Development of a Mechanistic Model for Hydrogen Generation in Fuel-Coolant Interactions

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Abstract

A dynamic model for hygrogen generation by Fuel-Coolant Interactions(FCI) is developed with separate models for each FCI stage, coarse mixing and stratification. The model includes the physical concepts of FCI, semi-empirical heat and mass transfer correlation and the concentration diffusion equation with the general non-zero boundary condition. The calculated amount of hydrogen, which is mainly generated in stratification, is compared with the FITS experiments. The model developed in this study shows a good agreement within a range of 10 % fuel oxidation rate and predicts the controlled mechanism of the chemical reaction very well. And this model predicts more accurately than the previous works. It is shown from the sensitivity study that the higher initial temperature of fuel particle is, the larger the reaction rate is. Up to 2700 K of temperature of the particle, the reaction rate increases rapid, which can lead to metal ignition.

1. Introduction

In severe accidents where the reactor suffers from the core-melt, the molten fuel called corium may come into contact with the water remained in-vessel or ex-vessel. If the corium falls into the water, fuel-coolant interactions(FCIs) will occur. These FCIs can lead to the production of large amount of steam and hydrogen that may cause the containment over-pressurization and threat its integrity under some conditions. Moreover, the hydrogen generated during FCIs poses an additional threat from deflagrations or detonations of this combustible gas.

Basically, the interactions between molten metal and water during FCIs are familiar as a well-known problem for many chemical reacting processes (e. g., in metal and paper industries) which the reaction takes place only at solid or liquid surfaces. But, due to

temperature gradient, the prediction of the oxidation rate of molten metal in FCI is complicated by the diffusion resistance through stable vapor film, which is determined by the heat and mass transfer inside the vapor film. In the case of heterogeneous reaction like as for a FCI of nuclear severe accidents, there are complicated thermodynamic and mechanical phenomena which may produce significant effects on the convective heat and mass transfer.

A number of experimental studies with molten zirconium (Zr) metal quenched in water have been reported. Among these, experiments by Crooks et al. [1] and Baker and Just[2] were only carried out under controlled conditions. These two experiments used with more or less a pure metal of single species, but the FITS(Fully Instrumented Test Site)[3] experiment was carried out with the corium and the thermite under circumstances which consider accident condi-

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tions.

Baker and Just[2] developed a simple theoretical model for a molten Zr metal sphere in water. With mass and heat transfer around and inside the metal sphere, heat and mass transfer coefficients were derived to treat the physical model of FCI, which underestimates the steam reactant taking part in chemical reaction. It was assumed that the Nusselt number was 2, which is the minimal value for a sphere, and the Lewis number was 1 based on the equality between the diffusion coefficient and thermal diffusivity. For the reaction mechanism, the chemical reaction was simply assumed to be controlled by only one stage of the two. One stage is chemical processes limited by steam diffusion through a steam/hydrogen mixture, the other is steam diffusion through zirconium oxide layer. The latter is often called "parabolic law". Thus, a better fundamental understanding of the heat and mass transfer processes is needed.

The analysis of Epstein et al. [4] was also divided into two parts. Epstein et al. were the first who present a more complete boundary layer treatment of film boiling around a hot sphere for steam diffusion through steam/hydrogen mixture. A steady-state theory based on mass, momentum, and energy conservation for axisymmetric stagnation flow over a circular disk was developed. For parabolic law, Epstein used the empirical correlation introduced by Baker and Just.

The model developed by Epstein et al. [4] is complex but incomplete because the empirical correlation developed by Baker and Just was directly used when the steam diffusion through the oxide layer controls the chemical reaction. The complexity of the initial phase seems incompatible with the empirical treatment of the second phase.

Corradini et al. [5] developed the different models for three FCI cases separately, based on the observation of FITS experiments. In their model, it is assumed that, since the molten fuel has very high temperature surrounded by stable vapor film, the steam diffusion through the vapor film will govern the chem-

ical reaction mechanism for oxidation. Using the governing equation for equimolar counter-diffusion of two perfect gases, they obtained the comparable results with that of the FITS experiments for each of three FCI cases. However, the calculated amount of hydrogen is much larger than that of the experimental results, and the model no longer describes a significant difference between the FCI phases. In addition, comparing with the CWII experiments in which the smaller hydrogen generation showed due to the subcooled water, the model over-predicted the amount of generation.

