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I.   INTRODUCTION

The modeling of sodium pool fires constitutes an important ingredient in conducting LMFBR accident analysis. Such modeling capability has recently come under scrutiny at Westinghouse Hanford Company (WHC) within the context of developing CONACS, the Containment Analysis Code System. One of the efforts in the CONACS program is to model various combustion processes anticipated to occur during postulated accident paths. This effort includes the selection or modification of an existing model and development of a new model if it clearly contributes to the program purpose. As part of this effort, a new sodium pool fire model has been developed that is directed at removing some of the deficiencies in the existing models, such as SOFIRE-II and FEUNA.

II.   EXPERIMENTAL OBSERVATIONS

Extensive sodium pool fire experiments have been performed in the United States as well as abroad. The important observations of sodium pool fires listed below form the bases for the pool fire modeling.
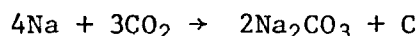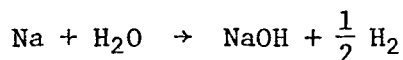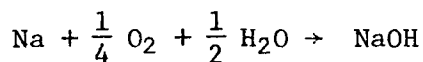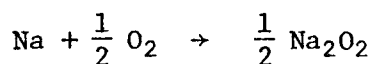
1. The flame of sodium pool fire is a diffusion flame (i.e., any flame in which the fuel and oxidizer are initially separated) as illustrated in Figure 1a, where sodium vapor diffuses from the pool to combine with the oxidizers (O_2, H_2O and CO_2) that diffuse to the flame from the containment atmosphere. Since the ratio of the heat of vaporization to the heat of combustion is on the order of 0.3, a large fraction of heat of combustion must flow to the pool in order to evaporate sufficient sodium to sustain the combustion. This is very different than the burning of hydrocarbon fuels where only about one thousandth of heat of combustion is needed to evaporate the liquid fuel. Hence, the flame lies very close to the pool surface ($\sim$1 mm) like a flame sheet. This very nature makes 1-D models for conservation equations possible.

2. About 60-70% combustion products (Na_2O, Na_2O_2, NaOH, etc) are falling into the pool directly from the flame. A sketch to illustrate the dispersal of combustion products is shown in Figure 1b. The combustion products are in forms of liquid or solid particles and their densities are much higher than that of atmosphere. Furthermore, since the flame sheet is so close to the pool surface, there is lack of convective flow to carry away these particles from the flame. Again, this is in contrast to the condition of burning hydrocarbon fuel where almost all the combustion products are drafted away from the flame by the strong fire induced flow current. This

phenomena requires the consideration of the thermal energy of falling aerosol in the region between the flame and pool surface as well as the within ʃf the pool in the formulation of energy equations.

3. The sodium burning rates are directly proportional to the pool temperature when the oxidizer concentration remains virtually unchanged. This experimental observation suggests that the temperature of the sodium pool should be carefully formulated since it plays an important role in the burning rate of pool fires. Moreover, in a postulated LMFBR accident path, the combustion may not be the only source of transferring energy to the pool and the nuclear heating, such as γ-radiation and core debris heating, may also coexist.

III. CHEMICAL REACTIONS

The chemical composition of the containment atmosphere varies considerably and is dependent upon the time interval into the accident as well as the different initial conditions for the accident scenarios. It is believed that the O_2, H_2O and CO_2 can exist in the atmosphere in sufficient amounts to initiate a chemical reaction. The following chemical reactions make up the various combustion processes in the CONACS pool model: [

$$Na + \frac{1}{4} O_2 \rightarrow \frac{1}{2} Na_2O$$

$$Na + \frac{1}{2} O_2 \rightarrow \frac{1}{2} Na_2O_2$$

$$Na + \frac{1}{4} O_2 + \frac{1}{2} H_2O \rightarrow NaOH$$

$$Na + H_2O \rightarrow NaOH + \frac{1}{2} H_2$$

$$4Na + 3CO_2 \rightarrow 2Na_2CO_3 + C$$
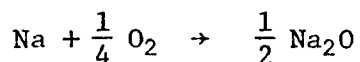
IV. THE MATHEMATICAL MODEL

The diffusion flame is governed by three mechanisms: 1) the diffusion of the oxidizer from the atmosphere to the flame sheet, 2) the diffusion of the sodium vapor from the pool to the flame sheet, and 3) the energy feedback to the pool to evaporate the liquid sodium and the energy transferred to the atmosphere by induced flow current.

