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Improvement and Verification of
Fast Reactor Safety Analysis Techniques

Progress Report

MASTER

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ABSTRACT

This report details a mathematical model for the dissipation of heat from an internally heated liquid pool which is contained in a hollow cylinder of finite inside and outside diameter. The model includes a temperature profile for the previously described cylinder, empirical correlations for Nusselt numbers at the walls of the container and a film theory correction of the heat transfer coefficients for mass transfer.

Also included in this report is a description of the experimental work conducted as a preliminary step to verification or rejection of the proposed mathematical model. This experimental work consisted of reacting Dimethyl Sulfoxide (DMSO) with Acetyl Chloride (AC), using Acetone as a solvent, in a hollow wax cylinder and observing the geometry and dimensions of the melt.

INTRODUCTION

The purpose for the development of this model is to provide a mathematical description of the geometry of the melt in a liquid metal fast breeder reactor (LMFBR) in the event of a hypothetical core disruptive accident (HCDA). As the heat transfer from an internally heated liquid pool to the walls of the vessel in which it is contained is considered, two cases must be evaluated. The first case involves heat transfer to the side walls or sideward heat transfer. In sideward heat transfer the bulk motion of the pool is parallel to the sidewall. The second case involves heat transfer to the floor of the vessel or downward heat transfer.

Since the amount of the container melted would be a function of the amount of heat transferred, it was deemed appropriate to use this phenomenon as a measure of how accurate the predictions of the mathematical model would be. This experimental method of verification was felt to be particularly appropriate in light of the intended application in nuclear reactors.

MATHEMATICAL MODEL

The heat balance for an internally heated liquid pool contained in a vessel may be expressed as

$$Q_T = Q_V + Q_M + Q_1 + Q_W + Q_Z \quad (1)$$

where

Q_T = Total heat generated in pool per unit time.
 Q_V = Heat lost as latent heat of vaporization per unit time.
 Q_M = Heat lost as latent heat of melting per unit time.
 Q_1 = Heat lost as sensible heat to the liquid per unit time.
 Q_W = Heat lost as sensible heat to the wall per unit time.
 Q_Z = Viscous terms.

$$Q_V = \lambda_V \rho_l \left[\frac{dV_l}{dt} - \beta \frac{dV_w}{dt} \right] \quad (2)$$

where

λ_V = Heat of vaporization of the liquid
 ρ_l = Density of the liquid
 V_l = Volume of liquid
 V_w = Volume of wall
 t = Time
 β = Expansion factor ($\rho_{\text{melted wall}} / \rho_{\text{solid wall}}$)

$$Q_M = \lambda_m \rho_w \frac{dV_w}{dt} \quad (3)$$

where

λ_m = Latent heat of melting of wall
 ρ_w = Density of solid wall

$$Q_1 = \rho_w \hat{c}_{pw} (T_b - T_M) \frac{dV_w}{dt} \quad (4)$$

where

$\hat{c}_{pw}$ = Heat capacity of liquid wall per unit mass
 T_b = Boiling temperature of liquid
 T_M = Melting temperature of wall.

Using Fourier's law and written for cylindrical geometry

$$Q_W = -Ak_w \left. \frac{dT}{dr} \right|_{r=R} \quad (5)$$

where

T_W = Wall temperature
 R = Radius of interface
 k_W = Thermal conductivity of solid wall
 A = Area for heat transfer

The sensible heat required to raise the boundary wall temperature from the initial temperature T_0 to the melting temperature T_m and the initial reaction mixture from the initial temperature T_0 to the boiling temperature, T_B , have been neglected as negligible. The viscous terms have been neglected based on the work of Wheeler (1978) with the same Dimethyl Sulfoxide (DMSO) and Acetyl Chloride (AC) system. Heat transferred from the surface of the mixture to the atmosphere is assumed to be by convection from the vapors generated in the pool. Heat lost by this mechanism is accounted for in the Q_V term.