To more accurately predict the amount of the hydrogen generation in FCI, three parts of the model must be presented. First, the physical processes of FCI should be treated in tractable ways. Most previous models assumed a single particle with constant size, which does not simulate the FCI situation. Thus, in this study, the dynamic mixing of fragmentation process will be included. Second, it might be emphasized that the reactant supplies rely on the amount of the steam transferred through the vapor film, and therefore it is important to analyze the heat and mass transfer in film boiling. In this study the semi-empirical heat and mass transfer model for each of FCI cases are introduced. Third, it has been known that the reaction front of the metal-water interaction may be anywhere between the steam/oxide layer boundary and the oxide layer/fresh metal boundary. The assumption of previous works that the reaction front lies on either the steam/oxide layer boundary or the oxide layer/fresh metal needs to be corrected. By the concept of the coupled rate-controlling reaction mechanism, the general chemical reaction model will be described with considering the thermal and diffusional effects.

2. Model Descriptions

2.1. Physical Processes

A FCI is a phenomenon where a hot liquid(fuel)

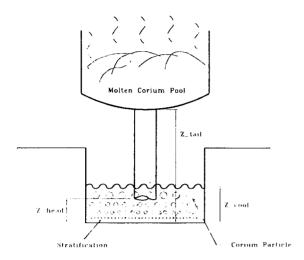


Fig. 1. The Schematic of FCI Physical Process

contacts a cold and more volatile liquid(coolant) and the hot liquid rapidly fragments with transferring its heat to the cold liquid to generate the steam, and lead to a locally high pressure. This phenomenon can be a form of energetic(steam explosion) or non-energetic(steam spike) reaction. Fig. 1 depicts the physical process of the fuel-coolant mixing. Recent researches into FCI have been directed at predicting the physical limits of mixing and the dynamic behavior of mixture[6]. But in previous works for predicting of hydrogen generation, the fuel was presumed the constant size of a fragmented particles, which does not consider the dynamic mixing process of FCI.

In FTTS experiments, some cases showed the steam explosion but others not even though the amount of hydrogen generation was measured. However, the general trend of the effect of steam explosion for hydrogen generation was not obtained. Since the explosion occurs in very short period with huge amount of heat transfer and do not show the physical process of stratification, this study treats only non-explosive case where coarse mixing is followed by a stratification of the molten fuel over the cavity floor, as shown in Fig. 1, and implements the analysis separately for each stage.

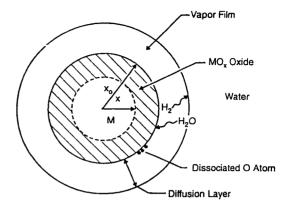


Fig. 2. The Physical Concept of a Coarse Mixing Stage

2.1.1. Coarse Mixing

In the coarse mixing, a spherical molten fuel droplet immerses in an infinite pool of subcooled water and falls at its terminal velocity with film boiling. Fig. 2 depicts the realistic representative of this concept, where the molten droplet is falling with a prescribed size and then undergoing the fragmentation(or, breakup) during the dynamic mixing. Furthermore, the minimum break-up size of droplet particles is adopted by results of previous works as discussed below.

For a break-up of the fuel droplet, Fauske and Henry[7,8] proposed the physical concept that the fuel can break up and premix with the water to a uniform size no smaller than that which would prevent the liquid from entering the mixture zone as the steam flows out. The minimum diameter was given as

$$D_{\min} = \frac{6 \, m_f q_{DROP}}{\rho_f A_c q_{CHF}}. \tag{1}$$

where q'CHF is the critical heat flux, used as the limit for steam outflow and water inflow. Corradini[9] suggested that limit to fuel-coolant mixing was determined by fuel or coolant liquid fluidization; e. g.,

$$D_{min} = \left[\frac{3}{4} \left(\frac{\alpha_f}{\alpha_v}\right)^2 \left(\frac{6 \, q_{DROP}}{\rho_v \, h_{fg}}\right)^2 \left(\frac{C_D \, H_c}{g}\right)^2 \left(\frac{\rho_v}{\rho_f}\right)\right]^{1/3}$$
(2)

where α_i and α_v are the fuel and vapor volume fraction at any time as the mixture evolves. Generally, this limit may never be reached because it takes time for the fuel to dynamically break up to this size, and an energetic fuel-coolant interaction or a agglomeration of the fuel may occur at the bottom having a finite depth.

