Validation of the Sodium Fire Models in the CONTAIN-LMR/1B-Mod.1 Code against the ABCOVE Experiments

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1. Introduction

The KAERI has developed the design and analysis technique of a pool-type sodium-cooled fast reactor as the prototype Gen-IV sodium-cooled fast reactor (PGSFR), since 1987. This reactor uses sodium as a reactor coolant to transfer the core heat energy to the turbine. Leaked sodium violently reacts with oxygen in the containment atmosphere under postulated accident conditions. The heat generated from the combustion reaction between leaked sodium and oxygen increases the temperature and pressure of the containment atmosphere. The structural integrity of the containment building which is a final radiological defense barrier could be threatened by the sodium fire accidents. For estimation of transient pressure and temperature of the containment atmosphere during a sodium fire accident, the CONTAIN-LMR/1B-Mod.1 code[1] was selected as a design tool for the PGSFR containment.

The purpose of this study is to validate the sodium fire models in the CONTAIN-LMR/1B(-Mod.1) code against the ABCOVE experimental data and to compare the results with the MELCOR results without using the sodium fire models.

2. CONTAIN-LMR/1B-Mod.1 Code

CONTAIN is a best-estimate tool for the analysis of containment phenomena during severe reactor accidents, which is supported by the USNRC and has been developed and maintained by Sandia National Laboratories (SNL). CONTAIN-LMR has been developed for application to liquid metal reactors (LMRs) using sodium coolant. The CONTAIN-LMR/1B code that has been used in this study was produced by applying LMR-specific updates to an official light water reactor (LWR) version of the CONTAIN 1.11 code[2] as the base version

3. Sodium Fire Models

Sodium is a soft silvery metal, which melts at 98°C. Sodium burns readily in an air atmosphere, especially in the presence of water vapor, forming various oxides.[3] Only two oxides, namely, sodium monoxide (Na_2O) and peroxide (Na_2O_2), are found to be abundant in the reaction products from the following chemical reactions.

$$4Na + O_2 \rightarrow 2Na_2O + \left(9.05\, MJ / kg\ of\ sodium\right) \quad (1)$$

$$2Na + O_2 \rightarrow Na_2O_2 + \left(10.97\, MJ / kg\ of\ sodium\right) \quad (2)$$

The following subsections briefly describe the sodium spray fire model and the sodium pool fire model implemented in the CONTAIN-LMR/1B.

3.1. Sodium Spray Fire Model

This model treats the combustion of sodium spray resulting from a postulated coolant pipe break or a breach of the upper head or vessel seal following an energetic slug impact in an LMR. The treatment of sodium spray fires is patterned after the phenomenological model used in the NACOM code[3].

An initial size distribution is determined from a correlation using a specified mean droplet diameter. The trajectory of the drops is taken as downward from the ceiling, with a velocity equal to the terminal velocity. The spray burning rate is the sum of the burning rates of all the droplets as follows:

$$\dot{m}_s(t) = \int_{D_i}\int_{t'} \dot{m}_f\left(D(D_i,t',t), V_f(D_i,t',t)\right) d^2N \quad (3)$$

where $\dot{m}_f$ is the sodium droplet burning rate as a function of the droplet diameter *D* and the droplet velocity V_f at a given droplet traveling time. D_i means the initial droplet diameter of size group *i*. d^2N is the number of droplets having diameters between *D* and *D* + *dD*, 6having elevations between *z* and *z* + *dz* at time *t*. These d^2N droplets are originated from the ceiling at time *t'*, having initial diameters between D_j and $D_j + dD_j$. The population of the group d^2N is assumed to be constant with time until the whole group is completely burned up.

The calculation begins by partitioning the injected sodium spray source among 11 discrete droplet-size classes according to the Nukiyama-Tanasama correlation [3], which may be written as

$$\frac{dR_V}{dD} = \left(\frac{3.915}{\bar{D}}\right)^6 \frac{D^5}{120} \exp\left(-\frac{3.915}{\bar{D}}\right) \quad (4)$$

Here, R_V is the volume fraction of spray which contains droplets of diameters smaller than *D*, and $\bar{D}$ is the volume mean diameter.

Then, the d^2N can be derived from the sodium leak rate $\dot{m}_l$ and drop size distribution as

$$d^2N = \frac{m_l(t')}{\frac{1}{6}\pi D_i^3 \rho_{Na}} \frac{dR_V}{dD_i} dt' dD_i = \frac{\dot{m}_l(t')}{\pi D_i^3 \rho_{Na}} \left(\frac{3.915}{\bar{D}}\right)^6 \frac{D_i^5}{20} \exp\left(-\frac{3.915 D_i}{\bar{D}}\right) dt' dD_i \quad (5)$$

where ρ_{Na} is the density of sodium.

