Modeling 2D transport of CO in protoplanetary disks: What ends up where?

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Introduction

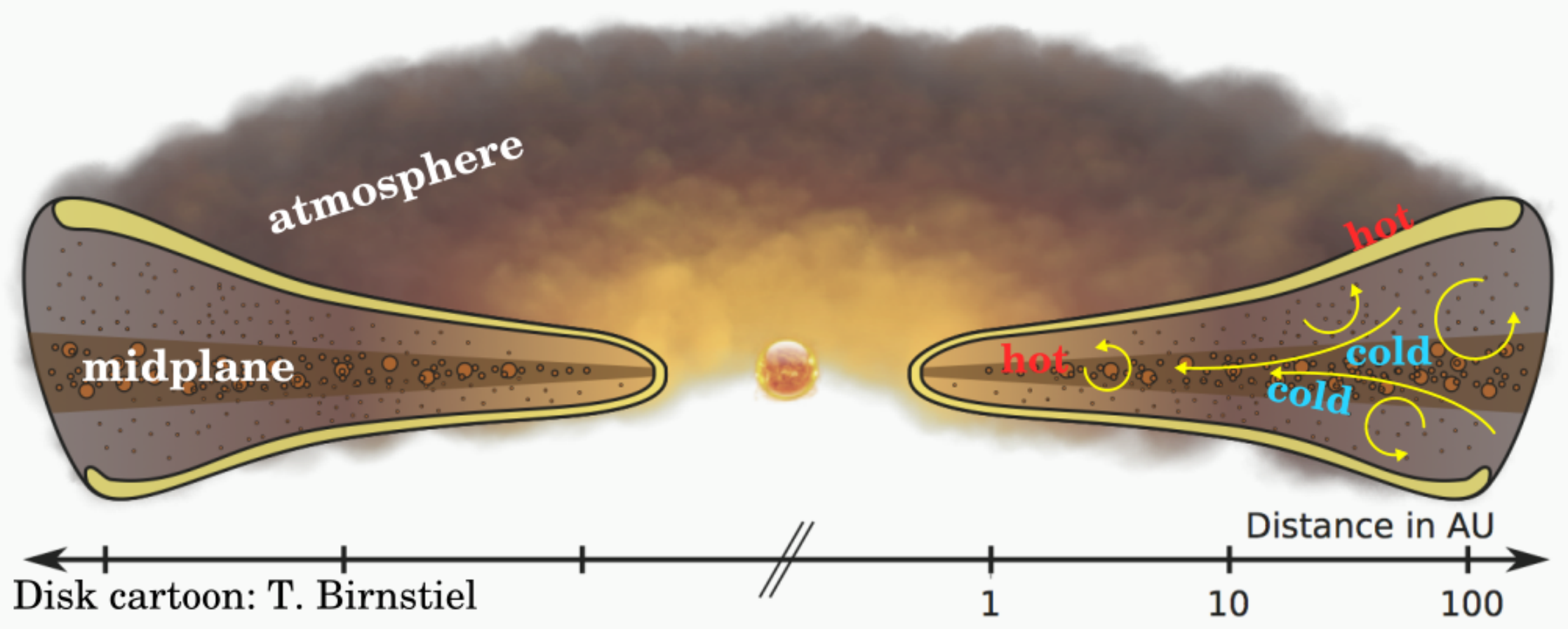


Fig. 1: Cartoon of a young protoplanetary disk. Planet formation takes place in the (cold) midplane, while CO emmision tends to trace warmer layers closer to the disk atmosphere. Transport of solids and gas is prevalant throughout the disk.

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 in which: (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].

Methodology

We have developed 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 (Fig. 2). 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 (Fig. 3), and sweep-up of small grains by pebbles.

At the same time, 2D transport equations (including advection and diffusion) are solved on a logarithmic spatial grid for gas-phase CO and small dust, while pebble dynamics (including vertical gravitational settling and radial drift) are described using Lagrangian tracer particles [2,3,9,10].

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.

