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AN EQUATION OF STATE FORMULATION FOR HICKS-MENZIES FCI EFFICIENCIES

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ABSTRACT

Energetic fuel-coolant interactions may occur in a nuclear reactor in the event that molten fuel comes in contact with the reactor coolant water. Reliable mechanistic models of these interactions have yet to be developed and so relatively simple thermodynamic models have been proposed for estimating the conversion of thermal energy to mechanical work. The present paper outlines a generalized thermodynamic model for fuel-coolant interactions which accounts for variable thermodynamic properties as well as the effect of latent heat in the fuel. The variable property model is shown to provide an upper bound (most conservative) estimate of the conversion efficiency compared to other formulations appearing in the literature.

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INTRODUCTION

An energetic fuel-coolant interaction (FCI) may occur whenever a hot liquid is mixed with a relatively cold liquid in which the temperature of the hot liquid is well above the nucleate boiling temperature of the cold liquid. This event, more commonly known as a "vapor explosion", is of concern to reactor safety in the event of a core meltdown due to the possible mixing of the exposed molten core (fuel) with the coolant liquid (water) used to cool the reactor vessel. The rapid vaporization and expansion of the coolant is propagated throughout the mixture in a manner somewhat analogous to a chemical explosion, converting the available thermal energy of the fuel into mechanical work. The threat posed to the containment structure by this process depends directly upon the efficiency of the thermal to mechanical work conversion. It is therefore of particular interest to reactor safety engineers to have accurate estimates of upper bound conversion efficiency so that the potential risk to the containment may be properly assessed.

Methods for determining FCI conversion efficiency have been developed by many researchers over the last several years using both experimental as well as analytical techniques (1,2). Direct calculation of the conversion efficiency using analytical techniques is difficult at best due to the present lack of detailed mechanistic models for the mixing and expansion phases of the explosion. Uncertainties in the dynamics of fuel-coolant mixing, the heat transferred during mixing, and the explosion propagation mechanism all contribute to exacerbate the modelling problem.

An alternate method for estimating FCI conversion efficiency is to use relatively simple thermodynamic models to describe the mixing and expansion phases. Since work is a path-dependent quantity, the work produced depends on the thermodynamic processes chosen to connect the initial and final equilibrium states of the fuel-coolant mixture. These connecting processes are typically quite simple, invoking isochoric, isobaric, or isentropic assumptions as exemplified by the work of Hicks and Menzies (3). This model is significant in that the assumptions of no heat loss or irreversibilities in the system provide for an upper bound (conservative) estimate of the conversion efficiency. McFarlane has developed a computer code based on the Hicks-Menzies thermodynamic model (4). This formulation does not account for the evolution of heat from the fuel as it solidifies and assumes the fuel and coolant to have constant thermodynamic properties.

In the present investigation, a generalized Hicks-Menzies model is developed which allows for variable properties in both the fuel and coolant, while taking into account the latent heat of the fuel during the expansion process. The governing thermodynamic equilibrium equations are expressed in a form which allows for an arbitrary number of constituents in the fuel-coolant system. It will be shown that incorporating these generalizations into the Hicks-Menzies process yields significantly higher conversion ratios than those predicted by McFarlane. Results from this model are also compared to the Hicks-Menzies efficiencies and also with a recent thermodynamic model proposed by Hall (5) for lower-bound efficiencies.

OVERVIEW OF FCI THERMODYNAMIC MODELS

Thermodynamic models used to describe energetic fuel- coolant interactions are best compared by considering their fundamental processes on a P-V diagram. For the present investigation, the thermodynamic efficiencies calculated by two models are analyzed.

Hicks-Menzies Model

The Hicks-Menzies thermodynamic model consists of the following processes.

1. Adiabatic, isochoric mixing of the fuel and coolant.
2. Isentropic expansion to a specified final pressure.

These processes are illustrated on the P-V diagram shown in Figure 1. Assuming the various processes occur adiabatically with no irreversibilities insures that the calculated work is a maximum.

