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SODIUM SPRAY AND JET FIRE MODEL DEVELOPMENT WITHIN THE CONTAIN-LMR CODE*

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ABSTRACT

An assessment was made of the sodium spray fire model implemented in the CONTAIN code. The original droplet burn model, which was based on the NACOM code, was improved in several aspects, especially concerning (1) evaluation of the droplet burning rate, (2) reaction chemistry and heat balance, (3) spray geometry and droplet motion, and (4) consistency with CONTAIN standards of gas property evaluation. An additional droplet burning model based on a proposal by Krolikowski was made available to include the effect of the chemical equilibrium conditions at the flame temperature. The models were validated against single-droplet burn experiments as well as spray and jet fire experiments. Reasonable agreement was found between the two burn models and experimental data. When the gas temperature in the burning compartment reaches high values, the Krolikowski model seems to be preferable. Critical parameters for spray fire evaluation were found to be (1) the spray characterization, especially the droplet size, which largely determines the burning efficiency, and (2) heat transfer conditions at the interface between the atmosphere and structures, which controls the thermal hydraulic behavior in the burn compartment.

I. INTRODUCTION

A variant of the CONTAIN code has been developed to analyze the thermal-hydraulic and radiological conditions in the containment of a liquid-metal reactor (LMR) during a severe accident.[1] This variant is based on the light-water-reactor (LWR) version of CONTAIN,[2] which provides a number of models that are either generic or readily converted to LMR analysis through a change in coolant type. A number of these models, such as those for aerosol behavior, heat transfer to structures, and intercompartment flow, are used in some of the experimental comparisons discussed below. However, because of space limitations, see Reference 2 for the details of these models. Also, see Reference 1 for a discussion of the sodium-specific models available in the current officially released LMR version, CONTAIN-LMR/1B-Mod. 1. The present discussion will focus on recent work on the assessment of the spray fire model in this released version and on the improvements in the modeling that were subsequently implemented.

II. CONTAIN-NACOM SPRAY FIRE MODEL

The spray fire model available originally in CONTAIN LMR/1B Mod. 1 is based on the NACOM code developed by Tsai.[3] The model can be activated in more than one cell and it may be combined with any other CONTAIN option, for instance, with pool fires or bulk atmosphere chemistry, which allows flexibility in experimental analysis as well as in accident description and evaluation.

The main model characteristics are the following:

(1) The burning compartment is described as one cell. The atmosphere is considered homogeneous and well mixed. Gas motion and the feedback to spray motion are not taken into account.

(2) The sodium spray orientation is assumed to be downward. The droplet size distribution is separated into 11 size classes and follows the Nukiyama-Tanasawa

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correlation.[4] The spray is characterized by the mass mean droplet diameter and fall height.

(3) The droplet velocity is taken equal to the terminal fall velocity. The burn history of one droplet of each size class is followed during its fall until it is either consumed or reaches the floor. The effect of the droplet swarm is taken as that of the single droplet multiplied by the number of droplets. No interaction between burning droplets is considered.

(4) The droplet burning model assumes immediate vapor-phase burning, without a preignition phase. The burning rate is based on the D^2-law, which expresses the observation that the square of the diameter of a burning droplet decreases linearly with time

$$D^2 = D_i^2 - Kt \tag{1}$$

From this equation, the burning rate of a stationary droplet is obtained as

$$BR_0 = \frac{\pi}{4} \rho_{Na} K D \tag{2}$$

The vapor-phase burning coefficient K is taken from Spalding[5]

$$K = \frac{8k_g}{C_{pg} \rho_{Na}} \ln(1 + B) \tag{3}$$

with the transfer coefficient B

$$B = \frac{1}{h_{fg}} \left(C_{pg}(T_g - T_{Na}) + h_{com} \frac{Y_{O2}}{i} \right) \tag{4}$$

For a moving droplet, the effect of forced convection is taken into account by setting

$$BR = BR_0 \left(1 + C_f Re^{1/2} Pr^{1/3}\right) \tag{5}$$

where the empirical constant C_f is chosen as 0.3.

