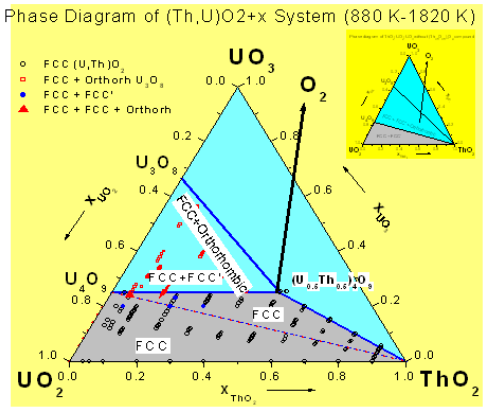
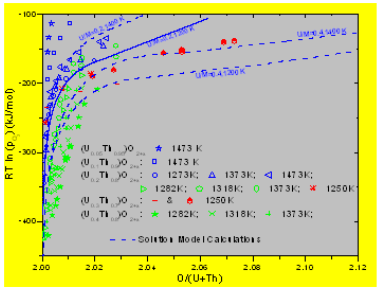
Thermodynamic properties of thoria based fuels



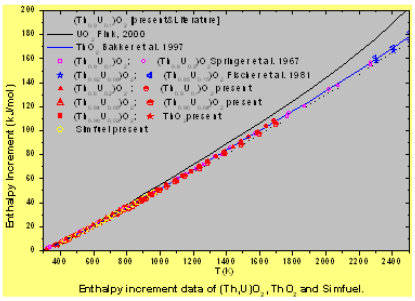
- 'Th' has +4 valency state but 'U' has +4, +5, +6 valency states so O/M > 2.0 with increase in U/M
- In absence of $(Th_{0.5}U_{0.5})_4O_9$ compound, $(Th,U)O_{2+x}$ will be biphasic for all values of x > 0.0, but due to its presence $(Th,U)O_{2+x}$ remains single phase FCC for reasonable value of 'x'.



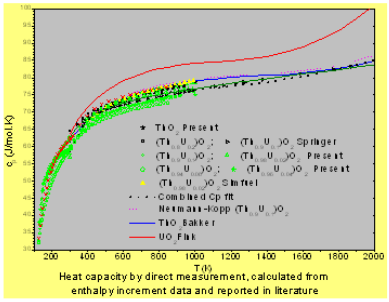
Solution model of ThO_2-UO_2-$UO_{2.33}$ was developed. It gave best fit with experimental data compared to all earlier models: Blackburn model, Cluster model of Franco et al., Lindemer and Besmann semi-empirical model & solution model of Labroche et al.

Results: Oxygen potential of $(Th,U)O_{2+x}$ increases with (i) decrease in U/M (ii) increase in temperature (iii) increase in O/M.

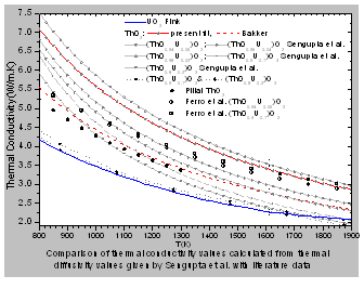
Phase Diagram and Oxygen potential of $(Th,U)O_{2+x}$ system



Enthalpy increment data of $(Th,U)O_2$, ThO_2 and Simfuel.



Heat capacity by direct measurement, calculated from enthalpy increment data and reported in literature

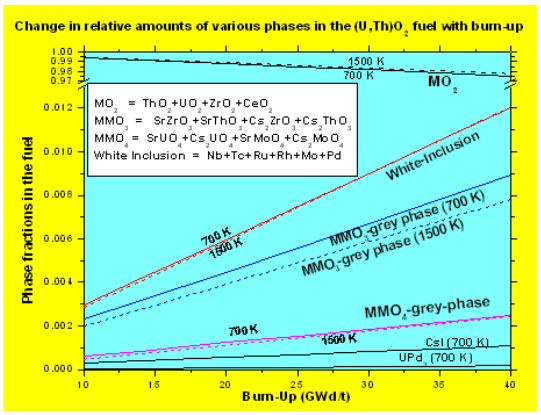


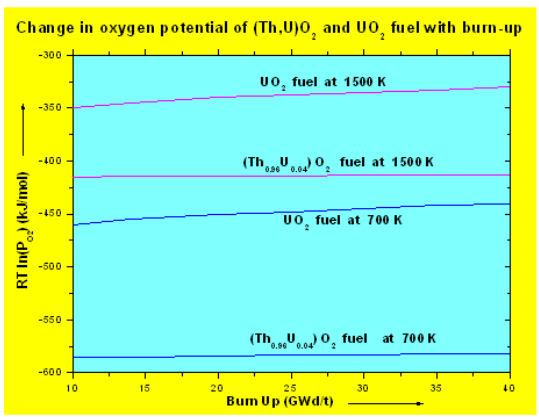
Comparison of thermal conductivity values calculated from thermal diffusivity values given by Sengupta et al. with literature data

Enthalpy increments of ThO_2, $(Th,U)O_2$, UO_2 and simfuels were measured by Calvet calorimeters (298 K – 1698 K) and heat capacities were measured by DSC-131 (127 K - 845 K). Thermal conductivities were calculated from measured thermal diffusivity and density data using measured Cp data and Newman-Kopp's Cp values.

➢Results:

- ❑ A slight negative deviation from additivity value on thoria rich side with maximum deviation at ~4 % UO_2.
- ❑ Simfuel has higher Cp than fuel.
- ❑ Additivity Cp values give reliable result for thermal conductivity calculations.





Chemical state of fission products of $(Th_{0.96}U_{0.04})O_{2.0}$ fuel were calculated as a function of burn-up using thermodynamic parameters of all possible compounds that can form in the fuel. Based on stability of fission products in different chemical states, oxygen potential of the fuel was calculated as a function of burn-up.

➢Results:

- Oxygen potential of $(U,Th)O_2$ fuel increases with burn-up .
- Oxygen potential of $(U,Th)O_2$ fuel is lower than that of UO_2 fuel