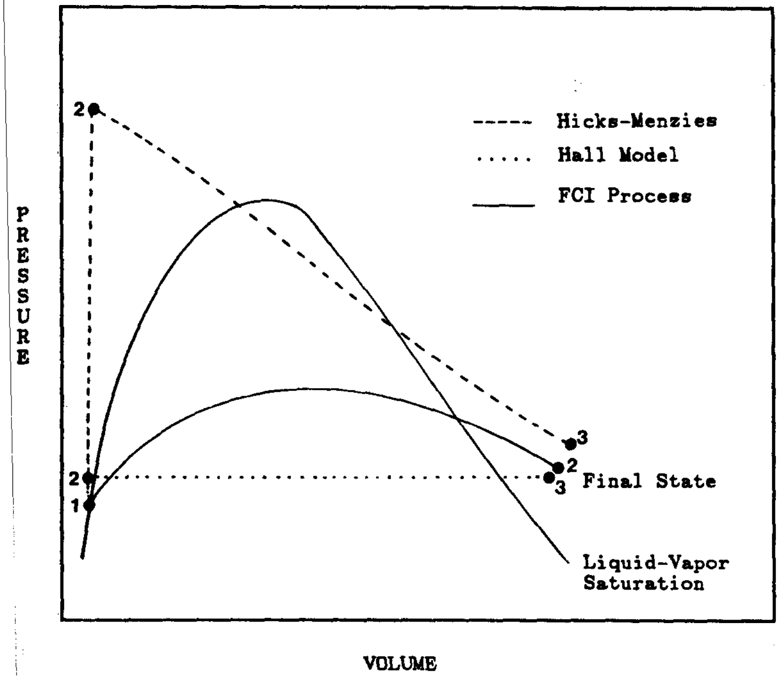

Figure 1. P-V Diagram Illustrating FCI Thermodynamic Processes

Hall Model

Because experimental evidence indicates that the Hicks-Menzies model can greatly over-estimate measured efficiencies, a lower limit (minimum work) model has been proposed by Hall (5). This model consists of the following processes shown in Figure 1.

1. Adiabatic, isochoric mixing to the final system pressure.
2. Adiabatic, isobaric expansion to a specified final volume.

The above model represents the simplest quasi-static, reversible processes that can be identified which link the initial and final states of the system.

GENERALIZED HICKS-MENZIES MODEL

Thermodynamic Relationships

The generalized Hicks-Menzies formulation assumes the fuel thermodynamic properties are functions of temperature only, while the coolant properties may be determined as a function of both temperature and pressure. Initially, the fuel and coolant are assumed to be separate with temperatures T_f and T_1, respectively. Upon mixing, the fuel-coolant system attains an equilibrium temperature, T_2 at some system pressure P_2. For equilibrium of the system with no external work or heat transfer between the system and its surroundings, the first law of thermodynamics for the mixing process may be written as,

$$\sum_{i=1}^{k} m_{p,i}\, u_{p,i}(T_2) + m_c u_c(T_2,P_2)$$

$$= \sum_{i=1}^{k} m_{p,i}\, u_{p,i}(T_f) + m_c u_c(T_1,P_1) \qquad (1)$$

where $m_{p,i}$ denotes the mass fraction for the i^{th} constituent of the fuel. The specific internal energy for each fuel component is denoted by $u_{p,i}$. Coolant properties are identified by the subscript 'c'.

The isentropic expansion from state 2 may be specified by one of two alternate methods. In the first approach, it is assumed that a vapor blanket exists between the fuel droplets and the coolant which thermally isolates the two components in the system. Under these conditions the expansion to the final state is determined solely by the coolant entropy at state 2 and the pressure or temperature of the final state which is presumed to be known. In the second type of expansion process, it is assumed that the fuel and coolant are expanded as a system to a final end state determined by the total system entropy at state 2. This enables additional heat to be transferred between the fuel and coolant during the expansion. For expansion with no vapor blanketing entropy conservation for the system gives,

$$\sum_{i=1}^{k} m_{p,i}\, s_{p,i}(T_3) + m_c s_c(T_3,P_3)$$

$$= \sum_{i=1}^{k} m_{p,i}\, s_{p,i}(T_2) + m_c s_c(T_2,P_2) \qquad (2)$$

Here the quantity $s_{p,i}$ represents the specific entropy for the i^{th} component of the fuel. In each expansion method, consideration must be given to the fact that the coolant quality at the final state may be less that unity (saturated) or greater than unity (superheated).

