Thermodynamics of the C-H-O fluid at extreme conditions

S.K. SAXENA[1]*, R. HRUBIAK[1], V. DROZD[1],
A.B. BELONOSHKO[2], P. SHI[3] AND G. ERIKSSON[4]

[1]Department of mechanical and materials engineering, Florida International University, Miami, FL 33199, USA (*correspondence: saxenas@fiu.edu)
[2]Department of Metallurgy, Royal Technical University, Stockholm, Sweden
[3]Thermo-Calc AB, Stockholm, Sweden
[4]GTT-Technologies, Aachen, Germany

The superfluid model [1] for calculation of high pressure-temperature fluid fugacities builds on the combination of experimental data on pure and mixed fluids at temperatures lower than 1000 K over several kilobars and molecular dynamics generated data at extreme conditions (> 5 kbar and up to 100 GPa and 4000 K). The model is found to be generally consistent with post-publication (since 1992) experimental data. The calculated data on water at low pressure differs significantly from the Brodholt-Wood fluid inclusion data [2] but closely reproduces the densities measured by Abramson and Brown [3].The superfluid model and the model of Zhang and Duan [4] are closely similar.

We have used the model to calculate high pressure and temperature phase equilibrium in binary (MgO-CO_2, Al-H_2), ternary (Fe-H_2O-C, wustite-H_2O-C) and multicomponent (carbonaceous chondrite) systems. The results show that while a carbonate may be stable over the entire range of the mantle pressures and temperatures, it is not stable if the mantle is chondritic in composition. Iron carbide (Fe_3C), on the other hand, is stable to extreme pressure and temperatures in the ternary as well as in chondritic composition and may be a good candidate to be assimilated in the core. The conclusions are that a) the carbonate may not be the storage for CO_2 in the deep earth and b) carbon is more likely stored in Earth's core as carbide and as diamond in the mantle.

[1] Belonoshko, A.B, Shi, P., Saxena, S.K. (1992) *Computer and Geosciences* **18**, 1267–1269. [2] Brodholt, J.P., Wood, B.J. (1994) *Geochim. Cosmochim. Acta* **58**, 2143–2148. [3] Abramson, E.H., Brown, J.M. (2004) *Geochim. Cosmochim. Acta* **68**, 1827–1835. [4] Zhang, C., Duan, Z. (2009) *Geochimica et Cosmochimica Acta* **73**, 2089–2102.

Effect of magnetite addition on H_2S dynamics in coastal marine sediment

M. SAYAMA

National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba 305-8569, Japan (m.sayama@aist.go.jp)

It has been well known that magnetite is poorly reactive towards dissolved sulfide (H_2S) on a time scale of hours to days (Canfield *et al*., 1992; Raiswell and Canfield, 1996; poulton *et al*., 2004). However, microprofiles of H_2S in experimental sediment cores made wtih coastal marine surficial sediment showed a dramatic change by the addition of magnetite (Fig. 1). The depth of H_2S front at which H_2S concentration starts to increase stayed at the original even after four days incubation in the core with magnetite addition (Fig. 1, right), whereas the H_2S front moved up quickly and reached to the oxic-anoxic interface (OAI) within 24 hours in the control core (without magnetite addition) (Fig. 1, left). Possible mechanism to explain these results might be electrochemical oxidation of H_2S at deep with long distance electron (e^-)-transfer through solid state cycling of structural Fe^{2+} and Fe^{3+} in magnetite (Latta *et al*., 2011).