The amount of heat transferred to the wall, $Q_{W,T}$ may be written as

$$Q_{W,T} = Ah(T_l - T_W) \quad (6)$$

where

A = Area for heat transfer
 h = Heat transfer coefficient
 T_l = Bulk temperature of the liquid
 $Q_{W,T}$ = Total heat transferred to the wall. (Energy/time)

For the case of heat transfer to the sidewalls, (sideward heat transfer) several correlations have been proposed for calculating a Nusselt number and hence a heat transfer coefficient.

The first case to be considered is that of the non boiling internally heated liquid pool. The predominant mechanism is natural convection. It was proposed by L. Baker et al. (1974) that the correlations for heat transfer from a vertical plate to a fluid could be used with the modification that the heat transfer coefficient obtained would be corrected to take into account that the heat was being transferred

from an internally heated fluid to a plate.

The uncorrected equation for the Nusselt number as used by L. Baker et al. (1975) is

$$Nu_o = \frac{(4/3)(0.508)Pr^{1/2}Gr^{1/4}}{(0.952 + Pr)^{1/4}} \quad (7)$$

where

$$Nu_o = \frac{h_o L}{k} \quad \text{uncorrected Nusselt number}$$

$$Pr = \frac{C_p \mu}{k} \quad \text{Prandtl number}$$

$$Gr = \frac{g \beta \Delta T L^3 \rho^2}{\mu^2} \quad \text{Grashof number}$$

L = Pool height

h_o = Uncorrected heat transfer coefficient

β = Thermal coefficient of volumetric expansion

g = Gravitational constant

μ = Viscosity

Equation 7 works well for values of $GrPr < 10^9$. At greater values the flow becomes turbulent and the correlation breaks down. It is reported by W.H. McAdams (1954) that for the range $10^4 < GrPr < 10^9$ the correlation is described well by the equation

$$Nu_o = 0.59 (GrPr)^{1/4} \quad (8)$$

The corrected heat transfer coefficient is obtained as follows:

$$\frac{h}{h_o} = \frac{3.88}{3.88 - 12.91\phi + 46.5\phi^2} \quad (9)$$

where

h = Heat transfer coefficient for internal heat generation

h_o = Heat transfer coefficient without internal heat generation

$$\phi = \frac{qL^{1/2}}{(g\beta)^{1/2} \Delta T^{3/2} (\rho C_p)} \quad (10)$$

q = Volumetric heat generation Energy/(Time)(Volume)

The correction h/h_0 was found to be ~ 0.03 when $\phi < 0.01$.

The second case of sideward heat transfer to be treated is that of the boiling internally heated pool. Baker et al. (1975) calculated that as bubbles rise in the boiling pool the fluid motion in the center is in the direction of the rising bubbles. At the walls, however, the fluid motion is downward. At the bottom of the pool the motion of the fluid is from the sidewalls toward the center with the converse being true at the top of the pool.

At low boiling rates the flow near the wall may be assumed to be laminar and correlations for tangential flow past a flat plate may be used. In the laminar region the following theoretically derived expression may be used as described by Bird, Stewart and Lightfoot (1960)

$$Nu_x = 0.332 Re_x^{1/2} Pr^{1/3} \quad (11)$$

where

$$Nu_x = \frac{h_x l}{k} = \text{localized Nusselt number}$$

h_x = Localized heat transfer coefficient
 x = Position

$$Re_x = \frac{V_\infty \rho_f l}{\mu_f} = \text{Localized Reynolds number}$$

V_∞ = Approach or bulk velocity

ρ_f = Density at film conditions

μ_f = Viscosity at film conditions

$$Pr = \left(\frac{C_p}{\mu k} \right)_f = \text{Prandtl number (evaluated at film conditions)}$$

An average Nusselt number may be also obtained from Bird, Stewart and Lightfoot (1960) as

$$Nu = 0.664 \left(\frac{L V_\infty \rho_f}{\mu_f} \right) Pr^{1/3}$$

where

L = Length of plate

Both equations 11 and 12 are accurate to within 2% for $Pr > 0.6$. The correlations become inaccurate at lower Pr numbers.

