactivity gains due to sodium voiding.

The expansion history of the FCI zone is shown in Fig. IV-11. It is seen that at 38 ms the FCI zone occupies almost the entire lower channel.

2. **Progressive Fragmentation**

Figure IV-12 presents the volume-fraction distributions of the fragmented fuel particles for the bottom-initiated progressive fragmentation. Note that the peak value of the volume fraction propagates upward
as the fragmentation propagates in the same direction. The volume-fraction distributions of the total fuel are shown in Fig. IV-13. As pointed out earlier, the unfragmented fuel mass was assumed to be stationary. Thus, as the fragmented fuel particles are being convected into the nodes containing unfragmented fuel, the total volume fraction of fuel can become larger than the initial value.

The void fractions of the sodium vapor and fission gas in the mixture are shown in Fig. IV-14. At 5 ms, only the fuel in the lower six nodes become fragmented, and the pressure increase occurs mostly in these nodes, as can be seen in Fig. IV-15. As the pressure waves propagate, the mixtures in the nodes just above the lower six nodes are compressed so that the void fractions there decrease rapidly, as is shown in Fig. IV-14. Moreover, with the convection of the fragmented fuel particles, the mixture temperatures in the nodes containing unfragmented fuel would rise, causing the liquid sodium to expand. This could make the sodium-vapor quality even negative. In this case, the sodium was considered to be in a single-phase liquid state. The high pressures in the upper nodes at 15 ms (see Fig. IV-15) occurred while the sodium was in a liquid state and lasted only for a very short time.

![Fig. IV-12. Distributions of Fragmented-fuel Volume Fractions for Bottom-initiated Progressive Fragmentation ($d_p = 0.05$ cm).](image1)

![Fig. IV-13. Distributions of Fuel Volume Fraction for Bottom-initiated Progressive Fragmentation ($d_p = 0.05$ cm).](image2)
Figures IV-16 to IV-19 present the results for the case in which the fuel fragmentation started from the top node. The results are similar to those given in Figs. IV-12 to IV-15 for the bottom-initiated fragmentation. In Fig. IV-19 it is seen that the pressure wave propagates downwards as the fragmentation proceeds.

Fig. IV-20 shows the mass effluxes of the sodium mixture and the fuel particles from the initial FCI zone for the progressive fragmentation. The results appear to be rather insensitive to the location of fragmentation initiation (top or bottom). It is seen that, unlike the case of uniform fragmentation, the mass efflux of the sodium mixture exceeds that of fuel for a short time between 15 and 30 ms.
Fig. IV-16. Volume-fraction Distributions for Top-initiated Progressive Fragmentation ($d_p = 0.05$ cm).

Fig. IV-17. Distributions of Fuel Volume Fraction for Top-initiated Progressive Fragmentation ($d_p = 0.05$ cm).

Fig. IV-18. Void-fraction Distributions of Sodium Vapor and Fission Gas for Top-initiated Progressive Fragmentation ($d_p = 0.05$ cm).
Fig. IV-19. Pressure Distributions for Top-Initiated Progressive Fragmentation ($d_p = 0.05 \, \text{cm}$).

$10^7 \text{ dynes/cm}^2 = 1 \text{ MPa}$.

Fig. IV-20. Mass Effluxes of Fuel and Sodium-mixture for Progressive Fragmentation ($d_p = 0.05 \, \text{cm}$).
V. SUMMARY

An analysis has been made of combined motion of fuel and coolant due to fuel-coolant interactions following a massive fuel failure along the fuel-pin length. This problem is of interest in assessing potential autocatalytic effects under high-ramp transient overpower conditions.

The combined motion of fuel and coolant is described using a two-fluid model formulation in which the mixture of sodium liquid and vapor and fission gas, on the one hand, and the fuel particles, on the other, are treated as two superimposed continua. The method of solution used is a numerical procedure called the ACE method, a modified version of the IMF technique. It employs a completely Eulerian mesh of finite-difference cells in which field variables, such as fuel volume fraction, pressure, and density, are cell-centered quantities, whereas velocities are calculated at the cell boundaries. Full donor-cell differencing is used wherever applicable. Furthermore, the space variable is normalized so that the number of nodes in the FCI zone remains constant at all times. The normalization eliminates uncertainties involved in assigning new field variables after the rezoning that is otherwise required for the Eulerian mesh with moving boundaries. A computer program which operates on a stand-alone mode has been developed, so the effects of various physical processes, such as mixing, fragmentation, and heat transfer, may be examined separately.