The work done during the expansion process is given by the first law of thermodynamics for the fuel-coolant system,

$$W_{2-3} = m_f(u_2 - u_3)_f + m_c(u_2 - u_3)_c \qquad (3)$$

where the subscript 'f' implies fuel quantities. For expansion of the system under vapor blanketing conditions, only the latter work term is considered. The efficiency of the thermal conversion process is determined by the ratio of the expansion work to the available thermal energy in the fuel as calculated by the heat of reaction for the fuel Δh_r. This gives the efficiency for the process as,

$$\eta = \frac{W_{2-3}}{m_f\ \Delta h_r} \qquad (4)$$

Solution Procedure

From the generalized formulation a computer code has been developed called HMEOS (Hicks-Menzies Equation of State) for the purpose of calculating FCI conversion efficiencies. Solutions for the energy and entropy conservation equations are obtained using a nonlinear equation solver. In general the functional form for the fuel properties u and s are not known explicitly and must be provided in tabular form as a function of temperature. Thermodynamic properties for the fuel components are obtained from the JANAF tables in the present work (6). Coolant thermodynamic properties are provided by an extended form of the steam tables based on a Helmholtz function for the equation of state (7).

DISCUSSION OF RESULTS

Iron-Alumina Thermite Calculation

To demonstrate the solution capability of the HMEOS code, a series of calculations have been carried out for an Iron-Alumina thermite fuel. Thermite is used extensively in the experimental simulation of Corium melts because it is a safe, inexpensive material which is relatively easy to produce. In the thermite reaction, Iron-Oxide and Aluminum combine to form Iron and Alumina. Stoichiometric proportions of the two component system have been assumed for the present analysis. This yields a calculated heat of reaction of 3979.4 kJ/kg for which the corresponding adiabatic reaction temperature is 3100 K. From stoichiometry, the following mass fractions for each of the thermite reactants and products may be derived,

Reactants	Mass Fractions	Products	Mass Fractions
Iron-Oxide	0.747	Iron	0.523
Aluminum	0.253	Alumina	0.477

The coolant for the present study was taken to be water with an initial temperature and pressure of 298.15 K and 0.1 MPa, respectively. The corresponding coolant specific volume was 0.001 m^3/kg. In all case studies, the expansion process was allowed to proceed until a specified end pressure of 0.143 MPa was achieved.

Figure 2 presents a comparison of the calculated equilibrium mixture temperature at state 2 as a function of the coolant to fuel volume ratio. The small discontinuities in the slope of the temperature curve calculated by the HMEOS code reflect the evolution of latent heat from the thermite. The agreement between the two solution trends are quite good, with the HMEOS code predicting significantly higher equilibrium temperatures than the McFarlane code for volume ratios less than 8.

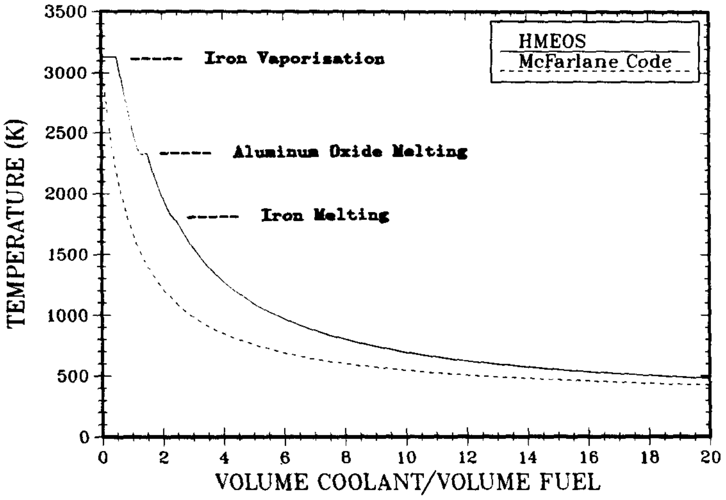

Figure 2. Comparison of Equilibrium Mixing Temperatures for Stoichiometric Iron-Alumina Thermite