Based on the work of Fair, Lambright and Anderson (1962), Baker et al. (1975) suggested that V_{∞} would be proportional to the superficial vapor velocity U_V . On this basis V_{∞} in equations 11 and 12 may be replaced by U_V and a proportionality constant c . Equation 12 becomes

$$Nu = c \left(\frac{L U_V \rho_f}{\mu_f} \right)^{1/2} Pr^{1/3} = c Re^{1/2} Pr^{1/3} \quad (13)$$

where c = proportionality constant.

As the bubbling rate increases the flow near the wall becomes more turbulent. This process may be thought of as turbulent diffusion of packets of fluid from the pool interior to the side wall.

For an average packet residence time at the wall of θ , Baker et al. (1975) describe the heat transfer coefficient as

$$h = \frac{\sqrt{4 C_p \rho k}}{\pi \theta} \quad (14)$$

where θ = mean packet residence time at the wall.

In order to estimate θ several assumptions are made:

1) Bubble size is independent of boiling rate. Since the distribution of bubble diameters is in a narrow range the bubble rise velocity or terminal velocity will be essentially the same. On this basis, increasing the vaporization rate will increase the frequency of bubble formation.

$$f = c' \left(\frac{W}{AL} \right) = c' \left(\frac{U_V}{L} \right) \quad (15)$$

where

f = Frequency of bubble formation
 c' = Constant
 W = Volumetric vapor generation rate

A = Base area of pool
 L = Height of pool
 U_V = Superficial vapor velocity

2) The frequency of local bubble disturbance of the fluid at the wall is proportional to the frequency of bubble formation. On the basis of assumption 1, the disturbance of each bubble and the length of time of each disturbance would be the same. This results in a residence time at the wall of a packet of fluid between bubble disturbances of

$$\theta = \frac{c''}{f} = c''' \frac{L}{U_V} \quad (16)$$

where c'' and c''' = constants.

Substituting equation 16 into equation 14 the heat transfer coefficient in terms of the superficial vapor velocity becomes

$$h = c^{IV} \sqrt{\frac{C_p \rho k U_V}{L}} \quad (17)$$

where c^{IV} = a constant.

Equation 17 may be arranged in terms of a Nusselt number as

$$Nu = \frac{hL}{k} = c^{IV} [Re]^{1/2} [Pr]^{1/2} \quad (18)$$

where $Re = \frac{LU_V \rho}{\mu}$

It may be noted that in the laminar flow model the Prandtl number is raised to the 1/3 power, where in the turbulent flow model it is raised to the 1/2 power.

Baker et al. (1975) found using a boiling pool of $Zn SO_4 \cdot H_2O$ with resistive internal heat generation that the constants c and c^{IV} for use in equations 13 and 18 respectively to be

$$c = 1.76 \pm 0.101 = 1.76 (1 \pm 0.0572)$$

$$c^{IV} = 2.131 \pm 0.121 = 2.131 (1 \pm 0.0568)$$

For the case of laminar flow equation 13 becomes

$$Nu = 1.76 (1 \pm 0.0572) Re^{1/2} Pr^{1/3} \quad (19)$$

For the case of turbulent penetration equation 18 becomes

$$Nu = 2.131 (1 \pm 0.0568)(Re)^{1/2}(Pr)^{1/2} \quad (20)$$

Baker et al. (1975) further generalized the correlation for sideward heat transfer by introducing a velocity term referred to as a thermal convection reference velocity.

$$V_{TC} = (g\beta\Delta TL)^{1/2} = \left[\frac{g(\rho_w - \rho_p)}{\rho_{AV}} L \right]^{1/2} \quad (21)$$

where

$$\begin{aligned} V_{TC} &= \text{Thermal convection velocity} \\ \rho_w &= \text{Fluid density at the wall} \\ \rho_p &= \text{Bulk fluid density} \\ \rho_{AV} &= \text{Average fluid density} \end{aligned}$$

Using the thermal convection velocity the Nusselt number may be expressed as

$$Nu = 2.131 \left(\frac{LV\rho_{AV}}{\mu} \right)^{1/2} Pr^{1/3} \quad (22)$$

where

$$V = U_V \text{ (superficial vapor velocity) for boiling pools}$$

$$V = 0.078 V_{TC} \text{ for non boiling pools.}$$

The prediction of downward heat transfer must also be considered in terms of a boiling and non boiling case.