Illustrative calculations were made for a fuel rupture length of 60 cm in the FFTF geometry. Three different modes of fragmentation were considered. First, upon pin failure, motlen fuel is completely fragmented and uniformly distributed in the coolant (uniform fragmentation). Second, fragmentation is initiated at the bottom of the mixing zone and propagates upward (bottom-initiated progressive fragmentation). Third, fragmentation is initiated at the top of the mixing zone and propagates downward (top-initiated progressive fragmentation). The calculations seem to indicate that reactivity losses due to fuel dispersal are likely to offset reactivity gains due to sodium ejection, minimizing the potential for autocatalytic effects. However, it would be very difficult to make a conclusive argument until the physical processes that characterize the FCI zone including cladding failure, mixing, and heat transfer,
are better understood. This would require an experimental data base which is statistically meaningful.
APPENDIX

THERMODYNAMIC PROPERTIES OF SODIUM, FUEL, AND FISSION-PRODUCT GAS

PROPERTIES OF SODIUM

Density of liquid sodium:

For saturated liquid:

\[
\rho_{Na,l}^{(sat)} = 0.1818 + 0.75683 (1.0 - 3.659 \times 10^{-4} T)^{0.5885} [g/cm^3]
\]

For subcooled liquid:

\[
\rho_{Na,l} = \rho_{Na,l}^{(sat)} e^{-\beta_T (p - p_{sat})}
\]

Saturation pressure:

\[
p_{sat} = \exp(10.46861 - 12016.6/T_{Na}) [atm]
\]

Thermal-expansion coefficient of liquid sodium:

\[
\alpha_p = 0.21968 \times 10^{-3} + 0.81226 \times 10^{-7} T + 0.97135 \times 10^{-11} T^2
+ 0.68998 \times 10^{-15} T^3 [K^{-1}]
\]

Adiabatic compressibility of liquid sodium:

\[
\beta_s = 0.69651 \times 10^{-5} + 0.26741 \times 10^{-7} T - 0.14891 \times 10^{-10} T^2
+ 0.82082 \times 10^{-14} T^3 [atm^{-1}]
\]

Isothermal compressibility of liquid sodium:

\[
\beta_T = \beta_s + \frac{V_{T,Na} T^2}{C_{p,l} \rho} [atm^{-1}]
\]
where

\[ V_L = \text{specific volume of liquid sodium} \]

\[ C_{p,L} = \text{specific heat of liquid sodium at constant pressure} \]

Viscosity of liquid sodium:\(^{23}\)

\[ \mu_{Na,L} = 0.01 \exp(1.1762 + 508.07T^{-1}) \times T^{-0.4925} \text{(poise)} \]

Viscosity of sodium vapor:\(^{23}\)

\[ \mu_{Na,v} = 2.2075 \times 10^{-4} \text{(poise)} \]

Heat of vaporization of sodium:\(^{21}\)

\[ \Delta h_{L,v} = 4992 \times (1.0 - 3.659 \times 10^{-4}T)^{0.4262} \text{[J/g]} \]

Specific enthalpy of liquid sodium:\(^{21}\)

\[ h_{Na,L} = 3841.9 + 0.85563(T - 1644.3) - 0.5 \Delta h_{L,v} \text{[J/g]} \]

Specific enthalpy of sodium vapor:\(^{21}\)

\[ h_{Na,v} = 3841.9 + 0.85563(T - 1644.3) + 0.5 \Delta h_{L,v} \text{[J/g]} \]

Compressibility factor for sodium vapor:\(^{22}\)

\[ Z_c = -0.97258 + 0.42417 \times 10^{-2}T \]
\[ -0.28996 \times 10^{-5}T^2 + 0.55424 \times 10^{-9}T^3 \]

**PROPERTIES OF FUEL AND FISSION-PRODUCT GAS**

Thermal conductivity of \(\text{UO}_2\):

\[ k_p = 0.0242 \text{ [J/s - cm-K]} \]
Specific heat of UO$_2$:

$$C_{p,\text{fu}} = 0.548\ [\text{J/g-K}]$$

Heat of fusion of UO$_2$ = 310 [J/g]

Melting point of UO$_2$ = 3040 K

Fission-gas constant:

$$R_g = 6.25 \times 10^{-2}\ [\text{J/g-K}]$$

Viscosity of fission gas:

$$\mu_g = 0.0009\ \text{[poise]}$$
ACKNOWLEDGMENTS

The authors wish to thank H. K. Fauske, M. A. Grolmes, and M. Ishii for many helpful discussions. Sincere thanks are also due M. T. A. Moneim for his careful review of the manuscript.
REFERENCES