The mathematical model for the CONACS pool fire is 1-D. That is, in the formulation of the conservative equations, only the variations in the directions perpendicular to the pol surface are considered. This assumption is valid according to experimental observations except at the edges of the flame. It is noted that the convective effects at the edges of the flame to the overall energy and balance balances

are diminished as the pool size increases. In the case of containment analysis, sodium pools are sufficiently large to mitigate the net influence of edge effects.

The following three equations describe the mentioned mechanisms.

A. Oxidizer diffusion equation

The equation for the oxidizer mass transfer from the atmosphere to the flame sheet is expressed as[1]

$$N_o = K(x_a - x_f) + x_a(N_o + N_n) \tag{1}$$

where

N_o = flux of oxidizer through a reference plan at the ambient containment atmosphere where the concentration of the oxidizer remains constant

N_n = flux of inert gases through a reference plan at the ambient containment atmosphere where the concentration of inert gases remain constant

x_a = molar fraction of oxidizer at ambient atmosphere

x_f = molar fraction of oxidizer at the flame sheet

K = mass transfer coefficient

To obtain the mass transfer coefficient, K, in Eq. (1), the heat-mass transfer analogy is invoked.[1] The Fujii-Imura[2] empirical correlation for heat transfer from a heated horizontal plate to atmosphere is used to simulate the mass transfer of oxidizer from the ambient atmosphere to flame sheet. The expression is:

$$Sh = 0.16 (GrSc)^{1/3} \tag{2}$$

where

Sh = Sherwood number $\dfrac{KL}{cD}$

Gr = Grashof number $\dfrac{g\rho^2\beta(T_f-T_a)L^3}{\mu^2}$

Sc = Schmidt number $\dfrac{\mu}{\rho D}$

and

L = characteristic length of flame sheet

c = molar concentration

D = diffusion coefficient (binary)

g = gravity acceleration

ρ = density of the containment atmosphere

β = coefficient of volumetric expansion of containment atmosphere

T_f = temperature of the flame sheet

T_a = temperature of the ambient atmosphere of containment

μ = viscosity of atmosphere

Consider now the Eq. (1) oxidizer mass transfer at the flame sheet. Since there is no sink for inert species at the flame sheet, N_n is zero. Observations confirm that in a combustion process, the chemical reaction rate is much faster (i.e., several orders of magnitude) than that of mass transfer process, so that $x_f = 0$. With these conditions, Eq. (1) can be rewritten as

$$N_o = \frac{kx_a}{1-x_a} \tag{3}$$

For a given thermochemical state, a proportional constant, s, can be obtained from the stoichiometrical relationship as given in Section III that relates the sodium burning rate, $(\dot{m}_b)$ to the oxidizer mass diffusion rate. With the use of Eq.s (2) and (3), one obtains:

$$\dot{m}_b = sN_o = s\left(\frac{x_a}{1-x_a}\right)\frac{cD}{L}\left\{0.16(GrSc)^{1/3}\right\} \tag{4}$$

B. Energy balance equation at the pool surface

The energy balance at the pool surface is written as:

$$\dot{m}_e H_{fg} + q_{s,p} - q_{f,s} = 0 \quad , \tag{5}$$

where

$\dot{m}_e$ = evaporization rate of sodium at pool surface

H_{fg} = heat of vaporation of sodium

$q_{s,p}$ = heat transfer rate from the pool surface to the interior of the pool

$= k_p \left.\frac{\partial T}{\partial X}\right|_{X=0^-}$

$q_{f,s}$ = heat transfer rate from flame sheet to pool surface by conduction and radiation

$$= k_m \left. \frac{\partial T}{\partial X} \right|_{X=0^+} + \sigma F_{f,s} (T_f^4 - T_s^4)$$

and

k_p = thermal conductivity of the pool

0^- = means the temperature gradient is evaluated beneath the pool surface

k_m = thermal conductivity in the region between the flame sheet and the pool surface

0^+ = means the temperature gradient is evaluated above the pool surface

σ = Stefan-Boltzmann constant

$F_{f,s}$ = overall radiation exchange factor between flame sheet and pool surface

T_s = temperature of pool surface

The equation is simply stated that the heat flow from the flame sheet to the pool surface by conduction and radiation is balanced by the heat of evaporation of sodium and the heat transferred into the pool by conduction.