Based on the work of Kulachi and Goldstein (1972), and Jahn and Reineke (1974), Baker et al. (1975) suggest that the predominant heat transfer mechanism for the non boiling case is conduction.

As a preliminary step to characterizing the upward and downward heat transfer, thermal layers may be considered to exist with upper and lower horizontal thermal boundaries of a uniform temperature. ($T_1 = T_0$ where T_1 = upper thermal boundary temperature, T_0 = lower thermal boundary temperature.) The thermal layer may then be divided at the

plane of maximum horizontally averaged temperature, $\hat{T}$, into an upper and lower sublayer. All of the heat generated in the lower sublayer is then assumed to transfer down and all the heat generated in the upper sublayer is assumed to transfer upward. Based on this model Kulachi and Goldstein defined an internal Rayleigh number and two Nusselt numbers as

$$Ra_{KG} = \frac{g\beta qL^5}{64\alpha\nu k} \quad (23)$$

$$Nu_1 = \frac{Q_1 L}{(\hat{T} - T_1)k} \quad (24)$$

$$Nu_0 = \frac{Q_0 L}{(\hat{T} - T_0)k} \quad (25)$$

where

- Ra_{KG} = External Rayleigh number.
- L = Thermal diffusivity
- ν = Kinematic viscosity
- Q_1 = Upward heat flux
- Q_0 = Downward heat flux
- $\hat{T}$ = Maximum horizontally averaged layer temperature
- T_1 = Upper boundary temperature
- T_0 = Lower boundary temperature
- Nu_1 = Upper sublayer Nusselt number
- Nu_0 = Lower sublayer Nusselt number

To extend the applicability of the work of Kulachi and Goldstein (1972) to systems where the boundary temperatures were not equal Baker et al. (1975) introduced an external Rayleigh number and the fraction of heat generated which is transferred downward, η .

$$Ra_E = \frac{g\beta L^3}{\alpha\nu} (T_1 - T_0) \quad (26)$$

where Ra_E = External Rayleigh number.

Dividing Ra_E by Ra_{KG} produces

$$\frac{Ra_E}{Ra_{KG}} = \frac{64 k (T_1 - T_0)}{qL^2} \quad (27)$$

Assuming uniform heat production, η may be written as

$$\eta = \frac{L_0}{L} \quad (28)$$

where

η = Fraction of heat transferred downward
 L_0 = Lower sublayer height
 L = Total layer height

Written in terms of η the sublayer Nusselt numbers become

$$Nu_1 = \frac{0.403 Ra_{KG}^{0.226} [32(1-\eta)^5]^{0.226}}{(1-\eta)} \quad (29)$$

$$Nu_0 = \frac{2}{\eta} \quad (30)$$

η may be found numerically from

$$\frac{(1-\eta)^{0.870}}{32 \eta^2 - Ra_E / Ra_{KG}} = 0.138 Ra_{KG}^{0.226} \quad (31)$$

From equation 26 it can be seen that Ra_E may be negative, positive or zero.