(5) Heat released from the burning zone is modeled through a balancing scheme. The reaction heat is distributed between the unburned sodium, which is collected in a pool, and the atmospheric gas. Aerosols are considered to have no heat capacity. There is no direct heat transfer to structures. Heat exchange between gas and structures can be modeled through the standard CONTAIN options for convective and radiative heat transfer,[2] although radiative heat transfer was not invoked in the calculations discussed below.

III. REVISED SPRAY FIRE MODEL

As shown below, the analysis of spray fire experiments with the model as described in the previous section resulted in significant discrepancies for important fire parameters. Besides intrinsic difficulties related to the problem of droplet size specification, other reasons were identified. First, the CONTAIN module was, in some modeling aspects, a simplified version of the NACOM code. Second, the NACOM model itself had a number of limitations and approximations that needed closer inspection. The components of the spray fire model were therefore subjected to an extensive revision, and major improvements were implemented.

In the original NACOM code, a preignition model was available, but this was not activated in CONTAIN. It is, however, activated in the new spray fire model. It treats the reaction of sodium with oxygen at the droplet surface during the period after injection when the droplet temperature is too low to sustain vapor-phase burning. The reaction is controlled by oxygen diffusion to the droplet surface. The oxygen flow rate is determined by a heat-mass transfer analogy, which leads to the following formulation for the burning rate:

$$BR_p = \frac{\pi}{i} D C_{diff} \rho_g Y_{O2,g} Sh \tag{6}$$

The reaction heat is transferred to the droplet, which exchanges heat with the surrounding gas by natural convection. When the heated droplet reaches a temperature close to the boiling temperature of sodium, the preignition phase is terminated and vapor-phase burning starts.

The NACOM vapor-phase burning model has been basically retained as described in Section II, but several modifications have been made. The main changes are as follows:

(1) In Eq. (4), which defines the transfer coefficient B, the value of the heat of combustion h_{com} used in the NACOM code is the reference value of the heat of formation. According to Spalding,[5] h_{com} must be the

reaction heat of the fuel in the vapor phase. Therefore, h_{com} was changed to $h_{com} = h_{com,ref} + h_{fg}$. It may be mentioned that Spalding's theory was developed for hydrocarbon fuel, for which the evaporation heat is very small compared to the combustion heat and may be neglected in practical applications. This is not the case for sodium.

(2) In the original model, the user has control over the reaction product composition through the input variable FNA2O2, which defines the stoichiometric ratio i of Eq. (4). The analysis of aerosols produced in sodium fires indicates a high fraction of peroxide. However, thermodynamic considerations suggest that at the temperature of the flame zone, monoxide is the principal stable reaction product. Therefore, in Eq. (4), the value of i is now internally set to that for monoxide formation. The reaction of monoxide to peroxide in the new model occurs outside of the flame zone depending on the bulk gas temperature. During the preignition phase, the reaction occurs at a relatively low temperature. Direct peroxide formation is assumed in this case, and the stoichiometric ratio i is chosen accordingly. The user can no longer specify the fraction of peroxide formed.

(3) Consistent use of gas properties evaluated at the boundary layer temperature $T_{bl} = 1/2(T_g + T_{Na})$ is made, which was not the case in the original NACOM formation.

(4) To model the droplet motion more accurately, an acceleration equation has been built into the model. The droplet velocity is now calculated according to the equation

$$\frac{dv}{dt} = g - \frac{3\,\rho_g\,v^2\,C_{dr}}{4\,\rho_{Na}\,D} \tag{7}$$

In the solution of the acceleration equation, the sodium mass loss from burning and the density variation from temperature changes are taken into account. The user may specify an initial velocity corresponding to the injection velocity of the sodium into the spray cell. A negative initial velocity describes an upward spray. If an upward-moving droplet hits the celling, then its velocity is set to zero, and it starts to fall downward.