C. Energy balance equation at the flame sheet

The flame sheet is realistically modeled instead of using the surface burning approximation used in SOFIRE-II and FEUNA. At the flame sheet, the energy balance is written as:

$$\dot{m}_b \Delta H - q_{f,a} - q_{f,p} - q_{f,w}^r = 0 , \tag{6}$$

where

$\dot{m}_b$ = sodium burning rate and equals to $\dot{m}_e$ by the requirement of the conservative law of mass

ΔH = heat of combustion

$$= H^o + a_{Na} \left(\int_{T^o}^{T_s} C_p dT \right)_{Na} + \left(\sum_i a_i \int_{T^o}^{T_a} C_{pi} dT \right)_{oxidizer}$$

$$- \left(\sum_i \alpha_i b_i \int_{T^o}^{T_s} c_{pi} dT \right)_{\substack{product \\ to \ pool}} - \left(\sum (1-\alpha_i) b_i \int_{T^o}^{T_s} c_{pi} dT \right)_{\substack{product \ to \\ atmosphere}}$$

$q_{f,a}$ = heat transfer rate from flame sheet to atmosphere by conduction, convection and radiation

$$= k_a \left. \frac{\partial T}{\partial X} \right|_{X=\ell} + h_{f,a} (T_f - T_a) + \sigma F_{f,a} (T_f^4 - T_a^4)$$

$q_{f,w}^r$ = heat transfer rate from flame sheet to the containment walls by radiation

$$= \sum_i \sigma F_{f,wi} (T_f^4 - T_{wi}^4)$$

and

H^o = standard heat of combustion at temperature T^o (e.g., T^o = 298.15 K)

a_i = stoichiometric coefficients for ith reactants

b_i = stoichiometric coefficients for ith products

α_i = fraction of ith combustion products that fall into the pool

c_{pi} = specific heat of constant pressure for ith chemical species

k_a = thermal conductivity of containment atmosphere

$h_{f,a}$ = convective heat transfer coefficient between flame sheet and containment atmosphere

$F_{f,a}$ = overall radiation exchange factor between flame sheet and atmosphere

$F_{f,wi}$ = overall radiation exchange factor between flame sheet and the ith containment wall

T_{wi} = temperature of ith containment wall

ℓ = the distance from pool surface to the flame sheet

X = coordinate measured vertically from pool surface to the flame sheet

Given the values of T_a, x_a and T_{wi}, the sodium burning rate, $\dot{m}_b$, and the flame temperature, T_f, can be determined by solving the Eqs. (4), (5) and (6) simultaneously. However, a careful examination of these equations one finds there are four unknowns that cannot be obtained without additional information; namely,

$$\left.\frac{\partial T}{\partial X}\right|_{X=0^+} \quad , \quad \left.\frac{\partial T}{\partial X}\right|_{X=\ell} \quad , \quad \left.\frac{\partial T}{\partial X}\right|_{X=0^-} \quad \text{and} \quad T_s$$

The first two unknowns can be obtained by solving the energy equation in the region between the flame sheet and the pool surface and the other two unknowns can be obtained by solving the energy equation of sodium pool.