Negative values of Ra_E correspond to the lower boundary temperature being greater than the upper boundary temperature. The limit of this case is when all of the heat generated is transferred upward and $\eta \rightarrow 0$. This limit occurs at

$$Ra_E \geq 72.6 Ra_{KG}^{0.774} \quad (32)$$

For the converse where the upper boundary temperature is greater than the lower boundary temperature the limit of applicability of equation 31 occurs when the stability limit of the upper sublayer is reached. This condition exists when the Nusselt number defined in terms of the actual sublayer height, Nu_1' , is equal to two.

$$Nu_1' = \frac{q L_1}{(\hat{T} - T_1)k} \quad (33)$$

where

Nu_1' = Nusselt number for upper sublayer
defined in terms of actual sublayer height
 L_1 = Upper sublayer height

Based on the work of Kulacki and Emara (1975) and modified by Baker et al. (1975)

$$Nu_1' = 0.403 [32 Ra_{KG} (\frac{Nu_1}{Nu_1 + Nu_0})^5]^{0.226} \quad (34)$$

When $Nu_1' \geq 2$ the heat transfer mechanism throughout the layer is that of conduction. When this occurs the sublayer Nusselt numbers become

$$Nu_1 = \frac{2}{1-\eta} \quad (35)$$

$$Nu_0 = \frac{2}{\eta} \quad (36)$$

When $Nu_1' \geq 2$ equation 37 is employed in the calculation of η rather than equation 31.

$$\eta = 0.5 + \frac{Ra_E}{64 Ra_{KG}} \quad (37)$$

The boundary between the total conduction regime and the conduction-convection regime is calculated by substituting equation 37 into equation 31 to obtain

$$\eta = 1 - 2.064 Ra_{KG}^{-0.200} \quad (38)$$

which defines the boundary between the regimes.

Since η is bounded between 0 and 1 an additional limit exists as $\eta \rightarrow 1$. At this limit all the heat generated is transferred downward.

For the case of boiling downward heat transfer Baker et al. (1975) found the ratio of the sideward heat flux to the downward heat flux to vary as a function of the boiling heat flux. As the boiling flux increased the ratio of the sideward heat flux approached a fairly constant value of 3.8. This finding indicates that as the boiling rate is increased the disturbance created by the vapor bubbles

predominates. This results in a uniform effect on both the sideward and downward heat transfer.

Baker et al. (1975) also compared the downward heat transfer from a boiling pool to that predicted by the conduction model alone. They found that at the lower values of the boiling heat flux that the downward heat flux was less than that predicted from conduction along. At larger values of the boiling heat flux they found that the ratio of downward heat transfer to that predicted by conduction only levels out in a range of 2 to 4.

All of the correlations previously described were derived in the absence of mass transfer. To correct for the presence of mass transfer the heat transfer coefficients are corrected using a film theory convection factor as outlined by Bird, Stewart and Lightfoot (1960).

$$h_{cor} = h \frac{\phi_T}{R_T} \quad (39)$$

where h_{cor} = heat transfer coefficient corrected for mass transfer.

$$\phi_T = \frac{N_{ao} \tilde{C}_{pa} + N_{bo} \tilde{C}_{pb}}{h_{Loc}} \quad (40)$$

where

N_{ao} = Molar flux of component a at the interface

N_{bo} = Molar flux of component b at the interface

$\tilde{C}_{pa}$ = Molar heat capacity of component a

$\tilde{C}_{pb}$ = Molar heat capacity of component b

$$R_T = \exp(\phi_T) - 1 \quad (41)$$

In the film theory correction it is assumed that beyond the boundary thickness that the temperature is uniform. The thickness of the thermal boundary is calculated as

$$\delta_T = \frac{k}{h_{Loc}} \quad (42)$$

where δ_T = thermal boundary thickness.

The heat transferred to the wall is absorbed as latent heat as the wall is melted or is dissipated as sensible heat

$$Q_{W,T} = Q_M + Q_W \quad (43)$$

where

$$\begin{aligned} Q_{W,T} &= \text{Heat flux to the wall} \\ Q_M &= \text{Heat absorbed in melting wall} \\ Q_W &= \text{Heat dissipated in wall} \end{aligned}$$

Assuming Fourier's law to be valid

$$Q_W = -Ak \left. \frac{dT}{dr} \right|_{r=R} \quad (44)$$

For evaluation of the derivative the temperature profile for a non moving boundary is assumed. On this basis the equation of energy takes the form in cylindrical coordinates

$$\frac{\partial T}{\partial t} - \frac{\alpha}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) = 0 \quad (45)$$