The droplet-size distribution calculated by the code is a function of the user-specified mass mean droplet diameter. The fall time of each droplet class is approximated from its user-specified fall height and its terminal velocity.

The combustion rate is integrated over the droplet's fall to obtain the total mass of sodium burned. A combustion rate is computed for each size class as a function of the fall velocity, the gas and droplet temperatures, the oxygen content in the atmosphere, and the mass ratio of the oxygen reacted to sodium. The heat of combustion depends upon the kinetics of oxidation and, in particular, upon the relative proportions of Na_2O and Na_2O_2 in the reaction products, which can be specified by the user input parameter.

3.2. Sodium Pool Fire Model

The sodium pool fire model in CONTAIN-LMR/1B simulates the chemical reaction between sodium located in a pool and the oxygen in the atmosphere above the pool. The model is taken from the SOFIRE II code[4], in which the sodium burning rate is assumed to be proportional to the oxygen concentration. It is also assumed that oxygen in the atmosphere must diffuse to the pool surface through a convective boundary layer before the reaction can occur. This diffusion controls the burning rate. The diffusion coefficient for oxygen-nitrogen mixtures is found by Slattery-Bird expression:

$$D_{O_2-N_2} = 6.4315\times10^{-5}\frac{T^{1.823}}{P} \tag{6}$$

where T is the gas (film) temperature and P is the pressure.

During a number of pool fire tests, it was determined that the sodium burning rate was proportional to the oxygen concentration and was controlled by the diffusion of oxygen to the sodium surface. Thus, the burning rate can be computed by

$$\left(\frac{dm}{dt}\cdot\frac{1}{A_S}\right) = H_G C \rho_G S \tag{7}$$

Here, m is the mass of sodium burned, and t is the burning time, A_S is the surface area of sodium pool, C is the mass fraction of oxygen, ρ_G is the density of gas, and S is the stoichiometric combustion ratio. The gas transport coefficient, H_G, is derived from the free convection equation for the heat transfer coefficient invoking heat and mass transfer analogy. Thermal conductivity is replaced by the diffusion coefficient and the Prandtl number is replaced by the Schmidt number.

$$H_G = 0.14 D_{O_2-N_2}\left[gS_C\frac{\beta}{v^2}\left(T_{SS}-T_G\right)\right]^{1/3},\ \text{[ft/hr]} \tag{8}$$

where g is the gravitational constant, β is coefficient of gas expansion, v is kinematic viscosity, T_{SS} is the sodium surface temperature, and T_G is the gas temperature. The sodium burning rates calculated by the pool fire model depend on the temperature differential between the pool and the atmosphere. This temperature differential in turn depends on the heat flux between the pool and the atmosphere.

Sodium pool fires produce sodium peroxide and sodium monoxide aerosols. By default in the CONTAIN-LMR/1B, all of the peroxide is assumed to be aerosolized and all of the monoxide is assumed to enter the pool.

4. Validation against the ABCOVE Experiments

A program for aerosol behavior code validation and evaluation (ABCOVE) had been developed in accordance with the LMFBR Safety Program Plan.[5] A series of large-scale confirmatory tests were performed in the Containment Systems Test Facility (CSTF) vessel in the Hanford Engineering Development Laboratory (HEDL), covering a range of aerosol source release rates, source duration times, and complexity of aerosol composition.

Since 2013, SFR-capabilities of the MELCOR code had been developed by implementing the sodium properties data from the SIMMER-III, and the containment sodium fire models and the sodium atmospheric chemistry from the CONTAIN-LMR code.[6] In this previous study[6], code-to-code comparisons between the CONTAIN-LMR and the improved MELCOR were performed, but the compared CONTAIN-LMR code was a later version of the available CONTAIN-LMR/1B-Mod.1 code and validations with AB-6 and AB-7 experimental data was not included. In this study, the CONTAIN-LMR/1B calculation results for the ABCOVE experimental data are compared with the MELCOR calculations[7] without using the sodium fire models.

4.1. AB-5 Test

The ABCOVE AB-5 test is a single-species aerosol test by spraying sodium at high rate into an air atmosphere, performed in 1982. Figure 1 shows the CSTF vessel arrangement for the AB-5 test. The CSTF containment vessel is an $852m^3$ carbon steel vessel installed in a concrete pit. Aerosols were generated by a sodium spray fire. 223 kg of sodium was sprayed over a period of 872s (from 13s to 885s), with all the sodium converted to a 60% Na_2O and 40% NaOH aerosols. Compressed air (23.3% O_2) was injected at several times in the test to make up for sampling losses and to prevent the containment pressure from going negative. The containment vessel was kept sealed for $5.136X10^5$s (5.94days). The maximum containment pressure and mean atmospheric temperature attained were 214kPa and 553K.

