Development of a new thermochemistry code for multiphysics simulations of nuclear materials

Parikshit Bajpai[1], Max Poschmann[1], David Andrs[2], Markus Piro[1]

[1] Nuclear Fuels and Materials Group, Ontario Tech University, Oshawa, Canada

[2] Modeling and Simulation Group, Idaho National Lab, Idaho Falls, USA

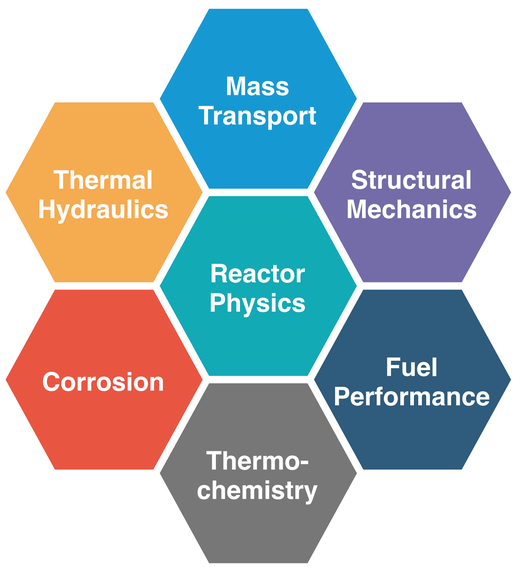
parikshit.bajpai@uoit.net https://nuclear.uoit.ca/piro

Objectives

Recently, there has been an increasing interest in direct coupling of thermodynamic computations with multiphysics codes such as INL's MOOSE. **A new thermochemistry code is being developed to provide rapid access to thermodynamic databases and perform thermochemical calculations for a range of different materials including nuclear fuels.** This poster describes the preliminary work done in this direction and plans for developing capabilities of practical interest to the nuclear industry.

Introduction

Nuclear reactors are highly complex multiscale, multiphysics systems with strong coupling between various phenomena such as temperature, creep, fission gas release etc.



Idaho National Laboratory's **Multiphysics Object Oriented Simulation Environment (MOOSE)** provides the computational foundation for performing multiphysics simulations suitable in such problems and a new MOOSE-based application called **Yellowjacket** is under development to model corrosion and fuel problems.

The thermochemistry solver within Yellowjacket will use **Gibbs Energy Minimisation** to provide material properties and boundary conditions such as the phase distribution and chemical potentials in molten salts.

Thermodynamic Equilibrium

Thermochemical equilibrium calculations are based on **minimising the integral Gibbs energy of a closed system at constant temperature and hydrostatic pressure**.

- Integral Gibbs energy of the system

$$G = RT\left(\sum_{\lambda=1}^{\Lambda} n_\lambda \sum_{i=1}^{N_\lambda} x_{i(\lambda)}\tilde{\mu}_i + \sum_{\omega=1}^{\Omega} n_\omega \tilde{\mu}_\omega\right)$$

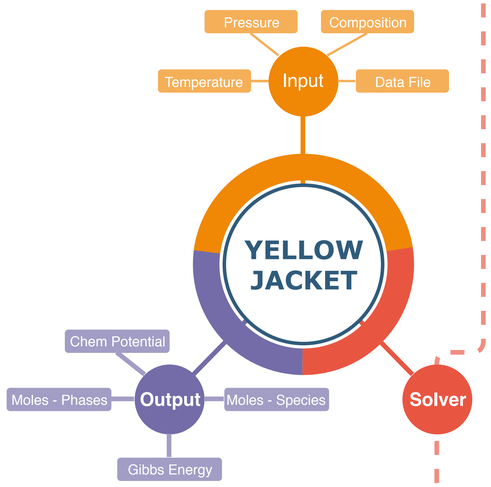
- Chemical potential of ideal phase species

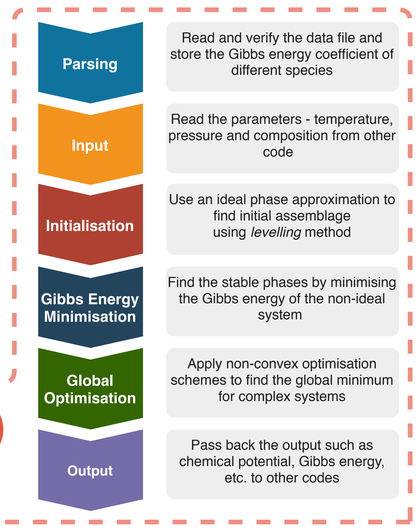
$$\tilde{\mu}_i = \tilde{g}^0_{i(\lambda)} + \ln(x_{i(\lambda)})$$