D. <u>Energy equation for the region between flame sheet and pool surface</u>

First, consider the region between flame sheet and the pool surface. The energy equation is written as:

$$(\rho C_p)_m \frac{\partial T}{\partial t} + (\dot{m} C_p)_{reactant} \frac{\partial T}{\partial X} - \sum (\dot{m} C_p)_{product} \frac{\partial T}{\partial X} = k_m \frac{\partial^2 T}{\partial X^2} \, , \qquad (7)$$

With initial condition:

$$T(t,X) = T_s^{\circ} \quad 0^+ \leq X \leq \ell, \quad t = 0 \qquad (8)$$

and boundary conditions:

$$T(t,X) = T_s (t), \quad \text{at} \quad X = 0 \, , \quad t>0 \, , \qquad (9)$$

$$T(t,X) = T_f (t), \quad \text{at} \quad X = \ell, \quad t>0 \, . \qquad (10)$$

where

t = time into the transient

$\dot{m}$ = mass flux (i.e., either reactant or combustion product)

and subscripts

m = mixture in the region between flame sheet and pool surface

Eq. (7), with the initial condition and boundary conditions, Eq. (8) and (9) can be solved numerically or analytically if a constant property assumption is invoked. The solutions of these two unknowns are in terms of $\dot{m}_b$, T_f, ℓ, and T_s. That is, they are functions of $\dot{m}_b$, T_f and ℓ; namely:

$$\left.\frac{\partial T}{\partial X}\right|_{X=0^+} = f_1(\dot{m}_b, T_f, \ell, T_s) \qquad (11)$$

$$\left.\frac{\partial T}{\partial X}\right|_{X=\ell} = f_2(\dot{m}_b, T_f, \ell, T_s) \qquad (12)$$

E. Energy equation for the pool

As mentioned previously, T_s is furnished by the solutions of pool energy equation, the substitutions of Eqs. (11) and (12) into Eqs. (4), (5) and (6) give three unknowns: $\dot{m}_b$, T_f and ℓ. Three unknowns and three nonlinear algebra equations, from the theory of equations, there should yield a meaningful solution physically.

It is realized that once the sodium burning rate, m_b, is obtained

- the consumption rates of oxidizers

- generation rates of aerosols

- energy addition to the atmosphere

- energy exchange between flame sheet and containment walls

- energy addition to the pool from the flame

- pressure changes of containment atmosphere

- aerosol falling rate to the pool

and other related quantities can be calculated through the stoichiometric relationship with the aid of the quantities or equations such as heat of combustion, equation-of-state, settling factor of aerosols, radiation exchange factor, etc.

To provide the other two unknowns for Eqs. (4), (5) and (6), i.e.,

$$\left. \frac{\partial T}{\partial X} \right|_{X=0^-} \quad \text{and} \quad T_s \, ,$$

one needs to solve the energy equation of sodium pool. The energy equation for the pool is written in a nodal form as:

$$(X_i A_p) \left\{ (1-V_i) \left(\rho C_p \frac{dT}{dt} \right)_i^{Na} + \sum_k \left(V \rho C_p \frac{dT}{dt} \right)_i^k \right\}$$

$$= (1-\xi_{i-1}) \sum_k (\dot{m}H)_{i-1}^k - (1-\xi_i) \sum_k (\dot{m}H)_i^k$$

$$+ q_{f,p}^c + q_{f,p}^r + q_{d,i} + q_{i-1,i} - q_{i,i+1} + \dot{Q}_i$$

$$k = Na_2O, Na_2O_2, NaOH, Na_2CO_3, \tag{13}$$

where

A_p = pool surface area

V_i = volumetric fraction of aerosol of the ith node

$\dot{m}_i^k$ = mass flux of kth chemical species in the form of aerosol at the boundary between the ith and $i+1$th nodes

H = enthalpy

$q_{f,p}^c$ = heat transfer from flame sheet to pool surface by conduction, when subscript i = 1, i.e., top node of the pool

= 0 for all interior nodes

$q_{f,p}^v$ = heat transfer from flame sheet to pool surface by radiation for the top node

= 0, for all interior nodes

$q_{i,i+1}$ = heat transfer by conduction between nodes i and i+1

$q_{d,i}$ = heat transfer from aerosol to sodium in the ith node

$\dot{Q}_i$ = internal heat generation for i^{th} node

ξ_i = settling coefficient of aerosol for i^{th} node

i = the subscript designate of the ith node of the pool

This parameter, "settling coefficient ξ," is introduced because of experimental observations on the various settling behavior of aerosols in the sodium pool under different conditions.[3,4] For example, WHC AB1 and AB2 tests[3] had found that the aerosol was accumulated on the top of sodium pool when atmosphere was dry; and the aerosol was settling on the bottom of the sodium pool when atmosphere was very wet. To simulate these cases one can simply set ξ_i = 0 for dry atmosphere and ξ_i = 1 for extremely wet atmosphere.

