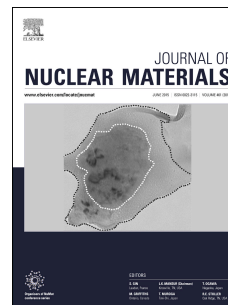


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Thermophysical properties of liquid UO_2 , ZrO_2 and corium by molecular dynamics and predictive models

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Abstract

Predicting the fate of accident-melted nuclear fuel-cladding requires the understanding of the thermophysical properties which are lacking or have large scatter due to high-temperature experimental challenges.

Using equilibrium classical molecular dynamics (MD), we predict the properties of melted UO_2 and ZrO_2 and compare them with the available experimental data and the predictive models. The existing interatomic potential models have been developed mainly for the polymorphic solid phases of these oxides, so they cannot be used to predict all the properties accurately. We compare and decipher the distinctions of those MD predictions using the specific property-related autocorrelation decays. The predicted properties are density, specific heat, heat of fusion, compressibility, viscosity, surface tension, and the molecular and electronic thermal conductivities. After the comparisons we provide readily usable temperature-dependent correlations (including UO_2 - ZrO_2 compounds, i.e., corium melt).

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Keywords : molten (liquid) corium; molten (liquid) UO_2 , molten (liquid) ZrO_2 , classical molecular dynamics; density; specific heat; heat of fusion; compressibility; viscosity; surface tension; thermal conductivity

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