The following dimensionless parameters are defined as:

$$\tau = \frac{\alpha t}{R^2} \quad \text{dimensionless time}$$

where R = initial phase boundary

$$\theta = \frac{T - T_2}{T_m - T_2} \quad \text{dimensionless temperature}$$

where T_2 = temperature at outside boundary.

$$\xi = \frac{r}{R} \quad \text{dimensionless radius.}$$

In dedimensionalized form equation 45 becomes

$$\frac{\partial \theta}{\partial \tau} - \frac{1}{\xi} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial \theta}{\partial \xi} \right) = 0 \quad (46)$$

To solve equation 46 assume θ to a product of two functions.

$$\theta = T Z \quad (47)$$

where

$$\begin{aligned} T &= f(\xi) \\ Z &= f(\tau) \end{aligned}$$

By substituting equation 47 into equation 46, equation 46 can be put in the form

$$\frac{1}{Z} \frac{dZ}{d\tau} = \frac{1}{\xi T} \frac{\partial}{\partial \xi} \left(\xi \frac{\partial T}{\partial \xi} \right) = 0, -\lambda^2, \delta^2 \quad (48)$$

where 0 represents the steady state solution and $-\lambda^2$ and δ^2 represent eigenvalues for the transient solution. The δ^2 solution produces an unrealistic solution and is therefore neglected. The T dependent portion of equation 48 becomes

$$(\lambda \xi)^2 \frac{d^2 T}{d(\lambda \xi)^2} + \lambda \xi \frac{dT}{d(\lambda \xi)} + [(\lambda \xi)^2 - 0]T = 0 \quad (49)$$

Equation 49 is a Bessel's differential equation of order zero. The solution for T is

$$T = C_1 J_0(\lambda \xi) + C_2 Y_0(\lambda \xi)$$

where C_1 and C_2 are constants.

The Z dependent portion of equation 48 is solved as

$$Z = C_3 e^{-\lambda^2 \tau}$$

where C_3 = a constant of integration. The steady state solution of equation 48 is

$$\theta = C_4 \ln(C_5 \xi)$$

where C_4 and C_5 are constants. Combining the steady state and the transient solution

$$\theta = C_4 \ln(C_5 \xi) + C_6 e^{-\lambda^2 \tau} [J_0(\lambda \xi) + C_7 Y_0(\lambda \xi)] \quad (50)$$

λ , C_4 , C_5 , C_6 , and C_7 are evaluated using the initial conditions and the boundary conditions of the particular problem.

EXPERIMENTAL

Equimolar amounts of a dimethyl sulfoxide (DMSO) solution

and an acetyl chloride (AC) solution were reacted in a wax cylinder. The solvent used was acetone. The wax used to construct the cylinder was Sun 3420 a product of the Sun Petroleum Products Company. The cylinder consisted of an outside diameter of approximately 4.8 cm, an inside diameter of 2.46 cm. and a height of between 19 cm and 25 cm depending on the concentration of the reactant used.

It was desired to observe the effect of the sideward heat transfer in the absence of any mass transfer effects which may be caused as a result of downward heat transfer. To accomplish this a glass plate was fused to the cylinder at a right angle to the axis of the cylinder (see fig. 1). This effectively formed a floor to the system from which no mass would be introduced into the system.

10 mls of the AC solution was placed into the cylinder. The DMSO solution was then injected into the AC solution by means of a syringe and mechanical syringe pump. 12, 8 and 4 molar solutions were used in this experiment.

Two procedures were followed at the conclusion of the boiling brought on by reaction. In procedure A the reactants were allowed to cool. After cooling (greater than 1 hour) the cylinder was bisected along the axis. Measurements of the geometry of the melt were taken. In procedure B the reaction mixture was removed from the cylinder immediately after boiling ceased. The cylinder was then allowed to cool and bisected. Measurements of the melt were then taken.

