MODELING 2D TRANSPORT OF CO IN PROTOPLANETARY DISKS: WHAT ENDS UP WHERE?

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Introduction: The spatial distribution of the abundances of major volatile species (e.g., water, CO) in protoplanetary disks is expected to change dramatically during the disk's 1-10 Myr lifetime. Astrochemical models indicate volatiles freeze out in cold, dense regions while remaining in the gas-phase in hot, tenuous, and/or UV-irradiated regions [e.g., 1]. At the same time, various mechanisms can transport large amounts of gas (through diffusion and advection) and solids (gravitational settling, turbulent mixing, and radial drift) in the vertical and radial directions [2,3]. Recent observations of mm-dust, molecular CO and various other tracers [4,5,6] hint at a common narrative: (i) volatiles are depleted from disk surfaces and presumed to be locked up in solids at the disk midplane; (ii) these solids then drift inward, redistributing the volatiles and potentially enriching the planet formation zone in carbon and oxygen [7]. At this point however, we lack a complete understanding of the interplay of these various processes and how they influence each other, making it difficult to connect different observables in single, well-studied systems (e.g., TW Hya or HL Tau), let alone draw comparisons between disks in different evolutionary stages.

Towards a New Hybrid Model: We present a new global, two-dimensional model that is capable of simulating the transport and interaction between volatile species (both in the form of vapor or ice), small microscopic dust grains, and larger coagulated pebbles in a simultaneous and self-consistent manner.

The method is based on treating these three ingredients separately, but not independently (see Fig. 1). The CO vapor and small dust components are treated as concentrations on a 2D Cartesian grid with logarithmically spaced grid cells, while the pebbles are described using Lagrangian tracer particles, each representing a larger number of physical particles.

The transport of vapor and small dust is simulated by solving 2D transport equations (including advection and diffusion) on the logarithmic grid, while pebble motions are calculated using a random-walk-like Monte Carlo scheme that includes the effects of turbulent diffusion, vertical settling, and radial drift [2,3]. Different interactions between the components are included, such as freeze-out of CO molecules onto small dust, evaporation of CO ice present on dust grains or pebbles, and sweep-up of small grains by pebbles. The key advantage of this hybrid approach is that we can describe the pebbles as particles with unique histories (every pebble's current size and chemical make-up is a function of its journey through the disk) and still solve interactions between vapor and microscopic grains in regions where the total mass of solids is small.

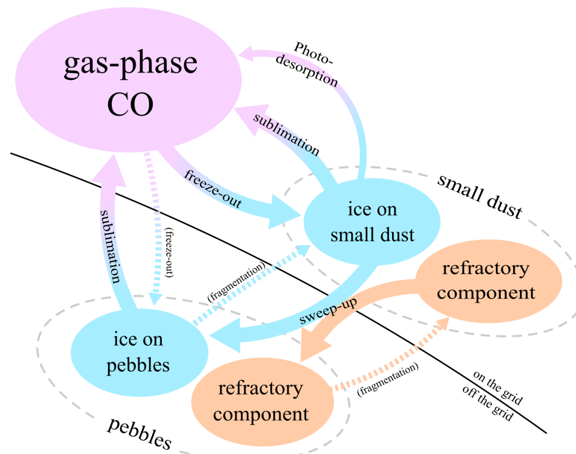

Figure 1: Conceptual model of the hybrid approach. Vapor and small dust grains (and their ice) live on a 2D grid, while pebbles are described using Lagrangian tracer particles.

Results: Figure 2 shows snapshots of models for a disk resembling the Minimum Mass Solar Nebula. The initial conditions (Fig. 2A) assume small dust is present everywhere with a constant dust-to-gas mass ratio of 0.005, while pebbles start out in a settled disk between 100-140 AU, with individual sizes around 1 mm and a surface density (relative to the gas) of 0.005. At t=0, we assume freeze-out/desorption equilibrium, which results in very little vapor in the midplane outside of r~70 AU.

Figure 2B shows the situation after 0.5 Myr of evolution, assuming all solids (dust & pebbles) are stationary. In this scenario, transport of ices is non-existent, and the continuous mixing of CO vapor to the midplane depletes the upper layers of the disk at those radii where freeze-out closer to the midplane is possible [5,8]. In this particular case, most vapor does not make it all the way down to the midplane, but freezes out onto small dust grains (not shown here) in the region highlighted by the blue contour. Knowing where and under which conditions ices are being formed is relevant for understanding their structure [e.g., 9].