(5) An option was introduced to describe the gas motion in the burning compartment and to estimate the possible influence on the droplet trajectory. The burn compartment is separated into a number of cells that describe, for instance, the spray cone and other volumes like those adjacent to walls. The cells are connected by open flow paths. In this manner, a limited capability for modeling gravity-driven convection inside a compartment is provided. From the gas flow through the spray cone calculated by CONTAIN, an effective gas velocity is deduced and the droplet velocity is corrected accordingly.

(6) There is experimental evidence that a maximum droplet size is not exceeded.[6] This is consistent with the criterion that a droplet becomes unstable if its Weber number exceeds a value of 12.[7] This leads to the relation

$$D_{crit} = 2\sqrt{\frac{\sigma_{Na}}{g\,\rho_{Na}}} \tag{8}$$

which results, for typical sodium properties, in $D_{crit} \approx$ 8 mm. An option has been added which redistributes a droplet spectrum with given mean diameter if size classes with $D > 8$ mm occur. In this case, the oversize droplets are reduced to a stable diameter, and the excess mass is added to a size class with a diameter of about 2 mm, the observed size after breakup.

The NACOM model assumes zero oxygen concentration in the flame zone. However, at high temperatures, the dissociation of the reaction products leads to the situation that sodium vapor, oxygen, and reaction products are in chemical equilibrium with non-negligible concentrations in the flame zone. Therefore, a second burn model, following a proposal of Krolikowski,[8] has been implemented into the CONTAIN spray fire module. This second model utilizes the preignition, drop size, and drop trajectory modeling of the improved NACOM model, but in contrast, the second model actually models the flame zone conditions. The model is based on the assumptions of (1) diffusion-controlled oxygen flux to the flame (2) diffusion of sodium to the flame in a stoichiometric ratio, and (3) maintenance of chemical equilibrium for the combustion reaction in the burning zone at the flame temperature. From these assumptions, one obtains three equations for the oxygen molar flux to the flame, for the oxygen molar concentration in the flame zone, which is formulated in Eq. (10) for the case of pure monoxide production, and for the flame temperature, deduced from a heat balance:

$$N_{O2} = c_m \frac{Y_{O2,g} - Y_{O2,f}}{1 - Y_{O2,f}} \tag{9}$$

$$\Delta F = R\, T_f \ln\left(16\ (p\ Y_{O2,f})^{5/2}\right) \tag{10}$$

$$N_{O2}\, Q_c = \sigma\, \varepsilon \left(T_f^4 - T_g^4\right) + h\,(T_f - T_g) \tag{11}$$

Heat and mass transfer coefficients are obtained from Nusselt and Sherwood correlations. In contrast to the original model by Krolikowski, the CONTAIN model assumes a composite reaction product, depending on the flame temperature. In addition, the flame diameter D_f is taken as the characteristic length used in evaluating the boundary conditions. D_f is estimated, following Newman,[9] by setting the liquid sodium to flame surface area ratio equal to the fraction of heat output received by the droplet:

$$\frac{D}{D_f} = \sqrt{\frac{h_{fg}}{h_{com}}} \tag{12}$$

A comparison of droplet burning rates obtained with the NACOM model and the Krolikowski model at low temperatures shows good agreement in magnitude as well as in dependencies on principal governing parameters. Figure 1 gives as an example the burning rate as a function of the gas velocity around the droplet. The burning rate at high gas temperature, however, is completely different as shown in Figure 2. The NACOM burning rate increases with gas temperature, which means that