The purpose for employing the two procedures was to determine the extent of the melt which occurred after the void had collapsed and a non boiling pool existed. The results of this experiment may be seen in Figures 2 through 10.

From the data presented graphically in Figure 7, the average melted volume for the 12 M solution in which the mixture was allowed to cool in the wax reaction vessel was 21.2 cc. The average melted volume for the 12 M solution from the which the reaction mixture was removed immediately after the void collapsed was 19.4 cc. This results in a 9% melted volume increase when the reaction mixture remains in the vessel and is allowed to cool.

From the data presented in Figure 8 the average melted volume for the 8 M solution which was allowed to cool in the vessel was 11.6 cc while the average melted volume for the 8 M solution which was immediately removed after the void had collapsed was 6.9 cc. This represents a 68% melted volume increase when allowed to remain in the vessel.

The large discrepancy between the 12 M and 8 M solutions in the increased melt volume for the two procedures is due to the difference in the heat generation rate. It appears that in the 12 M solution the reaction has gone nearly to completion prior to the collapse of the void. In the 8 M case the reaction continues for a significant length of time after the void collapse but without sufficient intensity to generate a void.

It may be observed in Figures 7 through 10 that in each case a shoulder exists in the melt profile at a height of approximately 2.5 cm. From motion pictures taken earlier of the reaction transpiring in a glass vessel it was observed that two distinct regimes existed. The regime existing in the lower portions of the vessel more nearly resembled a liquid while that in the upper portions of the vessel was characterized by being highly dispersed and very bubbly. The

difference in the volumetric heat generation may account for the difference in the melt geometry occupied by the respective regimes. This subject will be further investigated in subsequent research.

The specific gravity of the final reaction mixture (the mixture at the conclusion of the chemical reaction) was determined after having conducted the reaction in a glass vessel. The results of this experiment may be seen in Table 1.

The coefficient of expansion for the transition from solid wax to liquid wax was determined. The volume of a sample of the solid wax was determined by immersing it in a graduated cylinder containing a known volume of liquid and noting the volume increase. The volume of the molten wax was determined by melting the same sample in a graduated cylinder and noting the volume and temperature. The coefficient of expansion for the wax from solid to liquid was found to be 1.18 or a volume increase of 18% from the solid to the liquid.

The solubility of the wax in the final reaction mixture was determined at each of the reactant concentrations used in the experiment. The volume of the solution was noted. A sample of wax of known weight was introduced. The weight of the cylinder, solution and wax was noted. The system was heated until the wax was melted. A phase boundary existed between the reaction mixture and the molten wax. The volume of molten wax phase was noted. The system was again weighed to determine the amount of the solution vaporized. Any weight difference was considered to be vapor lost. Any wax not found to be in the liquid wax phase was assumed to be in solution in the reaction mixture. The solubility was then calculated as volume of liquid wax per volume of reaction mixture. These results are reported in Table 1.

Continuing Research

In order to evaluate the correlations previously mentioned in this report, further work remains to be performed to characterize the physical properties of the system. These properties include heat capacities of the wax and reaction mixture; thermal conductivity of the reaction mixture, viscosity of the reaction mixture, thermal coefficient of expansion of the reaction mixture, viscosity of the reaction mixture and the volumetric heat generation as a function of time.

Work is continuing on improving the mathematical model which describes the melt. Work is also continuing in the improvement of the mass transfer correction and temperature profiles.

The downward heat flux will be investigated in the absence of mass transfer effects from the sidewall. The reaction will then be conducted in a cylinder where mass transfer takes place from both sidewalls and floor. A cylinder will be bisected axially and fused to a glass plate. This will then constitute a sidewall through which the reaction can be observed and the time dependency of the melt determined.

The observed melt will be compared with that calculated from the proposed mathematical model.

