# Molecular dynamics approach to sodium–water reaction compensating macroscopic heat and mass flow dynamics for LMFBR safety

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Many theoretical and experimental studies concerning the sodium–water reaction in a heat exchanger have been performed to evaluate the safety of a liquid metal cooled fast breeder nuclear reactor (LMFBR). When vapor accidentally leaks from piping in a turbine system into the sodium forming the vapor jet, the following sodium–water reaction occurs on the vapor–sodium boundary:

$$Na+H_2O \rightarrow NaOH+(1/2)H_2,$$
$$2Na+H_2O \rightarrow Na_2O+H_2.$$
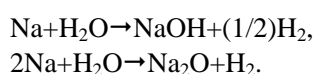
Theoretical studies have used macroscopic Navier–Stokes equations and heat-mass-transfer equations. However, these equations require chemical and physical data concerning the reaction rate and reaction energy. The present study targets the analysis of the reaction and energy production rates in terms of classical molecular dynamics using the quantum molecular orbital method [1-3]. The quantum electronic state calculation determines the atom-atom interaction potential using Gaussian quadratures in the local density functional scheme. Initially, the classical molecular dynamics with a two-dimensional solid sphere model was performed in order to evaluate the collision between H_2O molecules and sodium surface atoms and initial momentums assigned to H_2O molecules obeyed the Boltsmann distribution. The collision rate between H_2O molecules and the sodium surface was derived as a function of the vapor pressures and temperatures.* The averaged heat and mass generated on the macroscopic reaction surface will be utilized in macroscopic heat and mass flow dynamics.**

References
[1] K. Fukushima, J. Mizuno, K. Fujima and H. Adachi, J. Phys. Soc. Jpn. 51 (1982) 4028.
[2] K. Fukushima, Int. J. Quant. Chem. 109 (2009) 2664.
[3] K. Fukushima "Atom-atom interaction potential by the Gaussian Quadrature and classical molecular dynamics", The 6th International Conference on DV-Xα Method (DV- Xα 2010) (Taejeon, Korea, 2010).

Appendix: Collision in reaction and microscopic analysis available to macroscopic flow dynamics

*The reaction rate is expressed as a product of the H_2O–Na collision rate, H_2O form (atomic configuration) factor (including a dimension factor) and activation factor due to the activation energy barrier.

**For detailed calculations, the space distribution of the propagated reaction energy, which exceeds the thermal energy and is derived via microscopic molecular dynamics, is directly available to the macroscopic flow dynamics. This is realized when the locally small variable mesh width (as on a logarithmic scale), normal to the reaction boundary in macroscopic flow dynamics, the mesh width of which is large in the mainstream, coincides with the molecular dynamics region width. This procedure is supported, e.g. by the $k-\varepsilon$ model, which renormalizes the kinematic viscosity coefficient as a function of the scale-independent constants.