NUOX4: TCS Nuclear Oxides Database

Database name:	TCS Nuclear Oxides Database	*Database acronym:*	NUOX
Database owner:	Thermo-Calc Software AB	*Database version:*	4.2

NUOX4 is suitable for nuclear oxide solution system calculations. This database is developed to study molten core-concrete interactions. However, it can also be applied to any relevant system or application which comprises essentially the constituent oxides. It can also be coupled with pure substance databases (e.g. NUMT and SSUB) or solution databases (e.g. SSOL and TCFE) to increase the range of applications which can be studied.

Included Elements

Al Ba Ca Ce La Mg O Si Sr U Zr

Included Phases

AL11LAO18	BA2SIO4	CAMGSIO4	LA2O7SI2	PROTO_ENSTATITE
AL12BAO19	BA3SI5O13	CAZRO3	LA2O7ZR2	PSEUDO_WOLLASTONITE
AL12SRO19	BA5SI8O21	CE2O7ZR2	LA2ZR2O7	QUARTZ
AL2BA3O6	BACEO3	CE2SI2O7	LA4O12SI3	RANKINITE
AL2BAO4	BALA2O4	CEO1_72	LA4O7SR	SISR2O4
AL2SR3O6	BASI2O5	CEO1_83	LA4O9SR3	SISR3O5
AL2SRO4_A	BASIO3	CEO3SR	LIQUID_OXIDE:L	SISRO3
AL2SRO4_B	BAUO3	CLINO_ENSTATITE	MELILITE	SPINEL:I
AL32SR84O132	BAZRO3	CORDIERITE	MGO12SI4SR3	SR2ZRO4
AL4SRO7	BETA_QUARTZ	CRISTOBALITE	MGO6SI2SR	SR3ZR2O7
AL7LA33O60	C12A7	DELTA	MGO7SI2SR2	SRZRO3
ALCEO3	C1A1	FCC_FLUORITE	MGO8SI2SR3	TETRA
ALLAO3	C1A2	GAMMA	MONO	TRIDYMITE
ALPHA	C1A6	HALITE:I	MULLITE:I	WOLLASTONITE
ALPHA_C2S	C3A1	HATRURITE	O7_96U3	ZIRCON
ANORTHITE	CA2MGSI2O7	HEXAGONAL	O9U4	
APRIME_C2S	CA3MGSI2O8	KAPPA	OLIVINE	
BA2SI3O8	CAMGSI2O6	LA2O5SI	ORTHO_ENSTATITE	

Assessed Systems

It contains data for a collection of assessed binary and ternary systems relevant to nuclear applications. The current version does not include gas phase data. Hence, for vaporization calculations, the database must be used in conjunction with another database which includes the gas phase species such as NUMT or SSUB. The current database has a full description of the following system: **UO2+x-ZrO2-SiO2-CaO-Al2O3-MgO-BaO-SrO-La2O3-CeO2-Ce2O3**

where all the component binary interactions have been assessed. A description of the fuel hyperstoichiometry in the FCC_FLUORITE phase (UO2+x) is included.

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 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.