NOMENCLATURE

A = Area

C = Constant

Cp = Heat capacity

f = Frequency of bubble formation

g = Gravitational constant

Gr = Grashof number

HCDA = Hypothetical core disruptive accident

K = Thermal conductivity

LMFBR = Liquid metal fast breeder reactor

N = Molar flux

Nu = Nusselt number

Pr = Prandtl Number

Q = Heat generation of dissipation Energy/Time, heat flux
Energy/(Time) (Area)

r = Radius

R = Radius at interphase or phase boundary, component of
mass transfer correction

Ra = Rayleigh number

t = Time

T = Temperature

U = Velocity

V = Velocity, volume

W = Volumetric vapor generation rate

α = Thermal diffusivity

β = Coefficient of volumetric expansion

δ = Boundary layer thickness, Eigenvalue
 ξ = Dimensionless radius
 Z = Component of dimensionless temperature function
 η = Fraction of heat transfered downward
 θ = Mean packet residence time at the wall, dimensionless temperature
 λ = Latent heat of change, Eigenvalue
 ν = Kinematic viscosity
 ρ = Density
 τ = Dimensionless time
 $\mathcal{T}$ = Component of dimensionless temperature function
 ϕ = Component of mass transfer corrections

Superscripts

$\sim$ = Per mole
 $\wedge$ = Per unit mass, horizontally averaged maximum
 $'$ = Defined in terms of actual sublayer

Subscripts

a = Component a
 AV = Average
 b = Boiling, component b
 cor = corrected
 E = External
 f = Evaluated at film conditions
 KG = Kulacki-Goldstein
 l = Liquid

loc = Local

M = Melt

p = Bulk phase conditions

T = Thermal, total

TC = Thermal convection

V = Vapor

W = Wall, wax

X = Localized value

Z = Viscous terms

0 = Initial value, uncorrected value, at interface, lower thermal
boundary

1 = Upper thermal boundary

∞ = At approach or bulk conditions

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Table 1
Properties of Final
Reaction Mixtures

<u>Initial Molar Concentration of reaction Mixture</u>	<u>Temperature (°C)</u>	<u>Density (g/ml)</u>	<u>Solubility of wax in Reaction Mixture (%)</u>
4	22	.902	0
	60	.900	1
8	22	1.038	0
	60	1.029	1
12	22	1.101	0
	60	1.09	.5

Figure 1. Glass bottom reaction vessel.

Figure 2. Radial melt pattern for the reaction of 10 ml of 12M acetyl chloride with 10 ml of 12M dimethyl sulfoxide in a wax cylinder. Reaction products were allowed to cool overnight before being removed from the cylinder. Two different runs are shown.

Figure 3. Radial melt pattern for the reaction of 10 ml of 8M acetyl chloride with 10 ml of 8M dimethyl sulfoxide in a wax cylinder. Reaction products were allowed to cool overnight before being removed from the cylinder. Three different runs are shown.

Figure 4. Radial melt pattern for the reaction of 10 ml of 4M acetyl chloride with 10 ml of 4M dimethyl sulfoxide in a wax cylinder. Reaction products were allowed to cool overnight before being removed from the cylinder. Three different runs are shown.

Figure 5. Radial melt pattern for the reaction of 10 ml of 12M acetyl chloride with 10 ml of 12M dimethyl sulfoxide in a wax cylinder. Reaction products were removed from the wax cylinder immediately after the void collapsed. Two different runs are shown.

Figure 6. Radial melt pattern for the reaction of 10 ml of 8M acetyl chloride with 10 ml of 8M dimethyl sulfoxide in a wax cylinder. Reaction products were removed from the wax cylinder immediately after the void collapsed. Three different runs are shown.

Figure 7. Comparison of mean diameters from Figures 2 and 5.
12 M Solution

Figure 8. Comparison of mean diameters from Figures 3 and 6.
8 M Solution

Figure 9. Comparison of mean diameters from Figures 2, 3, and 4. The reaction mixture was allowed to cool in the wax cylinder overnight.

Figure 10. Comparison of mean diameters from Figures 4, 5, and 6. The reaction mixture was removed immediately after the void had collapsed.