Addition of Vanadium oxides to the GTOX oxide database

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The GTOX oxide database containing CaO-MgO-Al_2O_3-CrO_x-FeO_x-K_2O-Na_2O-MnO_x-NiO-ZnO-P_2O_5-SiO_2-TiO_x (CaF_2, CaS, CrS, FeS, MgS, MnS) relevant for the development and production of refractory materials as well as for metallurgical slag applications, glass processing, coal combustion and gasification has been thermodynamically assessed using all available experimental data. Vanadium oxides V_2O_5 and V_2O_3 have so far been integrated into the reduced core system CaO-MgO-Al_2O_3-FeO-Fe_2O_3-Cr_2O_3-MnO-Mn_2O_3-SiO_2-TiO_2-Ti_2O_3. This resulted in the thermodynamic description of 12 binary and 7 ternary systems based on the presently available experimental data. The Gibbs energy of the liquid phase has been modelled using a non-ideal associate solution model. The compositions of the pure liquid oxide species as well as the associates have been chosen to have two moles of cations per associate thus keeping the successful method of Spear and Besmann [Bes2002].

The thermodynamic assessments of the Vanadium-Oxygen system given by Yang, Mao and Selleby [Yan2015] and of the Titanium-Vanadium-Oxygen system [Yan2017] were considered, the liquid phase was re-optimized in this work using the non-ideal associate solution model [Bes2002] with the associates V_2O_2, V_2O_3, V_2O_4 and V_2O_5 taken from the SGPS database. The liquid phase of the binary oxide systems containing V_2O_5 and V_2O_3 is described with similar sets of associates to provide a handle for the use in ternary assessments and later in quaternary systems. For systems of the type MeO-V_2O_3 one associate species $MeO{\cdot}V_2O_3$ was included.

Vanadium was also introduced into the thermodynamic description of solid solution phases such as MeO, Spinel, Corundum, Ca_2SiO_4-α and Pseudo brookite using available experimental information. In the vanadium oxides containing systems attention was given to the phase Spinel which forms the wide completely miscible solid solution Fe_3O_4-FeV_2O_4-MgV_2O_4-MnV_2O_4. The cation V^{+3} was introduced on the second sublattice of the present description of the Spinel phase (Fe^{+2}, Fe^{+3}, Mg^{+2}, Mn^{+2}, Ti^{+4}) (Al^{+3}, Fe^{+2}, Fe^{+3}, Mg^{+2}, Va, Mn^{+2}, Mn^{+3}, Ti^{+3}, V^{+3})$_2$(O^{-2})$_4$ with additional Gibbs energies where the missing values could be estimated using reciprocal equations.

The experimentally determined solubilities of Vanadium in MeO are described using the corresponding formulae (Al^{+3}, $\underline{Ca^{+2}}$, Cr^{+3}, $\underline{Fe^{+2}}$, Fe^{+3}, $\underline{Mg^{+2}}$, $\underline{Mn^{+2}}$, Mn^{+3}, Na^{+1}, Ti^{+4}, Ti^{+3}, Zn^{+2}, $\underline{Ni^{+2}}$, V^{+3}, V, $\underline{V^{+2}}$, Va)(O^{-2}). The phase Pseudobrookite was modelled using the following formula: (Al, Mg, Fe, Ti, V)(Al, Ti, Fe)(Ti)$(O)_5$ which allows to describe the experimentally determined wide solubility with respect to vanadium oxide.

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