PHOTOOXIDATION IN THE INNER SOLAR NEBULA. J. R. Lyons, Institute of Geophysics and Planetary Physics, and Department of Earth and Space Sciences, UCLA, Los Angeles, CA 90095-1567 (jrl@ess.ucla.edu).

Introduction:
Quantitative evaluation of gas-phase kinetic processes over temperatures ~ 500 to 2000 K is likely to be essential to understanding the evolution of oxygen isotopes and oxidation state in the solar nebula. Gas shocks generated during accretion of parent cloud material and by density waves, solar flares and other energetic processes, will push (perhaps only nudge) gases toward isotopic and chemical equilibrium. On the longer timescales of cooling of the inner nebula, high temperatures (~ 1500 K) drive both gases and solids to equilibrium [1]. Photochemical processes, due to uv and x-ray radiation from the protosun and nearby O and B stars, create disequilibrium in nebular gases. At the low temperatures in molecular clouds and in the outer regions of protoplanetary disks, chemical disequilibrium is well known to prevail. As the inner disk cools, a transition may occur from thermochemistry-dominated (and photochemistry-relevant) to photochemistry-influenced, at least with respect to trace gas abundances (e.g., \( \text{O}_2 \)).

Here I consider a preliminary model of photochemical kinetics for nebular gases in the inner nebula. The principal motivation for this work is the observation that chondrules in unequilibrated ordinary chondrites have fayalite fractions that require equilibrium with a gas considerably more oxidizing than a gas of solar composition. A recent chapter for Meteorites in the Early Solar System II [2] discusses the difficulty in understanding the fayalite content of chondrules in detail. (There is, of course, a large body of literature on this topic, and I refer the reader to [2] for a more complete discussion of earlier work.) Wood [3] originally proposed that dust enrichment could account for a nebular \( \text{fO}_2 \) greater than solar. Inward radial migration of water (e.g., [4]) in meter-sized icy boulders from the outer solar system will also lead to a nebular gas more oxidizing than solar. Fedkin and Grossman [2] computed the expected \( \text{fO}_2 \) and Fa fraction for condensation from a nebular gas with both enriched dust and water, and concluded that only very high dust and water enrichments can explain the observed Fa fractions over the entire range of nebular cooling rates, a solution which they do not consider to be robust. At the Oxygen in the Early Solar System meeting in Gatlinburg (Sept. 19-21, 2005), Grossman suggested that photochemistry may play a role in enhancing \( \text{fO}_2 \) in the nebula.

Nebular model: For the present calculations, I used the same nebular model used to compute CO self-shielding in the outer solar nebula [5]. At the high temperatures of the inner disk, both \( \text{H}_2 \) and CO will be present in the gas phase. Because \( \text{H}_2 \) is photolyzed at longer wavelengths than is CO, and is less affected by shielding from \( \text{H}_2 \) than is CO, \( \text{H}_2 \)O photolysis rates due to uv radiation will be at least an order of magnitude higher than those of CO. I have therefore created an initial model consisting only of H-O species, which greatly simplifies the high-temperature chemistry (no hydrocarbons). I have also (temporarily) removed oxygen isotopes from the model in part because \( \text{H}_2 \)O photolysis is not isotope selective, but also to simplify the chemistry. Because inward migration of water ice from the outer solar system may alter both bulk oxygen isotopes and bulk oxidation state (e.g., [6]), it is essential that both be treated simultaneously at high temperatures.

Results and discussion: Figure 1 shows kinetic results for a nebular gas with initial composition of \( \text{H}_2 \), He and \( \text{H}_2 \)O, the latter with a volume fraction of \( 2 \times 10^{-4} \). The calculations are at a heliocentric distance of 3 AU, and assume a temperature of 800 K (pressure of 1.6 microbar). I have assumed a 1000-fold enhancement in protosolar uv relative to the modern Sun, diminished by a factor of 10 to account (roughly) for grazing incidence on the disk surface. Absorption by uniformly distributed 0.1 micron dust is also included. Vertical mixing is prescribed as in [5], and Figures 1a and 1b show results for \( \alpha = 10^{-3} \) and \( 10^{-2} \), respectively. I will not specify the physical basis for mixing at 3 AU, but it is unlikely to be due to magneto-rotational instabilities because of insufficient ionization near the midplane.

The oxidative photochemistry in Figure 1 is initiated by

\[
\begin{align*}
\text{H}_2\text{O} + \text{hv} & \rightarrow \text{H} + \text{OH} \\
\text{OH} + \text{hv} & \rightarrow \text{O} + \text{H} \\
\text{O} + \text{OH} & \rightarrow \text{O}_2 + \text{H}
\end{align*}
\]

Molecular oxygen is destroyed by

\[
\begin{align*}
\text{O}_2 + \text{hv} & \rightarrow \text{O} + \text{O}(1\text{D}) \\
\text{O}_2 + \text{H} & \rightarrow \text{OH} + \text{O}
\end{align*}
\]

The steady state volume fraction of \( \text{O}_2 \) is very low (~ \( 10^{-17} \)) even in the case of strong vertical mixing. As shown in Figure 2, a region of enhanced \( \text{O}_2 \) volume fraction (~ \( 10^{-8} \)) is predicted several scale heights...
above the midplane. For both strong and weak vertical mixing, fairly high OH fraction (~ $10^{-12}$ to $10^{-10}$) is predicted at steady state, considerably higher than $O_2$.

Much remains to be done before these results can be compared directly to equilibrium models [2]. A comparison over a range of temperatures with the expected thermochemistry for the simple H-O system will be an important check on the high temperature kinetics. Ionized species such as $OH^+$ need to be added. Then, CO and a reduced set of hydrocarbons will be added. Finally, the calculations will be performed for realistic nebular midplane cooling histories.


Acknowledgements: Funding from the NASA Origins program is gratefully acknowledged.