The dynamic mixing is modeled by the modified Chu's correlation[10] developed for a water/air system as,

$$D_{\ell}(t) = D_{\ell 0} \exp(-C_1 \tau We^{0.254}).$$
 (3)

We is Weber number which is defined by

$$We = \rho_c U_f^2 D_0 / \sigma_f. \tag{4}$$

where ρ_c is the coolant density, U_t , D_{t0} and σ_t are the velocity, initial diameter and surface tension of the droplets, respectively. τ is the dimensionless time which is defined by,

$$\tau = (U_f t / D_0) (\rho_c / \rho_f)^{1/2}$$
. (5)

And constant C1 is given by

$$C_1 = 0.1232 - 0.149 (\rho_c / \rho_f)^{1/2}$$
 (6)

Assuming the constant velocity, {U_i}, Eq. (3) can be converted to a function of the elevation of the pool surface, z_{POOL}, as,

$$D_{f}(t) = D_{f0} \exp(-Z)$$

for $z_{BOT} \le z \le z_{POOL}$. (7)

where the variable Z is

$$Z = C_1 (We^{0.254} / D_{f0})$$

$$(\rho_c / \rho_f)^{1/2} (z_{POOL} - z).$$
 (8)

2.1.2. Stratification

When fragmented fuel falls down the cavity floor,

it may be begun to be stratified. In this study, simple conceptual picture for the stratification is assumed as followings. The molten fuel is underlying the coolant water, and the stratification stage is delayed until the last part of fuels falls down the cavity floor.

2.2. Heat and Mass Transfer

For each of FCI stages, the appropriate heat and mass transfer models should be established and will be described below.

2.2.1. Coarse Mixing

The energy generated as a result of exothermic chemical reaction would be transferred by the convection and radiation away from the fuel particle, and by the conduction into the bulk particle. For very high temperature of particles surrounded by the vapor film, the heat transfer by radiation through the vapor film is comparable to that by the convection. It is assumed that the temperature is uniform into the molten fuel droplet since the characteristic Biot number is below 0.1 for most sizes. Then, by the lumped parameter approach, the energy balance is given as.

$$m c_{p,f} \frac{dT}{dt} = h_{CONVECTION} A +$$

$$h_{RADIATION}A - e_{OXIDATION}\frac{dm}{dt}$$
 (9)

There are several different heat transfer coefficients for the film boiling around a sphere. The heat transfer correlation developed by Dhir and Purohit[11] for film boiling around a sphere on subcooled water is used in this study because it gives a good prediction of their data over a wide range of subcooled liquid temperatures. These correlations are corrected as follows:

-Natural Convection

$$Nu_{\text{convection}} \, = \, \frac{h \, D}{k_{\text{v}}} \, = \, Nu_{\text{o}} \, + \, Nu_{\text{nc}} \, \frac{Pr_{\,\text{v}} \, Scc}{Pr_{\,\text{c}} \, Spp \, \mu}$$

(10)

$$Nu_{radiation} = C_1 \frac{Pr_v}{Spp} \frac{\sigma(T_f^4 - T_{SAT}^4)D}{h_{fg} \mu_v}$$
 (11)

-Forced Convection

$$Nu_{convection} = Nu_{o} +$$

$$0.8 \, (\text{Re})^{1/2} \left(1 + \frac{\text{Scc Pr}_{v}}{\text{Spp Pr}_{c} \, \mu} \right)$$
 (12)

where

$$Scc = \frac{c_{p,c} \Delta T_{sub}}{h_{fo}}$$
 (13)

$$Spp = \frac{c_{p,v} \Delta T_f}{h_{f\sigma}}$$
 (14)

$$Nu_o = 0.8 \left[\frac{g \rho_v (\rho_c - \rho_v) h_{fg} D^3}{\mu_v k_v \Delta T_f} \right]^{1/4}$$
 (15)

$$Nu_{nc} = 0.9 \left[\frac{g \rho_c^2 - c_{p,c} \beta \Delta T_{sub} D^3}{u_c k_c} \right]^{1/4}$$
 (16)

Total heat transfer coefficient used in this study is the maximum of heat transfer coefficient by natural and forced convection plus radiation heat transfer coefficient for the conservatism.