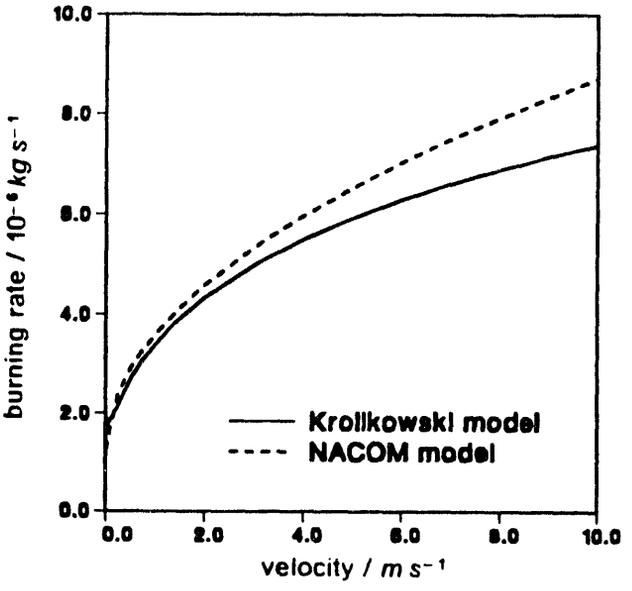

Figure 1. Comparison of NACOM and Krolikowski Droplet Burn Models

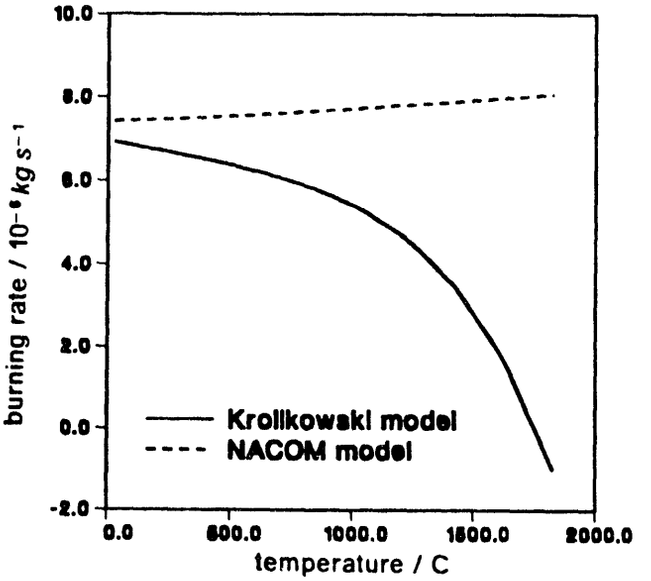

Figure 2. Comparison of NACOM and Krolikowski Droplet Burn Models

there is no limitation for the reaction process at high temperature. The Krolikowski model, more realistically, predicts a decreasing burning rate with increasing temperature, and it reaches zero at about 1750°C. This agrees with chemical stability considerations and with experimental evidence, which suggests a maximum sodium flame temperature in the range of 1500°C to 1800°C.[9]

It should be noted that the burn efficiency obtained calculations with a droplet burn model is very sensitive to the droplet size. For a given sodium mass flow rate, one can deduce from Eqs. (1)-(7) that the total burning rate varies as D^{-2} and $D^{-1.25}$ in the limit of very small and very large drops, respectively, for a monodisperse distribution of spherical drops. Even for controlled experiments, droplet diameter and size distribution are parameters that are difficult to determine; therefore, a certain arbitrariness exists in spray fire analysis. For accident analysis, the droplet size is even more difficult to predict since it depends on uncertain parameters such as leak size and shape, driving pressure, and shape and orientation of intercepting obstacles. The difficult problem of applying a droplet-based model to accident analysis will not be addressed here.

IV. COMPARISON WITH EXPERIMENTS

Burn experiments with stationary single sodium droplets were reported by Richard, who investigated the

Table 1. Comparison of Measured and Calculated Burning Rates (revised NACOM and Krolikowski) of Stationary Sodium Droplets at 21 % Oxygen in Air

		BR/D $10^{-3}kgm^{-1}s^{-1}$		
			Calculation	
		Experiment	NACOM	Krolikowski
Richard	T_g = 250C	0.85	0.30	0.41
D = 2 mm	300C	0.95	0.31	0.41
	350C	1.15	0.32	0.41
AI	high	1.08, 1.11, 1.19		
D = 7 mm	humidity	5.05		
	low	0.07, 0.12, 0.16	0.27	0.48
	humidity	0.59, 0.69		
		0.88, 0.90, 1.15		

dependency of the burning rate on parameters such as droplet size, oxygen mole fraction, and gas temperature.[10] At Atomics International (AI), the burn behavior of droplets of approximately 7 mm diameter were studied in atmospheres with different humidity.[11] Table 1 compares BR/D ratios, which should be independent of droplet size according to Eq. (2). One finds a significant scatter in the experimental values, especially in the AI data at low humidity, which have not been satisfactorily explained.