F. Preliminary assessment for the model

In the CONACS code system, equations (4), (5), (6), (7) and (13) will be solved simultaneously along with the other equations which govern surrounding regions and phenomena in the containment. In order to test the pool fire model, an isolated calculation was performed. This calculation decoupled all other models and used the WHC AB1 test[3] initial atmosphere and pool conditions.

The results on the temperature profiles of the pool, at the pool surface, and for the flame are plotted in Figure 2 along with the experimental results and SOFIRE-II calculation results. The predicted pool temperatures using the CONACS model closely agrees with the experimental results. Since the AB1 tests did not record the flame temperature and pool surface temperatures, direct comparisons of these profiles cannot be made. However, Newman's pool fire test indicated that the flame temperatures are about 1200-1300°K, which is in good agreement with the CONACS model. The SOFIRE-II predicted pool surface temperatures were 200°K higher

than the sodium boiling temperature and are physically unjustified. This is due to the fact that it assumes a burning surface exists on the liquid sodium. The reasonable predictions from the present model provide assurance that the correct approach to the mathematical formulation of the pool fire model in CONACS is being pursued. This test result qualifies the pool fire model for implementation into the CONACS model where extensive validation will be conducted.

REFERENCES

1. R. B. Bird, et al., Transport Phenomena, Ch. 21, John Wiley and Sons, Inc. New York, 1960.

2. T. Fujii and H. Imura, "Natural-Convection Heat Transfer from a Plate with Arbitrary Inclination," Int. J. Heat Mass Transfer, 15, 755 (1972).

3. R. K. Hilliard, et al., Aerosol Behavior During Sodium Pool Fire in a Large Vessel--CSTF Tests AB1 and AB2, HEDL-TME 79-28, Hanford Engineering Development Laboratory, Richland, WA, June 1979.

4. R. N. Newman and J. F. B. Payne, "The Burning Rates of Sodium Pool Fires," Combustion and Flame, 33 (1978) 291-297.
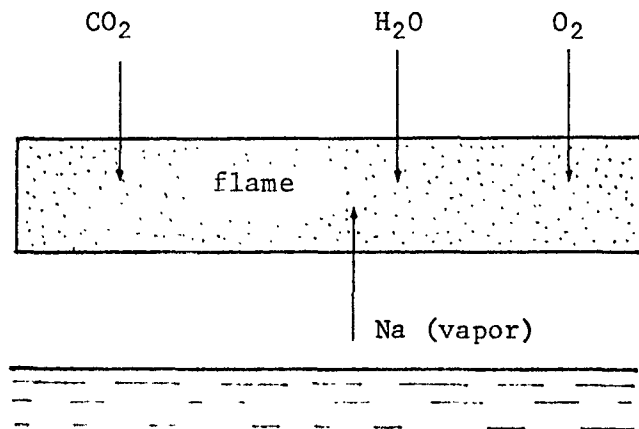
FIGURE 1a.   Sketch illustrating mass influx
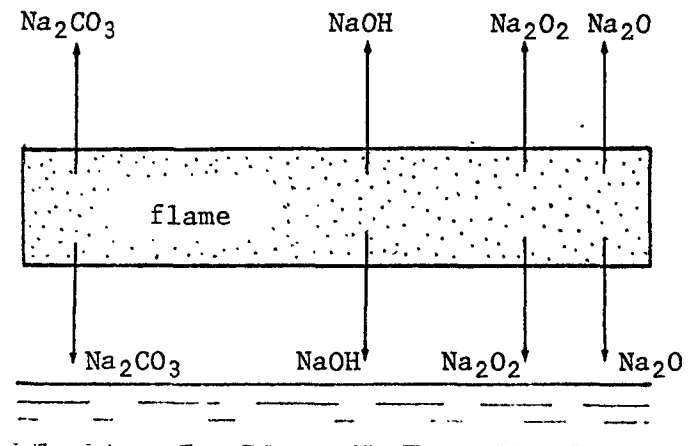to the flame sheet (reactants).

