Accepted Manuscript

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

Woong Kee Kim, Ji Hoon Shim, Massoud Kaviany

PII: S0022-3115(16)30686-9

DOI: 10.1016/j.jnucmat.2017.04.030

Reference: NUMA 50250

To appear in: *Journal of Nuclear Materials*

Received Date: 16 September 2016

Revised Date: 14 April 2017

Accepted Date: 20 April 2017

Please cite this article as: W.K. Kim, J.H. Shim, M. Kaviany, Thermophysical properties of liquid UO_2, ZrO_2 and corium by molecular dynamics and predictive models, *Journal of Nuclear Materials* (2017), doi: 10.1016/j.jnucmat.2017.04.030.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

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

Woong Kee Kim[a], Ji Hoon Shim[a,c,*] and Massoud Kaviany[a,b,*]

[a]*Division of Advanced Nuclear Engineering, Pohang University of Science and Technology, Pohang 37673, Korea*
[b]*Department of Mechanical Engineering, University of Michigan, Ann Arbor, Michigan 48109-2125, USA*
[c]*Department of Chemistry, Pohang University of Science and Technology, Pohang 37673, Korea*

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).

© 2012 Published by Elsevier Ltd. Selection and/or peer-review under responsibility of Global Science and Technology Forum Pte Ltd

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

E-mail address: kaviany@umich.edu (M. Kaviany), jhshim@postech.ac.kr (J.H. Shim)

Download English Version:

https://daneshyari.com/en/article/5454000

Download Persian Version:

https://daneshyari.com/article/5454000

Daneshyari.com