Figs. 2 and 3 compare the CSTF atmospheric pressure and temperature predicted by using the

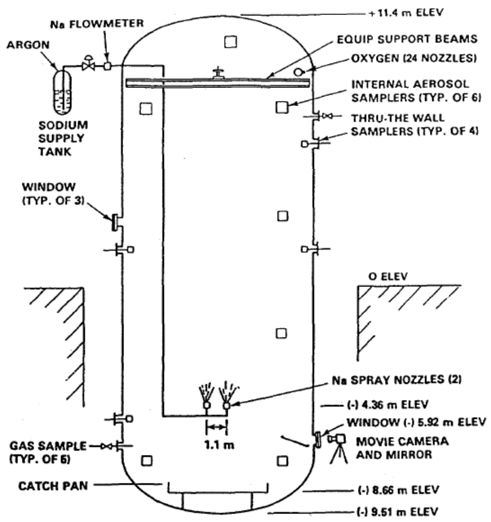

Fig. 1. CSTF Vessel Arrangement: Test AB-5.

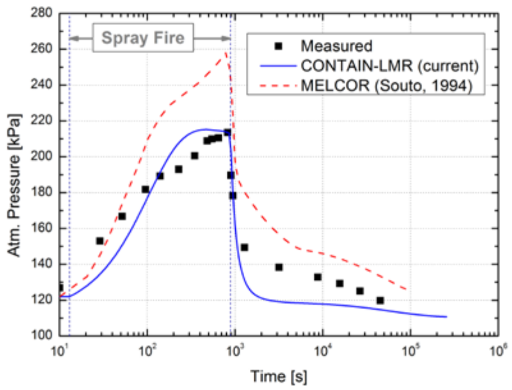

Fig. 2. CSTF Atmospheric Pressure of the Test AB-5.

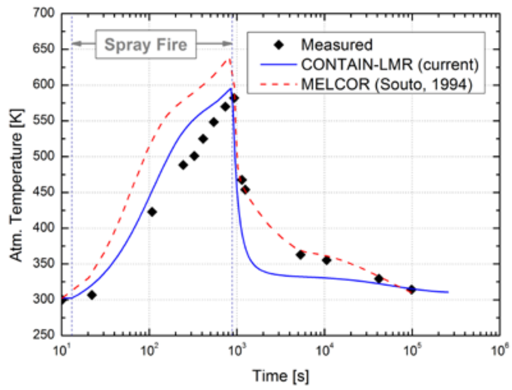

Fig. 3. CSTF Atmosphere Temperature of the Test AB-5.

CONTAIN-LMR/1B code with the experimental data[5] as well as the predicted values by using the MELCOR code [7]. As a result, the CONTAIN-LMR/1B predictions give more realistic atmospheric pressure and temperature values during the spray fire period than the MELCOR code. However, it is also observed that the CONTAIN-LMR/1B slightly under-estimates the atmospheric pressure and temperature after the sodium spray fire period.

4.2. AB-6 Test

The ABCOVE AB-6 test is a NaI aerosol release test in the presence of a sodium spray fire, performed in 1983.[8] AB-6 test was also performed in the CSTF vessel. The experimental conditions of the test simulated an accident in which a fission product aerosol, sodium iodide (NaI), was released in the presence of a sodium fire which released sodium combustion product aerosol. Therefore, a sodium iodide aerosol generator was added in the CSTF test configuration for test AB-6.

The test consisted of spraying 205kg of sodium into the CSTF over a period of 4780s (from 620s to 5,400s). Oxygen was also injected so that the oxygen concentration remained relatively constant during the test. All sodium was converted to an aerosol consisting primarily of a mixture of sodium peroxide and sodium hydroxide. The NaI source was terminated at 3000s, while the NaOx source continued for an additional 2400s. The maximum containment pressure and mean atmospheric temperature measured were 170kPa and 438.25K. From comparisons of the measured and the predicted atmospheric pressures and temperatures in Figs. 4 and 5, it was found that the CONTAIN-LMR/1B predictions give more realistic atmospheric pressure and temperature values during the spray fire period than the MELCOR code.