FIGURE 1b.   Sketch illustrating mass outflux
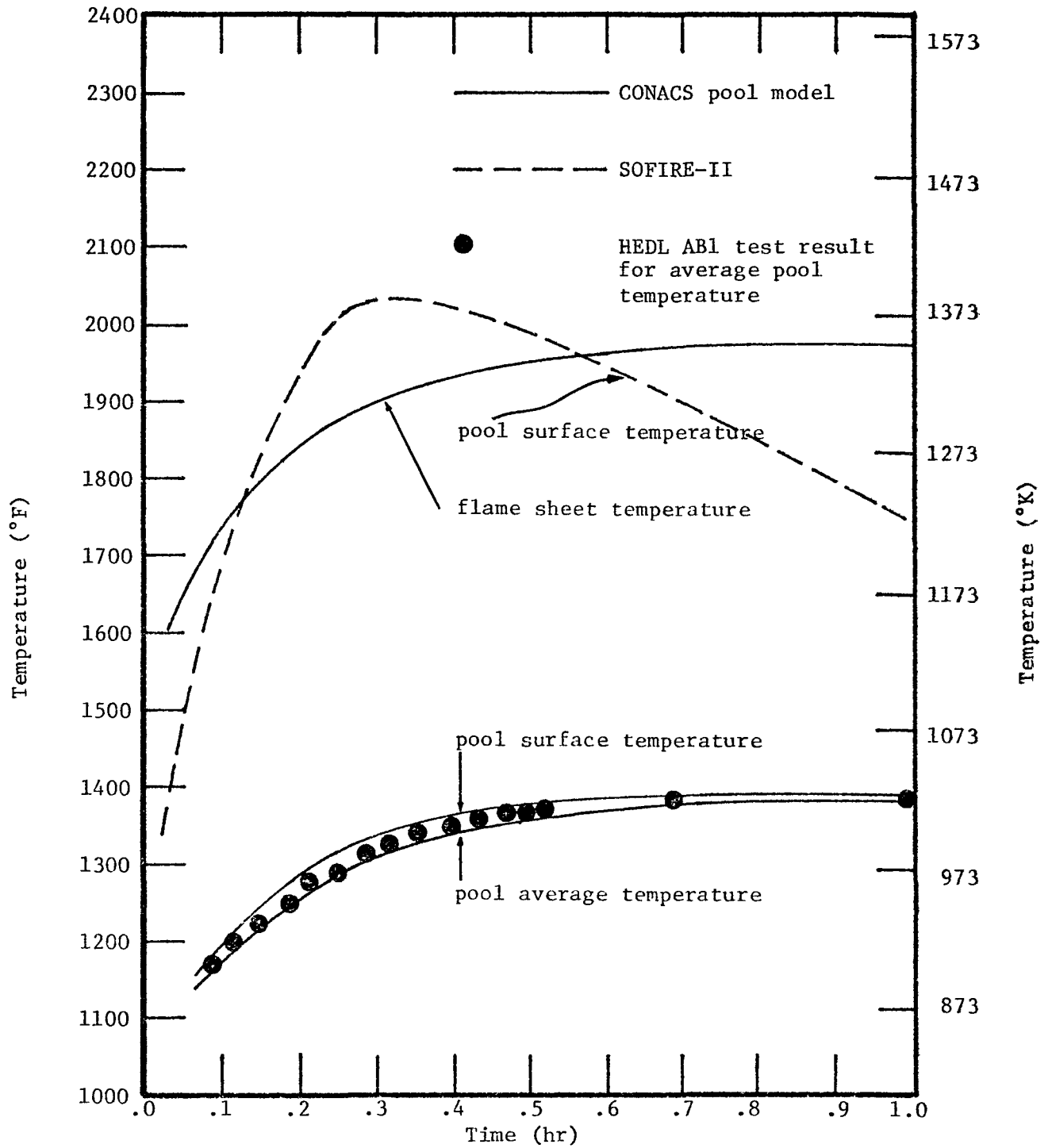from the flame sheets (combustion
products).

FIGURE 2. Comparison of predictions of CONACS pool model, SOFIRE-II and HEDL AB1 test.