For mass transfer, a consistent model is developed by the heat and mass analogy[12], which is based on the assumption that the physical properties are constant and the mass transfer rate is small. For this study, the physical properties of steam and water with film boiling are assumed to be at a saturated condition, and mass transfer rate in FCI is generally very low. Besides, this analogy has been confirmed experimentally for a number of flow systems[12].

-Natural convection

$$Sh_{conv} = \frac{k_m * D}{D_{s-H_2}} = Sh_0$$

$$+ Sh_{nc} * \left(\frac{Sc_v * Scc_m}{Sc_c * Spp_m * \mu}\right)$$
(17)

$$Sh_0 = 0.8 * \left(\frac{Sc_v * Gr_m * h_{fg}}{C_v \Delta T_f} \right)$$
 (18)

$$Sh_{nc} = 0.9 * (Gr_m * Sc_c)^{1/4}$$
 (19)

-Forced convection

$$Sh_{conv} = Sh_0 + 0.8 * Re^{1/2} *$$

$$\left(1 + \frac{Sc_v * Scc}{Sc_c * Spp * \mu}\right) (20)$$

2.2.2. Stratification

As mentioned in Sec. 2.1.2, the flat-shaped molten fuel pool contacts with and is cooled by overlying water. Thus, the same approach as in the coarse mixing is used except a modified Berrenson's correlation[13] for film boiling on a horizontal flat surface is used, and the transient heat conduction equation is used instead of lumped parameter equation due to its finite dimensions. The following equations are obtained with the heat and mass analogy.

-Convective heat transfer

$$h_{CONV} = 0.531 [k_{fm}^3 \rho_{fm} (\rho_c - \rho_{fm}) g h_{fg} / (D_1 \mu_{fm} \Delta T)]^{1/4}$$
 (21)

-Radiative heat transfer

$$h_{RAD} = \sigma_{SB} [1/\varepsilon_{SS} + 1/\varepsilon_{c} - 1]^{-1}$$

$$(T_{SURF}^{4} - T_{SAT}^{4})/\Delta T_{SAT} \qquad (22)$$

-Mass transfer

$$Sh = \frac{k_m D}{D_{s-H_2}} = 0.531 \times \left[\frac{Sc_v Gr_m h_{fg}}{C_{p,fm} \Delta T_{fm}} \right]^{1/4}$$
 (23)

2.3. Reaction Mechanism

To solve the transport of the reactants to the surface of molten metal, i. e. the chemical reaction front, the position of the chemical reaction front needs to be determined. In previous studies, it was assumed

that this would be a initial surface of metal with a rate-controlling mechanism of the two diffusion rates, or a determined surface depending on which the reactant(metal or oxygen) has the higher diffusion rate within oxide layer. But, the actual metal/water interaction in FCI would be a heterogeneous reaction and, in this case, can be treated by unreacted-coreshrink model[14] as described below.

A spherical particle or a flat pool in stratification, having an initial radius R or height H, respectively, is reacted by the steam. At first, this reaction takes place at the outside surface of the particle. As the reaction proceeds, the surface of the reaction will move into the interior of the particle. During the process, the reaction surface moves inward forming an unreacted core which shrinks with time, even though the external radius of the particle still remains the same because of assuming no deformation of the oxide layer that has been formed. Thus, in order for the steam to reach the surface of the unreacted core, it must move through various layers of resistances in series; the steam/hydrogen mixture around the surface of the particle, the porous oxide layer, and then the reaction surface at the core. Fig. 2 illustrates this concept of the reaction.

When the steam reaches the reaction surface, practically the reaction can take place under the thermo-chemical conditions. In other word, the reaction rate is determined the surface reaction rate constant governed by the reaction type. Corradini[15] assumed the surface reaction be occurred instantaneously and all steam be reacted. This assumption leads to a overestimated results in hydrogen generation. Thus, in this study, the general non-zero reaction rate boundary conditions are applied on the concentration diffusion equation.