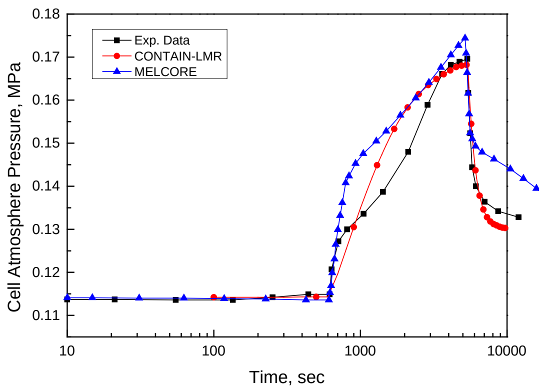

Fig. 4. CSTF Atmospheric Pressure of the Test AB-6.

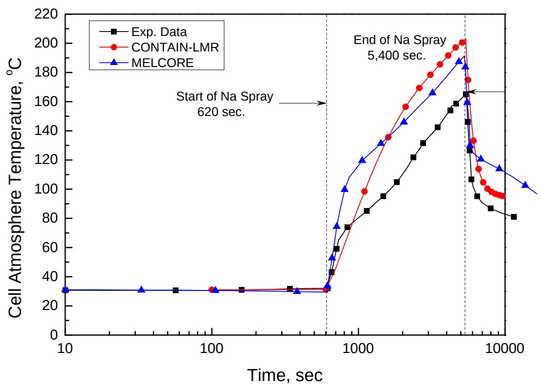

Fig. 5. CSTF Atmospheric Pressure of the Test AB-6.

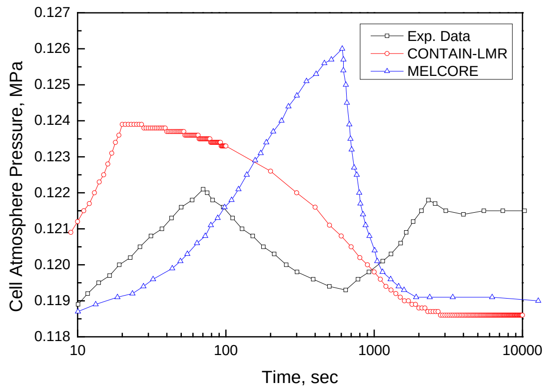

Fig. 6. CSTF Atmospheric Pressure of the Test AB-7.

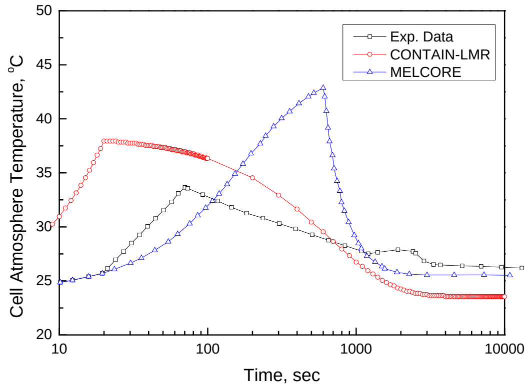

Fig. 7. CSTF Atmospheric Pressure of the Test AB-7.

4.3. AB-7 Test

The ABCOVE AB-7 test is a NaI aerosol release test after the end of a small sodium pool fire, performed in 1984.[9] Test AB-7 began with the injection of sodium into the containment vessel. The sodium spraying line failed immediately after the initiation of the sodium flow. The failure was such that sodium leaked from the line and fell about 10m down to the personnel deck at the -1.68m elevation, where it formed a pool and burned as a pool fire. The flow of sodium was stopped 20s after. The duration of the sodium fire is believed to have been approximately 10 minutes. The NaI aerosol was released at time 600s, and its generation remained constant until the end of the NaI source period at 2400s.

In the CONTAIN-LMR/1B simulation of the AB-7 test, a sodium spray fire was assumed with a spray height of 10.0m during the sodium leakage phase for 20s. Figure 6 and 7 show the measured and the predicted atmospheric pressures and temperatures, respectively. The peak pressure and temperature by using the MELCOR code without any sodium fire model are the maximum values, since it was assumed that all the injected sodium had been converted into NAOH and the total heat had been uniformly added to the CSTF atmosphere during the leak period of 600s.[9] On the other hand, the sodium spray fire of early 20s was assumed with a mean sodium droplet diameter of 0.00318 m. Though the CONTAIN-LMR/1B simulation with sodium fire models gives the better matched trends of the CSTF atmospheric pressure and temperature, sensitivity studies for some unknown parameters still remain for more detailed predictions.

5. Conclusions

In this research, the sodium fire models in the CONTAIN-LMR/1B code were investigated and validated successfully against the ABCOVE experimental data. From the validation results, it was confirmed that the CONTAIN-LMR/1B predicted conservatively the maximum atmospheric pressure and temperature in the containment under postulated accident conditions.

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