Richard's values suggest a relatively strong dependency on the gas temperature that is not reproduced by the models. There is an overall underprediction of the measured values, especially with regard to the NACOM model. It must be considered, however, that a stationary burning droplet creates a gas flow due to gravity-driven convection that is not simulated in the calculation. This may partly explain the difference.

Burn experiments of single sodium droplets falling from a 14.7-m height have been performed by Morewitz et al.[6] Measured quantities included fall distance to ignition and mass fractions burned. Figures 3 and 4 show comparisons with calculated values. Very good agreement is found for the fall distance of the droplets to ignition if one assumes an ignition temperature in the range of 1050 to 1150 K. Also, the fraction of mass consumed during the droplet fall is in excellent agreement for the whole range of droplet sizes that was investigated. Although only Krolikowski model results are shown, the revised NACOM model results are very similar.

The large-scale SOFICOV spray fire experiment was especially performed for code validation.[12] In the present calculations, the test vessel of 850-m^3 volume was

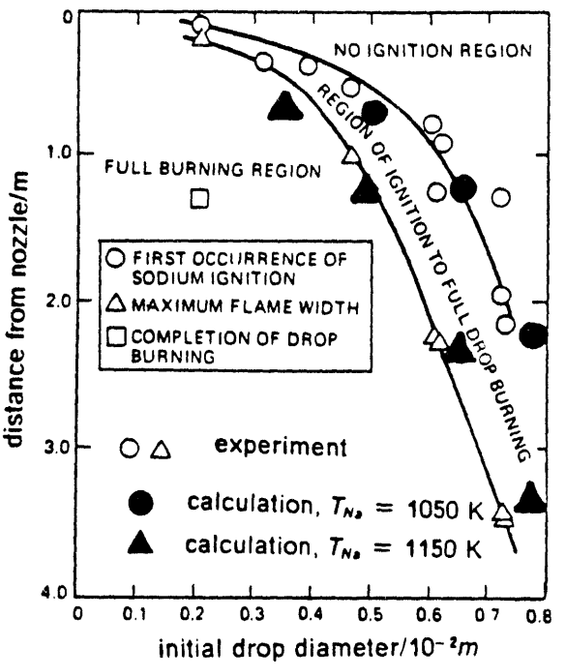

Figure 3. Burning Characteristics of Falling Sodium Drops in Air

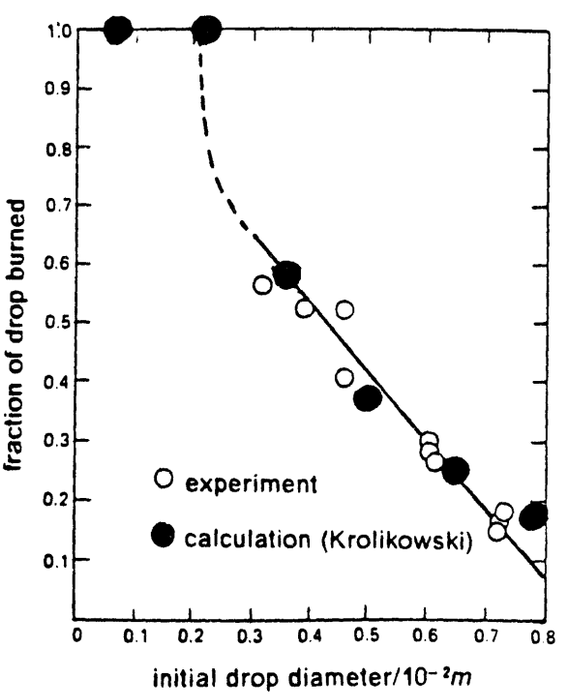

Figure 4. Fraction of Sodium Mass Consumed During Fall at 14.7-m Distance

modeled in five cells. One cell represented the spray cone of 3.5-m diameter and 13-m height, another the volume that surrounds the cone and contacts the cylindrical section of the vessel, and the others represented volumes for top and bottom vessel heads. The calculation included the effect of gas convection on droplet fall and the reaction with water vapor, which are treated in other CONTAIN modules. Figures 5 to 7 show temperature and pressure curves and aerosol concentrations obtained with the original and the revised NACOM model in comparison with measured data. The Krolikowski model results are very similar to the revised NACOM ones. For the revised model, one finds good agreement in the aerosol behavior during the whole analysis period and in the thermal-hydraulic behavior during the first 200 s of the fire. Overall, the new model underestimates pressure and temperature values. This is in line with the results of other spray fire codes that participated in the experiment analysis.