NUCL15: IRSN NUCLEA Nuclear Alloys-Oxides Database

Database name:	IRSN NUCLEA Nuclear Alloys-Oxides Database	*Database acronym:*	NUCL
Database owner:	IRSN	*Database version:*	15.4

The NUCL15 (IRSN NUCLEA-15_4) database contains critically-assessed and internally-consistent thermodynamic data for the entire field from metal to oxide domains within an 18-element framework + H-Ar (only for the gaseous phase, as well as for hydrides and hydrous oxides/silicates). It can be applied to study fundamental scientific issues and efficiently investigate practical engineering problems in both the In-Vessel and Ex-Vessel nuclear reactor circumstances. It effectively enables you to calculate the thermochemical equilibrium states at any step of an eventually-severe accident, and to utilize the calculation results for improving the predictions and treatments of thermo-hydraulic or other accidents, for enhancing the design and engineering of modern and safety-prioritized nuclear reactors, and for assisting the assessment and processing of nuclear fuel and waste managements.

Included Elements (18+2)

U	Zr	Fe	Cr	Ni	Ag	In	Ba	La	Ru	Sr	Al	Ca	Mg	Si
O	B	C									+	H	Ar	

Included Phases and Assessed Systems

Available solution and stoichiometric phases:

Condensed solution phases:	*(solids/liquid phases)*	59 phases
Condensed stoichiometric phases:	*(solid/liquid substances)*	507 phases
Gaseous mixture phase	*(ideal gaseous mixture)*	207 gaseous species

Note that the hydrogen element (H) being as a major component is added into the system, while its dissolution in condensed solid and liquid solution phases has not been taken into account yet. The Ar component is only present in the gaseous mixture phase. Included condensed stoichiometric phases (pure substances) are widely ranged: intermediate metallic compounds, oxides & hydroxides, silicates & hydrous silicates, hydrides, carbides & carbonates, borides & borates, and some simple inorganic/organic substances.

Available assessments and evaluations:

Binary subsystems:	*(metallic alloys, carbides, borides, oxides)*	153
Ternary subsystems	*(metallic alloys, carbides, borides, oxides, silicates)*	22
Pseudo-Binary subsystems:	*(oxides, silicates, borates)*	105
Pseudo-Ternary subsystems:	*(oxides, silicates, borates)*	27

Note that for many other ternary, quaternary and higher-order subsystems, the analytical descriptions of lower-order constituent subsystems are effectively combined and used (through appropriate extrapolations) to predict multicomponent systems, especially for compositions and temperatures which have not been experimentally evaluated. Depending on the complexity of multicomponent systems, such an analytical prediction is more or less accurate.

Limits

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary, quaternary and in some cases higher-order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.