- Chemical potential of non-ideal phase species

$$\tilde{\mu}_i = \tilde{g}^0_{i(\lambda)} + \tilde{g}^{ex}_{i(\lambda)} + \ln(x_{i(\lambda)})$$

Computational Framework



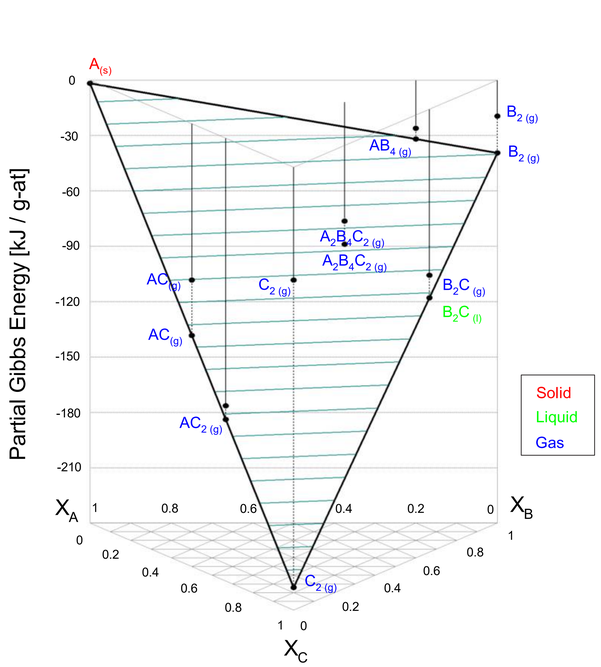


Coding Tools

- Environment: MOOSE
- Language: C++
- Data File Format: ChemSage (*.dat)
- Library: PETSc/Tao, LAPACK
- Documentation: MooseDocs
- Testing: CIVET

Gibbs Energy Minimisation

From a numerical point of view, the objective of computing thermochemical equilibria is to **determine a unique combination of phases and their composition that yields a global minimum in the integral Gibbs energy** subject to various linear and non-linear equality and inequality constraints.



Necessary conditions

- Conservation of mass

$$b_j = \sum_{\lambda=1}^{\Lambda} n_\lambda \sum_{i=1}^{N_\lambda} x_{i(\lambda)}\nu_{i,j} + \sum_{\omega=1}^{\Omega} n_\omega \nu_\omega$$

- Gibbs' phase rule

$$F = C - \Phi + 2$$

- Gibbs' criterion

$$\mu_i = \sum_{j=1}^{C} \nu_{i,j}\Gamma_j$$

Sufficient condition

- Integral Gibbs energy at global minimum

$$\pi_\lambda = \min_{\lambda} \sum_{i=1}^{N_\lambda} x_{i(\lambda)}\left(\mu_{i(\lambda)} - \sum_{j=1}^{C} a_{i,j}\Gamma_j\right)$$

Conclusion

The new MOOSE based app, **Yellowjacket**, is aimed at developing corrosion modelling capability for advanced reactors and will help in improving multiphysics simulations for nuclear reactor materials by coupling thermochemistry computations with continuum and meso-scales models.

Acknowledgement

This work was funded by the Department of Energy Nuclear Energy Advanced Modeling and Simulation program. This manuscript has been authored under Contract No. DE-AC07-05ID14517 with the US Department of Energy. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a nonexclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for United States Government purposes.

This research made use of the resources of the High-Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

References

[1] W. B. White, S. M. Johnson, and G. B. Dantzig. Chemical equilibrium in complex mixtures. *Journal of Chemical Physics*, 28(5):751–755, 1958.

[2] M. H. A. Piro, T. M. Besmann, S. Simunovic, B. J. Lewis, and W. T. Thompson. Numerical verification of equilibrium thermodynamic computations in nuclear fuel performance codes. *Journal of Nuclear Materials*, 414(3):399–407, 2011.