A pseudo-steady-state counter-diffusion equation relating with the steam is written as,

$$D_{ox}\left(\frac{\partial^{2}C_{v}}{\partial r^{2}} + \frac{2}{r}\frac{\partial C_{v}}{\partial r}\right) = 0, \quad x < r < x_{o}$$
(24)

at solid particle surface xo,

$$D_{ox} \left(\frac{\partial C_{v}}{\partial r} \right)_{x_{o}} = k_{m} \left(C_{v,o} - C_{v,SURF} \right)$$
 (25)

at the moving interface x,

$$D_{ox} \left(\frac{\partial C_{v}}{\partial r} \right)_{x} = a k_{s} C_{f} C_{v,ox}$$
 (26)

$$-D_{ox}\left(\frac{\partial C_{v}}{\partial r}\right)_{v} = a C_{f}\left(\frac{dx}{dt}\right)$$
 (27)

where k_m is the mass transfer coefficient of steam across the steam/hydrogen mixture, and C_t is the concentration of metal reactant. The initial condition is $x = x_0$ at t = 0.

Applying the boundary conditions, Eqs. (25) and (26), to Eq. (24), the concentration profile of steam can be obtained as.

$$\frac{C_{v}}{C_{v}} = \tag{28}$$

$$\frac{\left(1 + \frac{D_{ox}}{ak_sC_{s_o}x_o}\right)\frac{1}{x_{ox}} - \frac{1}{x}}{\left(1 + \frac{D_{ox}}{ak_sC_{s_o}x_o}\right)\frac{1}{x_o} - \left(1 - \frac{D_{ox}}{k_mx_o}\right)\frac{1}{x}}$$

And then, integrating the boundary condition, Eq. (27), from zero to the present time t, the time required for particle to reduce the unreacted core from x_0 to x is given by,

$$t = \frac{ax_{o}C_{f}}{C_{v,o}} \left[\frac{1}{3} \left(\frac{1}{k_{m}} - \frac{x_{o}}{D_{ox}} \right) \left(1 - \frac{x^{3}}{x_{o}^{3}} \right) - \frac{1}{ak_{s}C_{f}} \left(1 - \frac{x}{x_{o}} \right) + \frac{x_{o}}{2D_{ox}} \left(1 - \frac{x^{2}}{x_{o}^{2}} \right) \right] (29)$$

In other word, for a given time t, the reaction front of the particle is calculated by Eq. (29). Finally, the amount of steam reacting per unit time at the reaction front, M_s can be obtained from Eqs. (28) and (29),

$$M_{s} = \frac{4\pi C_{v,o}}{\frac{1}{x_{o}^{2}k_{m}} + \frac{1}{x^{2} ak_{s}C_{f}} + \frac{1}{D_{ox}}(\frac{1}{x} - \frac{1}{x_{o}})}$$
(30)

From Eq. (30) and the stoichiometry of the chemical reaction, the generated amount of hydrogen is calculated. On the other hand, the amount of hydrogen generation for stratification is derived in similar manner as:

$$M_{s} = \frac{C_{so}}{\frac{D_{ox}}{k_{m}} + x - x_{ox} + \frac{D_{ox}}{a k_{s} C_{f}}}$$
(31)

3. Results

3.1. Calculation Methods

The calculation for hydrogen generation during the coarse mixing begins with the commencement of FCI at the water surface and ends if last fragmented particles touch the cavity floor. Next, the calculation for stratification continues until saturated reaction rate reaches. The initial cylindrical column of the fuel determined by falling velocity and the vessel rupture size, is poured from the vessel into the coolant pool. At every time, the position of column is determined. As mentioned earlier, it is assumed that the stratification starts when the tail of column touches the cavity floor.