[12] Of all codes, however, the new CONTAIN model agrees best with the experimental data, and it represents a significant improvement over the original model. One reason for the differences still observed is the underprediction of the burn efficiency, which is calculated to be about 50% of the sodium injected, compared to the measured 80%. There is some question about the accuracy of the droplet size given in the SOFICOV report, since this parameter was not measured with sodium but deduced from data obtained with water. However, the median droplet size used in the calculation would have to be reduced from 5.5 mm to 3.5 mm to obtain the measured efficiency, a value which seems to lie outside the range of uncertainty. Other effects that could increase burn efficiency include splashing of unburned droplets on the catch pan and additional heating by a pool fire. Including the CONTAIN pool fire option, however, caused only a negligible effect. Figures 5 and 6 also suggest a different tendency in thermal-hydraulic behavior. The experiment shows an increasing temperature in the burn compartment, resulting in pressure and temperature maxima late in the burn period, while the calculation proposes early maxima with relatively little change later on. A possible reason could be a change of heat transfer conditions during the fire. Because of aerosol deposition on structures, one may expect an insulating effect for convective heat exchange and possibly an increased surface albedo. Figure 8 shows the results of two demonstration calculations, performed with an artificially increased burn efficiency to match the experimental one. The first calculation used the CONTAIN default convective heat transfer modeling with a coefficient of about 12 $Wm^{-2}K^{-1}$, the second a user-specified, time-dependent heat transfer coefficient of 25 $Wm^{-2}K^{-1}$ at the beginning of the burn, decreasing to 6 $Wm^{-2}K^{-1}$ at T = 1800 s. A rather good agreement for the thermal

