Current ChemApp Developments and Projects

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Abstract

A set of new subroutines was recently added to ChemApp which allows for the modification of thermochemical data once the data-file has been loaded into ChemApp:

Subroutine	Function
TQGDAT	Get selected thermodynamic data of a phase constituent
TQLPAR	List all excess Gibbs energy or all excess magnetic interactions of a phase
TQGPAR	Get selected excess Gibbs energy or excess magnetic parameters of a phase
TQCDAT	Change selected data of a specified phase constituent or of a specified phase
TQWASC	Write a thermodynamic data-file in ASCII format

The new subroutines will be briefly introduced and their use illustrated in a code example.

Currently work is under way to produce an OpenMP-parallelized version of ChemApp supporting multi-core computers. The current state of the effort will be presented plus an outlook into the near future and upcoming parallelization plans will be given.

Out of a number of interesting new projects that apply ChemApp, two projects from the area of nuclear fuels will be introduced.