For a stage of the coarse mixing, since the position of column varies with time and the radius of particles varies with height, it is not easy to treat numerically the particle fragmentation and heat/mass transfer at the same time. Thus, for this study it was taken numerically that the fuel column might be fallen down into coolant pool, where meshes of coolant pool are discretized finely below 1.0×10⁻⁴m. When the fuel column contacts the coolant, it can be fragmented into the particles with radius calculated by Eq. (7). Thereafter, the fragmented particles fall down exactly one mesh during one time step and the radius of particles changes with the representative value for each mesh of coolant pool by Eq. (8). So the particles have the same size within same mesh. When the fuel particle enters new mesh of the coolant pool, it is assumed that the "fresh" surface is ex-

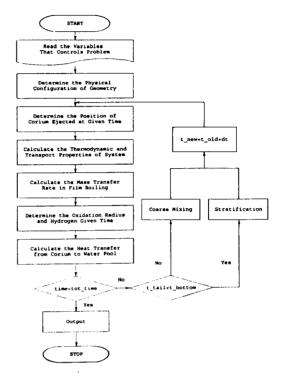


Fig. 3. Calculational Flow Chart for Hydrogen Generation

posed and surrounded by the steam reactant. And the physical data and properties of upper mesh are transferred in lower mesh at the same time. On the other hand, thermodynamic and transport properties of fuel, coolant, and steam vary with temperature.

For a calculational time step, the rate of oxidation reaction is determined by Eq. (29). Since Eq. (29) is non-linear for spatial variable, the reaction front, x, is calculated numerically by modified linear interpolation method[16]. The amount of hydrogen generated is determined by Eq. (30). Fig. 3 is the flow chart for the calculation of hydrogen generation.

3.2. Results

Calculational results compare with FITS experiments. FITS is an acronym for a test facility used to experimentally investigate FCIs. Among several FITS

Test	Fuel Ma ss	Water Mass	Mass Ratio	Water Temp	Ambient Pressure	Water Side	Water Depth	Melt Entrdy	Hydrogen Generated	Percnet M Oxidized	
	Deliv					Dime	ension	Velocity		FeO	Fe ₂ O ₃
	kg	kg	m₀/mf	K	MPa	m	m	m/s	gm		
FITS5C	19.6	110.4	5.6	351	0.510	0.61	0.31	6.0	49	13	9
FTTS2D	18.0	95.7	5.3	289	1.103	0.38	0.66	7.3	91	24	16
FTTS5D	19.5	21.3	1.1	368	0.083	0.38	0.15	7.3	120	31	21

Table 1. FITS Series Experimental Results

series, the two series, FITSC and FITSD[3] are intermediate-scale tests aimed at measuring hydrogen generation during FCIs. While two fuel compositions iron-alumina(55 w/o Fe and 45 w/o Al) and conum A+R were employed in experiments, the cases using iron — alunima composites are compared since this composite consists of pure metals. Table 1 summaries experimental conditions and results of the successful FITSC and FITSD series.

Table 2 shows the comparison of the experimental data with the predictions of this study and previous study[5]. Results indicate that the model developed in this study gives more or less overestimated results over data, but much closer results than the previous model. The predicted quantities of hydrogen is mainly generated in stratification stage. Since, for time scale occupied in each of FCI stage, the time interval of coarse mixing is much shorter than that of stratification, the portion of coarse mixing is below about 1%. Fig. 4 shows the percent of fuel oxidized by the reaction;

$$Fe + H_2O \rightarrow FeO + H_2$$
 (32)

The calculated value is slightly higher than the experimental data which is obtained from a final post-examination of the grab samples at times. When the FCI with high temperature particles(up to 2000 K) progresses, the oxidation rate rises rapidly. But as the particles cool down, the rate is gradually diminished and finally shows saturated oxidation rate.

In this study, the effect of initial fuel temperature on the amount of hydrogen generated is examined. Fig. 5 shows the same behavior as Just and Baker's

Table 2. Results of Calculations with Experiments

	Water	Mass of Hydrogen Generated					
Test	Subcooling	Measurement	Calculation (g)				
	(K)	(g)	Coarse Mixing	Stratification			
, FTTS 5C	75	49	0.11	68.5			
			(0.09)*	(205)			
FTTS 2D	168	91	1.09	138.2			
			(0.18)	(183)			
FITS 5D	0	120	0.9	176.8			
			(0.01)	(207)			

^{*:} the calculated results of Corradini et al. [5]

Calculated Results for FITS-2D

25
20
20
25
20
20
20
20
20
20
20
20
20
20
20
20
Time (sec)

Fig. 4. The Calculated Percentage of Fuel Oxidized

experiments predicted, that is, the higher the temperature of particle is the more violent the reaction becomes. But, over a certain temperature the reaction increases rapidly and leads to the metal ignition, which was also observed in previous study[15]. As seen in Fig. 5, this threshold temperature is about 2700 K and over.