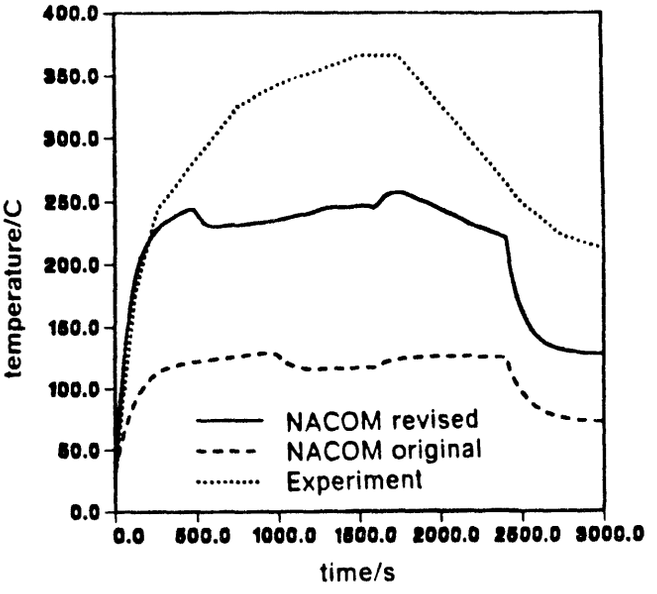

Figure 5. SOFICOV Experiment: Comparison of Gas Temperatures

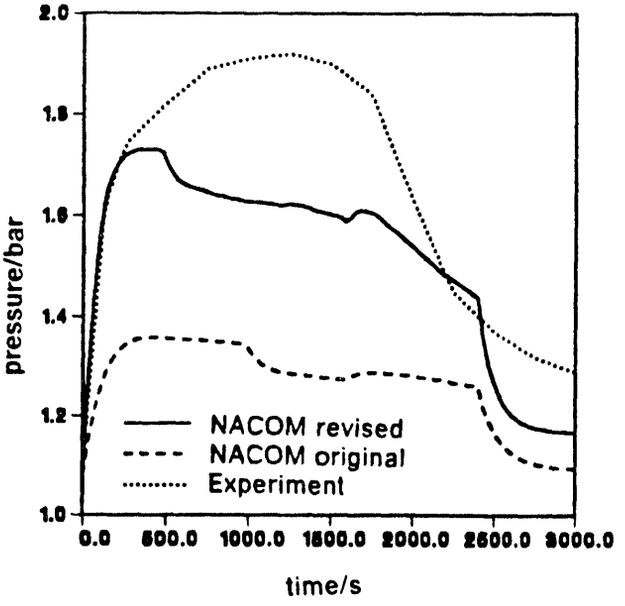

Figure 6. SOFICOV Experiment: Comparison of Pressure Evolution

hydraulic behavior in the burn compartment is found in the second case. This implies that the modeling of aerosol-dependent heat transfer conditions for convective an/or radiactive heat exchange may need to be improved.

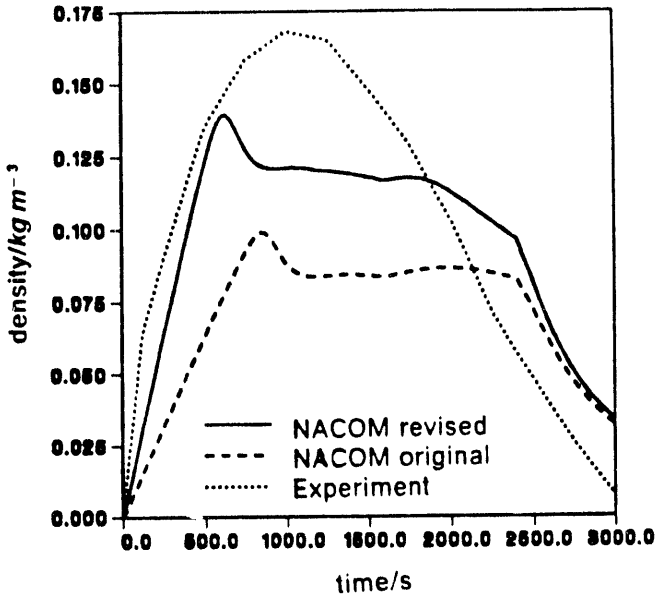

Figure 7. SOFICOV Experiment: Comparison of Aerosol Behavior

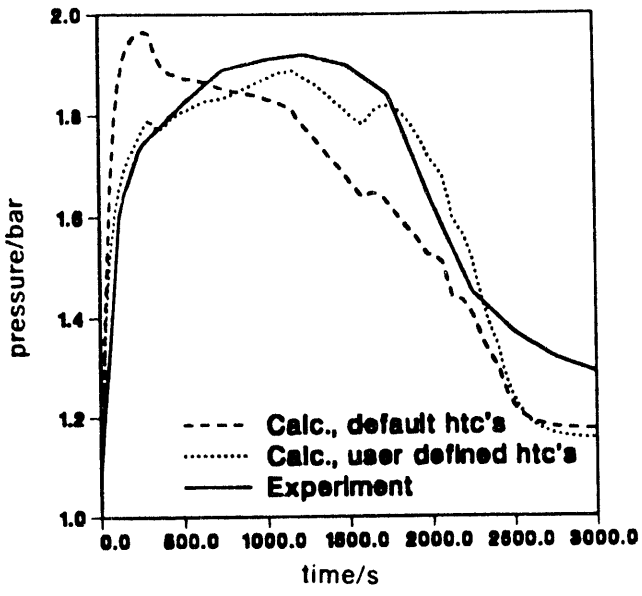

Figure 8. SOFICOV Experiment: Comparison of Pressure Evolution, Calculated with Default and Time-Dependent Heat Transfer Coefficients

Table 2. The FAUNA FS Experiments, Comparison of Calculated and Measured Peak Pressure Values

