Development of a Gibbs Energy Minimizer for Integration into Nuclear Fuel Performance Codes

M.H. Piro[a], B.J. Lewis[a], T.M. Besmann[b], W.T. Thompson[a]*
[a]*Department of Chemistry and Chemical Engineering, Royal Military College of Canada*
P.O. Box 17000, Kingston, ON, Canada K7K 7B4
[b]*Materials Science and Technology Division, Oak Ridge National Laboratory,*
P.O. Box 2008, Oak Ridge, TN 37831-6063, USA

**Corresponding author, Tel: +1 613.544.6159, Fax: +1 613.542.9489, Email: thompson-w@rmc.ca*

Abstract – A numerical tool is in an advanced state of development to compute compositions of species and phases in multicomponent systems in chemical equilibrium as well as related thermochemical properties. The programming is aimed at the specific requirement of being able to reliably handle a sufficiency of components necessary to capture all of the species possibly produced by nuclear fission. The resulting software is intended for direct insertion into nuclear fuel performance codes and other software requiring the computation of equilibrium chemistry as boundary conditions for heat and mass transport. An estimation technique is utilized which accelerates the rate of convergence, permitting calculations to be made sufficiently rapidly for frequent execution from other codes. The subsequent Gibbs energy minimization strategy is robust and efficient in calculating the coexistence of multiple phases in complex multicomponent systems. The programming is being structured to satisfy the requirements of nuclear fuel behaviour models under development at the Oak Ridge National Laboratory.