Additionally, the reaction mechanism controlling

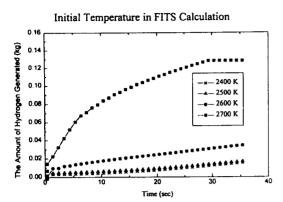


Fig. 5. The Effect of Initial Temperature of Fuel on Hydrogen Generation

the reaction rates can be described by the calculated results of this study. Three terms appearing in the denominator of Eq. (30) represent resistances in series for the reaction considered. The time behavior of these resistances is shown in Fig. 6, where the ellapsed times of the reaction extended arbitarily for the coarse mixing stage. The result confirms that the rate-controlling mechanism could be changed with time. At first, the steam/hydrogen mixture resistance controls the reaction, and then chemical reaction resistance supercedes the steam/hydrogen mixture. But the oxide layer takes a negligible role in rate-control-ling mechanism.

4. Conclusions

In this study, a mechanistic model is developed to analyze the hydrogen generation of FCIs. Considering the physical concept of FCI, the amount of hydrogen generated is predicted for each of FCI stages. It is concluded that results show better agreement to experiment data than that of previous works. The metal-water interaction is controlled by both heat and mass transfer and counter-diffusion with non-zero boundary condition in the circumstance of high pressure and low reactant concentration. The increase of initial fuel temperature shows the rapid increase in

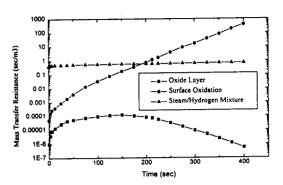


Fig. 6. The Reaction Mechanism Controlling the Chemical Reaction

the reaction rate beyond the ignition temperature of metal.

Additional work is needed in order to improve the results of the model. The following recommendations for future work might help to improve the prediction of hydrogen generation.

- (1) Through the comparision with the numerous experimental results using single particle of the fuel, the effects of several conditions in coarse mixing stage of FCIs might be investigated more precisely.
- (2) The diffusion coefficient of the fuel and steam through the oxide layers needs to be determined more accurately. The transport of the reactants to the reaction front is important for analyzing metal-water interactions, since some oxygen phase diagrams of the oxide layer are very changeable during the chemical reaction.

Nomenclature

A = area
a = stoichiometry

C = concentration

C₁ = empirical constant in eq.(11)

CD = drag coefficient for fuel

C_p = specific heat of fuel

D = equivalent diameter

DAR = diffusion of A species in B species D_1 = Laplace reference length = energy e. = gravitational acceleration g Gr = Grashof number = heat transfer coefficient h Hc. Zpool = depth of water pool = latent heat of vaporization hъ k =thermal conductivity = mass transfer coefficient k, = reaction rate constant k. M = mass rate of steam = mass of fuel m = Nusselt number Nu Pr =Prandtl number a" = heat flux R =radius of particle = raidal coordinate Re =Revnold number Sc =Schmidt number Scc =liquid subcooling parameter Spp = vapor superheat parameter T = liquid temperature =time U =falling velocity of We =Weber number X. x = coordinate variables Z = nondimensional axial falling distance z = axial position Greek =void fraction α =thermal coefficient of volumetric expan-В sion = viscosity, ratio of viscosites μ 3 = surface emittance = density ρ

CHF = critical heat flux
CONV = convection
DROP, f = fuel or its particle

fm = wapor film
m = mass
min = minimum
o = initial
ox = oxide layer

POOL -= water level of coolant

RAD = radiation

s = steam

SAT = saturation

SUB = subcooling

SURF = surface of fuel

v = vapor

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Subscripts

σ

τ

BOT = bottom of cavity

= surface tension

= Stefan-Boltzmann constant

= nondimensional time variable

c = coolant

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