MODEL SIMULATION OF MINERALOGICAL AND CHEMICAL CHANGES DURING ISOTHERMAL, FREE EVAPORATION OF A REDUCED CHONDRITIC PRECURSOR IN PURE H$_2$. A. V. Fedkin[1], M. S. Ghiorso[1] and L. Grossman[1,2]. [1]Dept. of the Geophysical Sciences, Univ. of Chicago, 5734 S. Ellis Ave., Chicago, IL 60637. avf@uchicago.edu. [2]Also Enrico Fermi Institute.

Introduction: Using the MELTS thermodynamic model [1] to compute the equilibrium phase assemblage and activities of all components in the liquid phase, a model has been developed for calculating equilibrium vapor pressures over multicomponent, iron- and alkali-bearing systems. In [2], this model was applied to published experimental measurements of evaporation rates of Mg, Fe, Na, K and Si for chondrule-like systems in H$_2$ to obtain evaporation coefficients (α_i) for the dominant evaporating species of these elements using the Hertz-Knudsen equation. The evaporation reaction of an oxide from a silicate liquid produces free oxygen or H$_2$O in vacuum or in H$_2$, resp. The vapor pressure of a volatile element like Na may generate a vapor pressure of O$_2$ or H$_2$O too high to be compatible with the valence of iron in the evaporating source material. Thus, the actual volatilization residue may be more reduced than the equilibrium assemblage for which vapor pressures are calculated. In our model, free oxygen otherwise released during each vaporization step in such a case is used to oxidize the residue until its oxidation state matches that of the equilibrium assemblage.

Technique: The model chondrule precursor was assumed to contain chondritic proportions of Si, Mg, Fe, Ni, Ca, Al, Na, K, Ti and Cr with enough oxygen to convert only 2.56% of the total Fe to FeO. The only evaporating solid phase was assumed to be metallic NiFe, for which we assumed $\alpha_{Ni} = \alpha_{Fe}$, which is nearly unity [3]. For silicate liquid, α_i for SiO$_{(g)}$, Mg$_{(g)}$, Fe$_{(g)}$, Na$_{(g)}$ and K$_{(g)}$ were taken from [2], and it was assumed that $\alpha_{Cr} = \alpha_{Ni} = \alpha_{Fe}$ and that $\ln \alpha_i = -7787/T(K) + b_i$ for all species. The initial radius was 0.5 mm and, at each evaporation step, the fractional surface area occupied by each phase was assumed equal to its volume fraction.

Results: For $P_H^{tot} = 10^{-4}$ bar, at all temperatures from 1500-1900K, metallic NiFe falls in abundance both by direct evaporation and by oxidation, the latter using oxygen released initially mostly by alkali loss and then mostly by $Fe_2SiO_{4(l)} \Leftrightarrow 2Fe_{(g)} + SiO_{2(l)} + O_{2(g)}$. X_{Fa} of olivine (ol) first increases by several mole % (from ~.02 to .05 or .06) until the oxidation state of Fe is equal in both the real and equilibrium assemblages, and then falls as Fe evaporated from silicate liquid cannot be replenished by further oxidation of metal (met) due to falling $f(O_2)$. At 1900K, the initial assemblage contains 51 wt% silicate liquid and ol+met+spinel (sp), the initial equilibrium $\log f(O_2) = IW + 3.5$, all alkalies are lost in <0.2 min, all metal in 11 min, and 10% of the total Fe in 0.8 min. At 1600K, there is initially only 24% silicate liquid (lowering evaporation rates) and ol+opx+sp+met, the initial $\log f(O_2) = IW + 1.1$, all alkalies are lost in 80 min, all metal in >300 min, and 10% of the total Fe in 29 min.

References: [1] Ghiorso M. S. and Sack R. O. 1995. *Contributions to Mineralogy & Petrology* 119:197–212. [2] Fedkin A. V. et al. 2005. Subm. to *Geochimica et Cosmochimica Acta*. [3] Tachibana S. 2005. Pers. comm.