In Fig. 2C, both the small dust grains and the pebbles are allowed to diffuse, settle, and drift. Since small, ice-covered grains can now return CO to the upper layers of the disk, the depletion as seen in case B practically vanishes. Thus, the removal of volatiles from the upper layers of the outer disk depends heavily on the ability of (small) grains to replenish vapor by transporting ices to these regions. After 0.5 Myr, most pebbles have moved inside the midplane snowline; their CO ice has evaporated and the disk has been enriched in CO vapor between 40-70 AU, with the radial extent of this enriched region depending on the height above the disk midplane.

For the simulations of Fig. 2, we have ignored dust-pebble interactions. If pebbles can efficiently accrete small grains however, the ability of small grains to replenish the vapor in the disk atmosphere will be reduced [10]. In that case, we still expect a considerable depletion of vapor from the upper layers [11]. A realistic disk is therefore expected to resemble an intermediate case between Figs. 2B and 2C.

The snapshots shown in Fig. 2 are by no means steady-state configurations. In fact, one of the outcomes of our simulations is that the abundances of ice, vapor, etc. vary significantly in time. Nonetheless, it is clear from Fig. 2 that both vertical and radial transport of volatiles, be it as vapor or ice, has a major impact on the spatial distribution of CO molecules.

Discussion: We introduce a novel 'hybrid' approach for modeling 2D transport of volatile species and solids in protoplanetary disks. The method is designed to intuitively connect several key observables: (1) vapor abundances in the upper parts of the outer disk; (2) vapor abundances close to, and inside of the midplane snowline; (3) the radial extent of the pebble disk; and (4) the distribution of small, microscopic grains. Solving the vapor abundance in two dimensions is critical for comparing to observations, as different tracers/wavelengths probe different layers of the protoplanetary nebula [e.g., 12].

By creating synthetic images of the model's output and comparing these predictions to resolved observations of nearby protoplanetary disks, we will be able to constrain the efficiency of various transport mechanisms in those systems (e.g., vertical settling/stirring, radial drift), allowing us in turn to extract key parameters such as the turbulence strength and the dust-to-gas ratio — parameters that, despite being very important for understanding disk evolution and planet formation, are notoriously hard to measure directly.

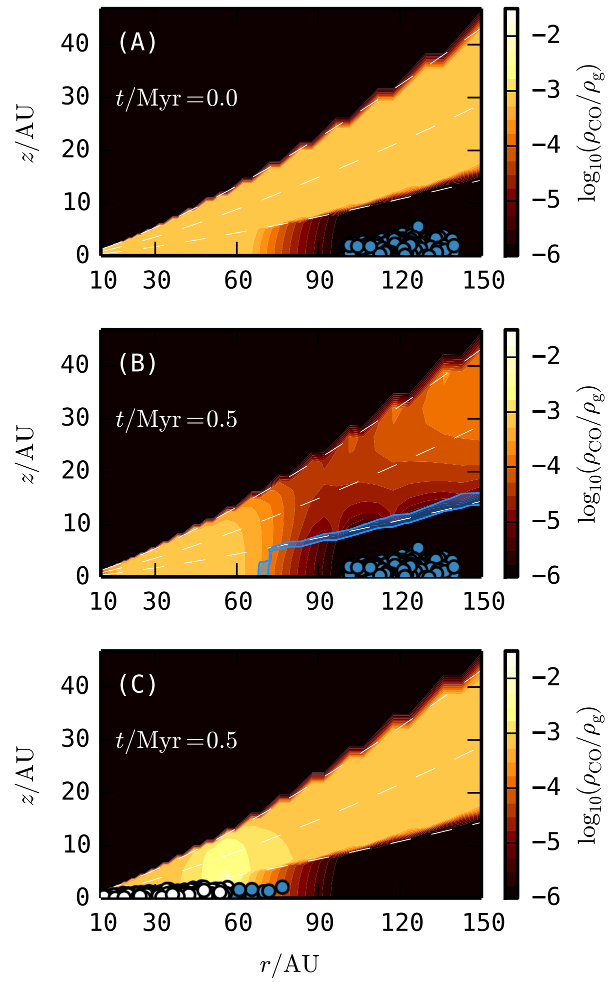

Figure 2: Snapshots of our model for different scenarios assuming an alpha turbulence of 5×10^{-4}. The background color indicates CO vapor density (relative to H_2) and the spherical symbols represent the pebble population (blue is ice-rich, white is ice-poor).

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