The thermal to mechanical conversion efficiencies for the coolant expansion phase (vapor blanketed fuel) are shown in Figure 3 for the previously described models. The HMEOS code predicts an increase in peak conversion efficiency approximately 30 % greater than the corresponding solutions obtained with the McFarlane code. Generally both codes predict a volume ratio of 2 for peak efficiency of the interaction. As the volume ratio decreases below this value, there is a decreasing amount of steam produced and therefore less expansion work is done by the system. For higher volume ratios, the addition of coolant mass reduces the efficiency due to the heating of residual coolant which remains in liquid form following the expansion. It is interesting to note the jumps in conversion efficiency which occur in the HMEOS vapor blanketed calculation at volume ratios of 1.25 and 2.25. Here the state 2 mixture temperature passes through 2300 K and 1800 K which correspond to the solidification temperatures of Aluminum-Oxide and Iron, respectively.

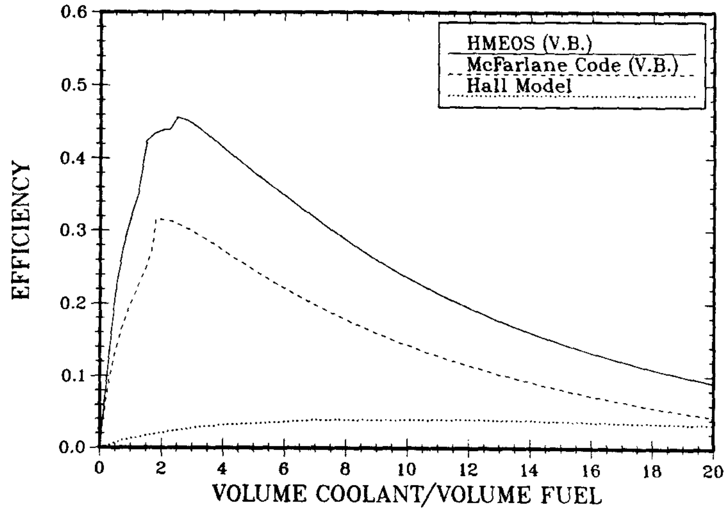

Figure 3. Effect of Vapor Blanketing During Expansion for Various Thermodynamic Models

The increase in thermal efficiency at each volume ratio is a result of having more energy transfer to the coolant as the thermite constituents give up their latent heat. Results from Hall's model for a lower bound estimate yield conversion efficiencies which are approximately an order of magnitude lower than the Hicks-Menzies efficiencies.

Corium Calculation

To investigate the effects of variable properties for realistic reactor fuels, a series of calculations were performed with the HMEOS code and the McFarlane code using Corium as the active metal. The Corium fuel was taken to consist of five component metals with the following mass fractions,

Component	Mass Fraction
Uranium Dioxide	0.540
Zircalloy	0.160
Iron	0.255
Chromium	0.030
Nickel	0.015

Mass weighted average values of the thermodynamic properties for the Corium components were used to describe the fuel in the McFarlane calculation.

Figure 4a shows a comparison of the resulting efficiencies as a function of coolant to fuel volume ratio for an initial Corium temperature of 3000 K. The predicted efficiency trends for both the blanketed (V.B.) and non-blanketed (N.V.B.) expansions appear very similar to the thermite results.

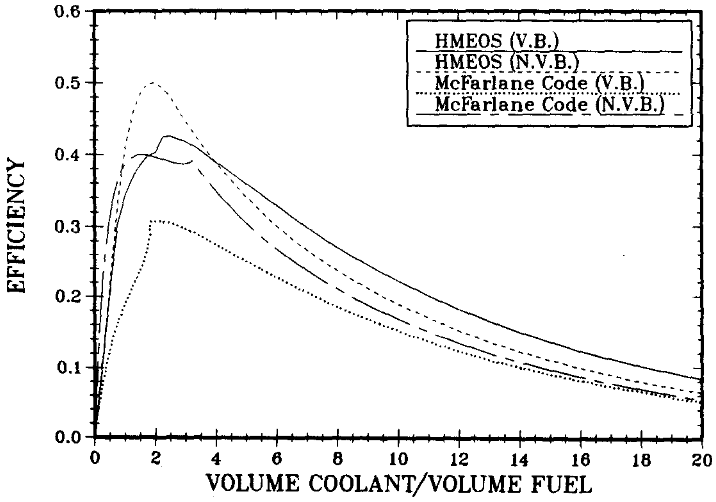

Figure 4a. Comparison of Hicks-Menzies Efficiencies for Molten Corium; T = 3000 K

