A UNIFIED MODEL OF PEBBLE GROWTH, DIFFUSION, AND CHEMISTRY IN PROTOPLANETARY DISKS
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Introduction: Observations of protoplanetary disks have revealed them to be complex, dynamically evolving objects. Gas and small dust are constantly in motion while larger pebbles and planetesimals grow; these changing conditions determine what chemical reactions dominate local regions of the disk, and thus which molecular compounds are available to be accreted into planets. Previous chemical models have generally focused on dynamically passive disks to explore spatial and temporal variations of molecular species [see 1 for a review of chemical models of disks]. Alternatively, dynamic models typically focus on dust dynamics through a gaseous disk, with little impact on the gas phase chemistry [2]. However, these processes would operate concurrently, leading to important feedbacks throughout the disk which must be understood [3].

Methodology: We present a new method for modeling pebble growth and its effects on evolving chemistry within a 1D slice of a diffusive disk. Gas and small dust particles are allowed to diffuse vertically within the disk, connecting chemistry at all elevations. Pebbles form from the dust present around the midplane, inheriting the composition of ices at this location. We use an astrochemical network modified to include self-shielding and gas-grain interactions to track the chemical reactions that occur as the dust abundance and optical depth change due to pebble formation. This new model allows us to link chemistry in the observed upper gaseous layers of the disk to the cold midplane region where planet formation occurs (and is generally shielded from view). Additionally, combining pebble growth with chemistry allows us to track the time-dependent composition of pebbles, giving insight to how properties of planet-building material evolve over the disk lifetime.

Results: We find that after 1 Myr of evolution, the growth of pebbles and the removal of small dust from upper layers of the disk allows penetration of UV photons deeper into the disk, driving photochemistry at regions closer to the midplane. Additionally, the removal of ice at the midplane leads to depletion of volatile species, such as CO, throughout the column by roughly an order of magnitude, consistent with observations of carbon depletion in protoplanetary disks [4]. Finally, we find that around major snowlines, some species are preferentially removed; for example inside the CO snow line, water ice is readily removed from the diffusing dust as pebbles form, leaving CO behind in the vapor. As a result, the chemistry becomes increasingly carbon rich and oxygen poor, leading to the creation of more hydrocarbon species.

The effects described here would also be important in examining the source of isotopic anomalies in the Solar System, as they have been proposed to be linked to self-shielding and photochemical processing within the disk [e.g. 5]. The location where molecules are photodissociated will evolve with time, meaning the secondary products that form from the photodissociated products will be determined over a range of physical conditions over time. This will impact how effectively, for example, liberated heavy-O from CO is able to combine with H to form H2O and enrich that compound in heavy isotopes. We will present results of our calculations which will track the isotopic evolution of carriers in our model.