			Maximum Overpressure (bar)						
							Calc./Exp.		
	Source Rate (kg/s)	Total Mass (kg)		NACOM			NACOM		
			Exp.	Orig.	Rev.	Krolikowski	Orig.	Rev.	Krolikowski
FS 11	0.82	30	1.07	0.26	0.97	0.91	0.24	0.91	0.85
FS 13	0.52	30	1.07	-	0.90	-	-	0.84	-
FS 21	0.84	90	1.37	-	1.76	1.55	-	1.28	1.13
FS 30	1.36	105	1.42	0.70	2.84	2.00	0.49	2.00	1.41
FS 31	2.19	105	1.63	-	3.47	2.37	-	2.12	1.45
FS 35	5.44	105	2.05	0.92	4.45	2.80	0.45	2.17	1.37

Sodium jet fire experiments were performed in the FAUNA facility at KfK.[13] Various nozzle types were used, from which jets were directed upward onto a plate located 6 m above the nozzle. The source rate was between 0.5 and 5.5 kg/s and the total sodium mass was 30 to 105 kg. The burn compartment of 220 m^3 volume was represented in the present calculation as a single cell. The sodium geometry was simulated as a spray falling from a 6-m height; the sodium jet itself was not modeled. The same mass mean droplet diameter of 4 mm was used for all experiments. Table 2 compares peak pressure values obtained experimentally to those obtained with CONTAIN using the original NACOM model, the revised NACOM model, and the Krolikowski model. One finds that the original model underpredicted the pressure values in all cases. The new models agree fairly well for low source rates and overpredict the pressure increase for high source rates. Here the overprediction by the Krolikowski model is less pronounced because of the reduced burn efficiency predicted by the Krolikowski model at the high

cell gas temperatures attained at the high source rates. It is likely that aerosol-mediated radiative heat transfer, which was not modeled, would significantly reduce the pressure predicted at the high source rates.

V. CONCLUSIONS

An assessment of the original NACOM-based spray fire model in the CONTAIN-LMR code has been conducted, and a number of modeling improvements have been made. Good agreement with single falling droplet experiments has been demonstrated, and significant improvement in the agreement with experimental results for other experiment geometries has typically been found. It appears, however, that good agreement with respect to burn efficiencies in single droplet measurements is not sufficient to ensure good agreement in spray and jet geometries, even when the droplet size distribution is fairly well characterized, as in the SOFICOV experiment. Therefore, it is likely that some collective effect of thedroplet swarm is important and is still not taken into account. When the spray burning efficiency is adjusted to fit the experimental value in the SOFICOV experiment, one observes that the pressure is initially too high, and then too low. The pressure can be forced to fit the experiment by assuming a larger than normal wall convective heat transfer coefficient at early times, and a smaller than normal coefficient at late times. Such variations in heat transfer may be related to aerosol effects, such as aerosol-mediated radiative heat transfer to cold walls and wall albedo changes, and insulative effects from aerosol deposition. These effects have not been taken into account in the present analyses.

NOMENCLATURE

B transfer coefficient
BR burning rate
BR_O burning rate, stationary droplet
BR_p burning rate, preignition phase
c_m mass transfer coefficient
c_p specific heat at constant pressure
C_{diff} diffusion coefficient
C_d drag coefficient = f(Re)
D droplet diameter
F Gibbs free energy
g acceleration resulting from gravity
h heat transfer coefficient
h_{fg} heat of evaporation of sodium
h_{com} combustion heat
i stoichiometric ratio
k conductivity
K burning coefficient
N molar flux
p pressure
Q_c reaction heat per mole O_2
R gas constant
t time
T temperature
v velocity
Y gas mole fraction

Greek Symbols

ε omissivity
ρ density
σ Stefan-Boltzmann constant
σ_{Na} surface tension of liquid sodium

Subscripts

d droplet
f flame
g gas
Na sodium
$O2$ oxygen

Dimensionless Quantities

Re Reynolds Number
Pr Prandtl Number
Gr Grashoff Number
Sh Sherwood Number

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