Figure 4b shows the predicted conversion efficiencies for a Corium temperature of 2000 K. It is interesting to notice the effect of decreased temperature on the non-blanketed results. As the temperature decreases the HMEOS solution shows relatively good agreement with the McFarlane code near the point of peak efficiency. At higher volume ratios, the McFarlane efficiencies are somewhat larger than those predicted by the variable property model. The reason for the discrepancy with the McFarlane solutions may be found by examining McFarlane's equation for the work contribution by the fuel. This is given as,

$$W_f = (mc)_f \; (T_2 - T_3) \qquad (5)$$

where c corresponds to the specific heat of the fuel taken at either constant pressure or volume (4). To be consistent with the first law of thermodynamics for a closed system, the HMEOS code calculates the work contributed by the fuel as,

$$W_f = \Delta U_f = (H_2 - H_3)_f - (P_2V - P_3V)_f \qquad (6)$$

Since $T_2 > T_3$ it follows that $(H_2 - H_3) > 0$. This term in general corresponds to the work calculated by Equation 5. The term $-(P_2 V - P_3 V)$, is less than zero since $P_2 >> P_3$. Considering the negative PV term, the work contribution by the fuel calculated by HMEOS is smaller than that given by the McFarlane code when the PV term is dominant. The addition of the fuel to the system reduces the expansion work because of the greater thermal energy needed to expand the added mass.

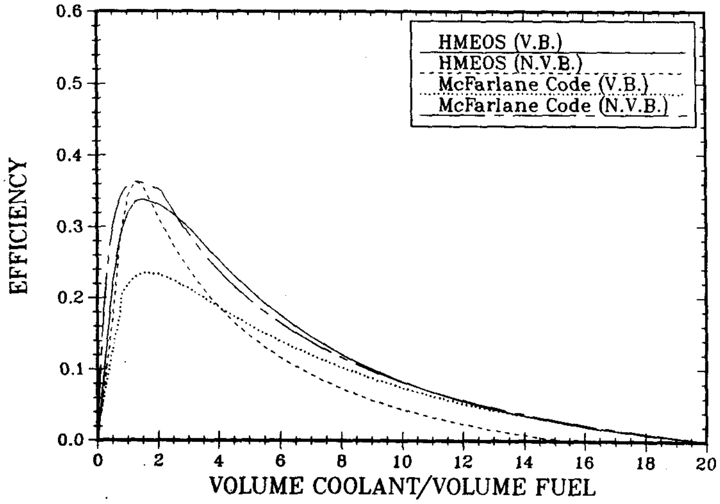

Figure 4b. Comparison of Hicks-Menzies Efficiencies for Molten Corium; T = 2000 K

CONCLUSIONS

A generalized computer code has been developed for the prediction of FCI conversion efficiency based on the thermodynamic model first proposed by Hicks and Menzies. Because of the assumptions inherent in the Hicks-Mezies process, the computed work represents the theoretical maximum which can be produced during the course of an FCI. In the sample cases presented the equation of state formulation predicts an increase in peak conversion efficiency as much as 30 % over the constant property formulation. Overall the efficiencies at lower initial fuel temperatures are closer in agreement as the effects of latent heat and variable properties are reduced. It should be emphasized that achieving the peak efficiencies predicted by this model is unlikely due to violation of the constant volume mixing assumption. Additional experimental and numerical studies are necessary in order to better understand the mixing process so that the amount of fuel and coolant which actually participates in the interaction may be determined. This will enable the thermodynamic paths of actual fuel-coolant interactions to be refined so that reliable estimates of conversion efficiency can be made.

ACKNOWLEDGEMENTS

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