

Computational Fluid Dynamics Coupled with Chemical Reaction in Sodium-Cooled Fast Reactor Technology

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Abstract

Computational fluid dynamics and chemical reaction play an important role in the safety evaluation of a liquid metal cooled fast reactor (LMFR). The LMFR is sodium cooled because of its preferable thermal-hydraulic performance, neutronic characteristics and compatibility with the structural materials. On the other hand, it is noted that the sodium is chemically active and combustible under oxygen and/or water vapor conditions. Therefore it is essential to solve engineering and scientific issues related to the usage of the sodium as the coolant of the LMFR. Since sodium reactions with oxygen and water vapor are complicated phenomena of reacting fluid flow, the physical and chemical processes are not well understood in detail. Important phenomena in sodium technology are chemical reaction of sodium with oxygen and water vapor in case of structural failure of a heat transport system. In this context, a research has been initiated to quantify fluid dynamics, chemical reaction of sodium and aerosol dynamics mostly based on computational methodology.

Figure 1 shows representative geometrical and physical scale of sodium thermal-hydraulics and chemical reaction in case of sodium fire. The largest scale is tens of meters that represent the size of a reactor building and rooms. In the sodium pool fire, the burning pool size ranges from 10 cm to 10 m. In the sodium spray fire, the size of sodium spray cloud is a few meters and the sodium liquid droplet size is a few millimeters. The boundary layer thickness of the diffusion flame is an order of a few millimeters since sodium saturated vapor pressure is low. It is known that the reaction products are sodium oxide and sodium hydroxide aerosols. The initial aerosol size is measured to be 0.1 μ m to 0.5 μ m. They are floating in the air with 0.1 μ m to 10 μ m diameter.

In the present study, two numerical methodologies for sodium reaction at sodium-oxidizer interface has been developed. One is the boundary layer equations approach and the other is the Navier-Stokes equation approach for the flow field simulation in the burning region. In both approaches, mass, momentum and energy conservation equations are solved to obtain thermal-hydraulic fields coupled with chemical reactions. The validity of the boundary layer approximation has been crosschecked by comparison with the Navier-Stokes equations solutions. The chemical reactions are evaluated with the chemical equilibrium model using Gibbs free energy minimization method. The chemical reaction and heat and mass transfer are solved interactively considering radiation heat transfer and behavior of reaction product aerosols. Regarding the chemical reaction products, the aerosol behavior is calculated in detail. Since the behavior greatly depends on the size of the aerosols, the diameter is discretized into multi-groups.

Numerical results are compared with sodium pool combustion experiments. The burning rates for the sodium pool combustion have been calculated at various pool temperatures and oxygen concentrations. Furthermore, the temperature and location of the flame are evaluated using the methodology. The computations reproduce the experimental observations concerning burning rate, flame temperature and flame height, consistently. Particularly, the mechanism of the experimental evidence that the pool temperatures do not exceed 1000 K is identified based on the computations. The sodium evaporation heat is approximately one third of the combustion heat. Therefore, about 30% of the combustion heat must be supplied to the sodium pool at least

to sustain the combustion. If the sodium pool temperature exceeds 1000K, the combustion flame moves away from the pool surface and less combustion heat is transferred to the pool. This is the mechanism that the combustion rate reaches an upper limit as the pool temperature increases in the sodium pool combustion. The heat transfer is affected by the interaction of thermal-hydraulics, chemical reaction and aerosol behavior. It is an intrinsic feature that the sodium pool combustion is self-limited and negative feedback seems to be at work.

Concerning the reaction products aerosol behavior, computed aerosol release rates are compared with experiments. Here the aerosol release rate is defined as the fraction of the aerosol mass released to the atmospheric gas to the total production by the combustion. The aerosol release rates are also in good agreement with the measurement. They increase as the combustion flame moves away from the pool surface. The movement of the sodium oxide aerosol that diameter is of 0.1 to 1 μm is mostly dominated by the gas flow and thermophoresis. Hence the aerosol release rate is strongly dependent on the temperature gradient in the flame region and location of the reaction zone. At low pool temperatures, the flame is close to the pool surface and thermal conduction to pool is the major heat transfer mechanism. The aerosols move toward the pool surface because of the thermophoresis caused by the temperature gradient. On the other hand, as the pool temperature increases, the vaporized pressure of sodium increases and the flame goes apart from the pool surface. In this situation, radiation heat transfer to atmospheric gas becomes most dominant and the aerosols are transferred to the atmosphere by a convective gas flow.

Comparing with Navier-Stokes equations solutions, the author found that the sodium burning rates are in consistent with the boundary layer analysis. Since the Navier-Stokes equation solutions are costly, parametric analyses are not practical. It is found that the local sodium burning rates are dependent on the radial coordinate. In other words, at the edge of the sodium pool, oscillating flow and slightly higher burning rate has been analyzed. Transient course of the total burning rate is periodically oscillating because of the fluctuation of natural convection airflow

In conclusions, the sodium reaction rate has been reasonably evaluated if the thermal-hydraulics and chemical reaction are solved interactively. The computational results are in consistent with the experimental data in various aspects and the boundary layer equations model can predict the sodium combustion phenomena. Navier-Stokes equations model is also available.

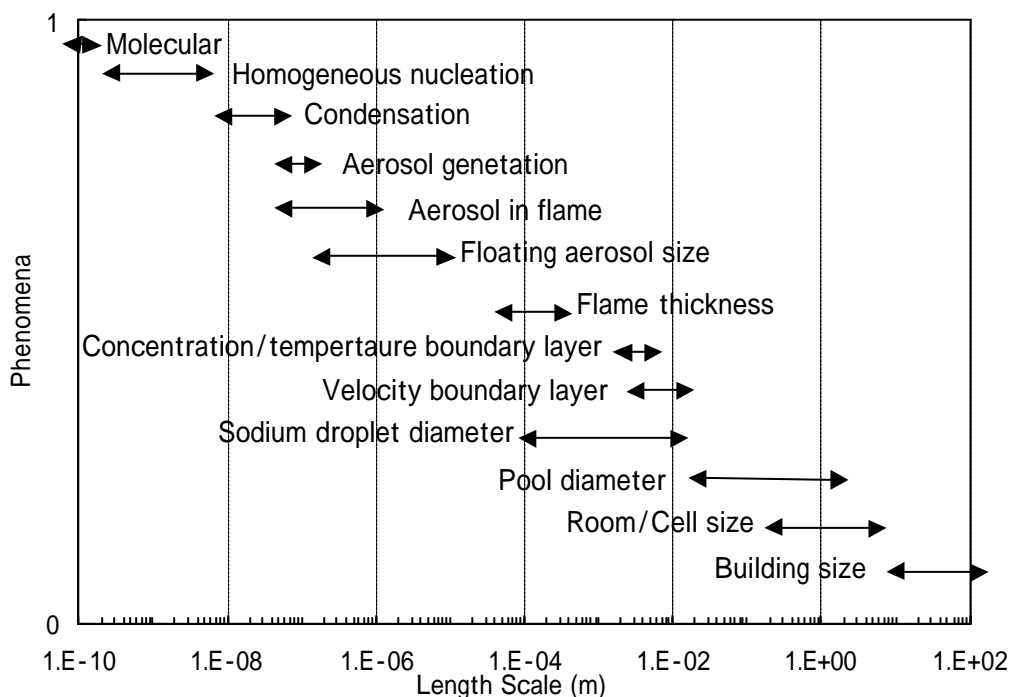


Figure 1 Magnitude of scale for sodium reaction with oxidizer.