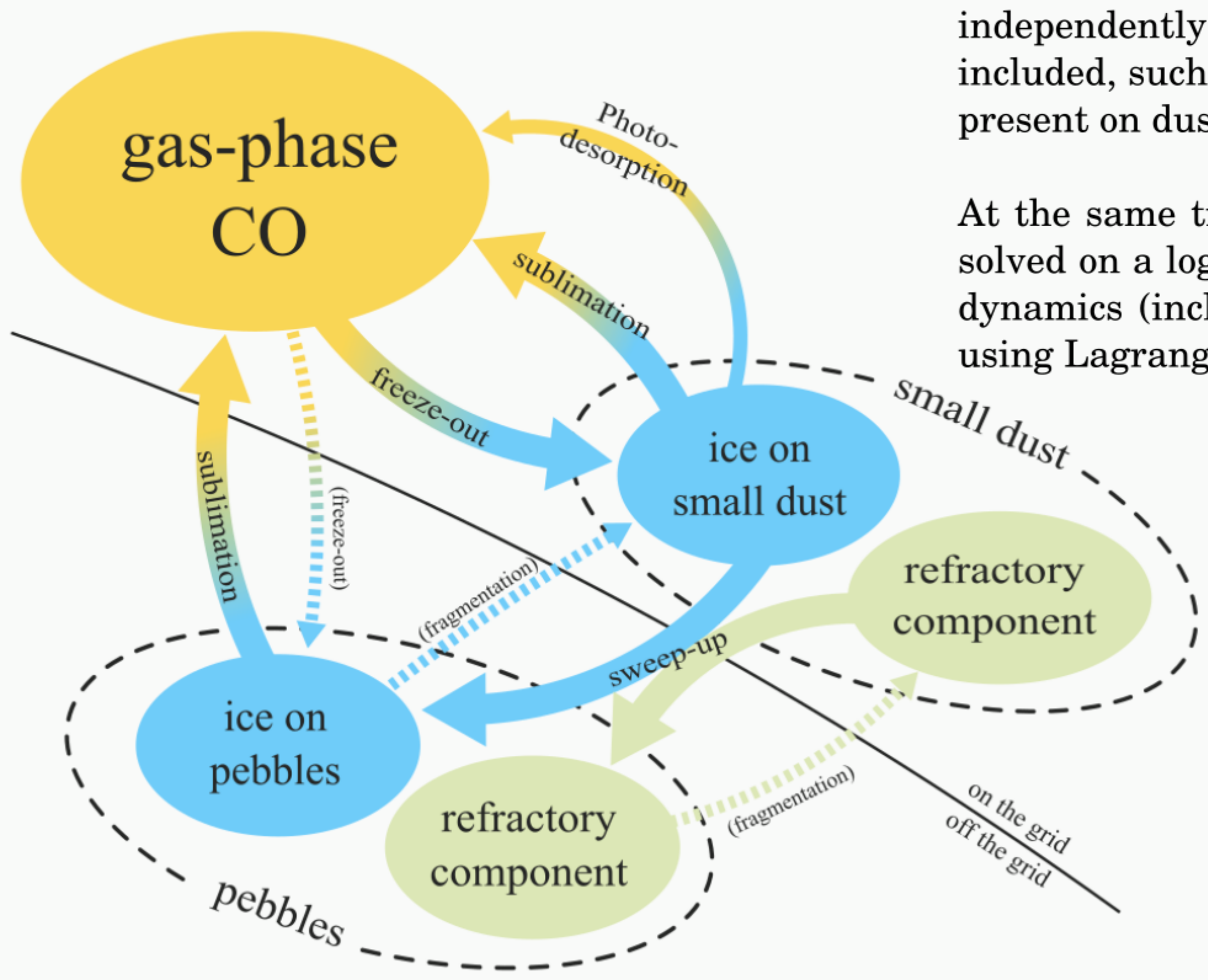


Fig. 2: Conceptual model of the hybrid approach. Locally, CO vapor, small dust grains, and pebbles (and their ice) interact in various ways. Globally, transport of gas-phase CO and small dust is calculated on a 2D grid while pebbles are modeled as Lagrangian tracer particles.

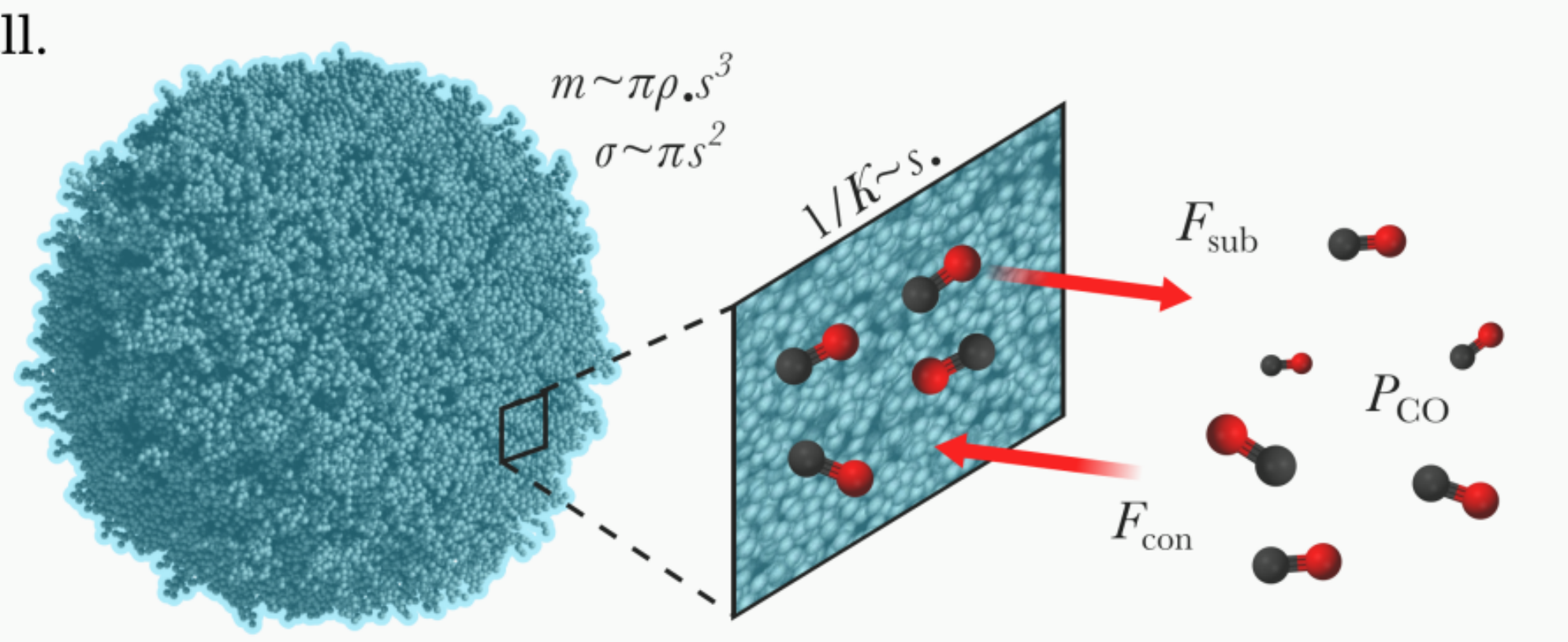


Fig. 3: CO molecules interacting with the surface of a dust grain. Based on Fig. 1 of Krijt et al. 2016 [10].

Results

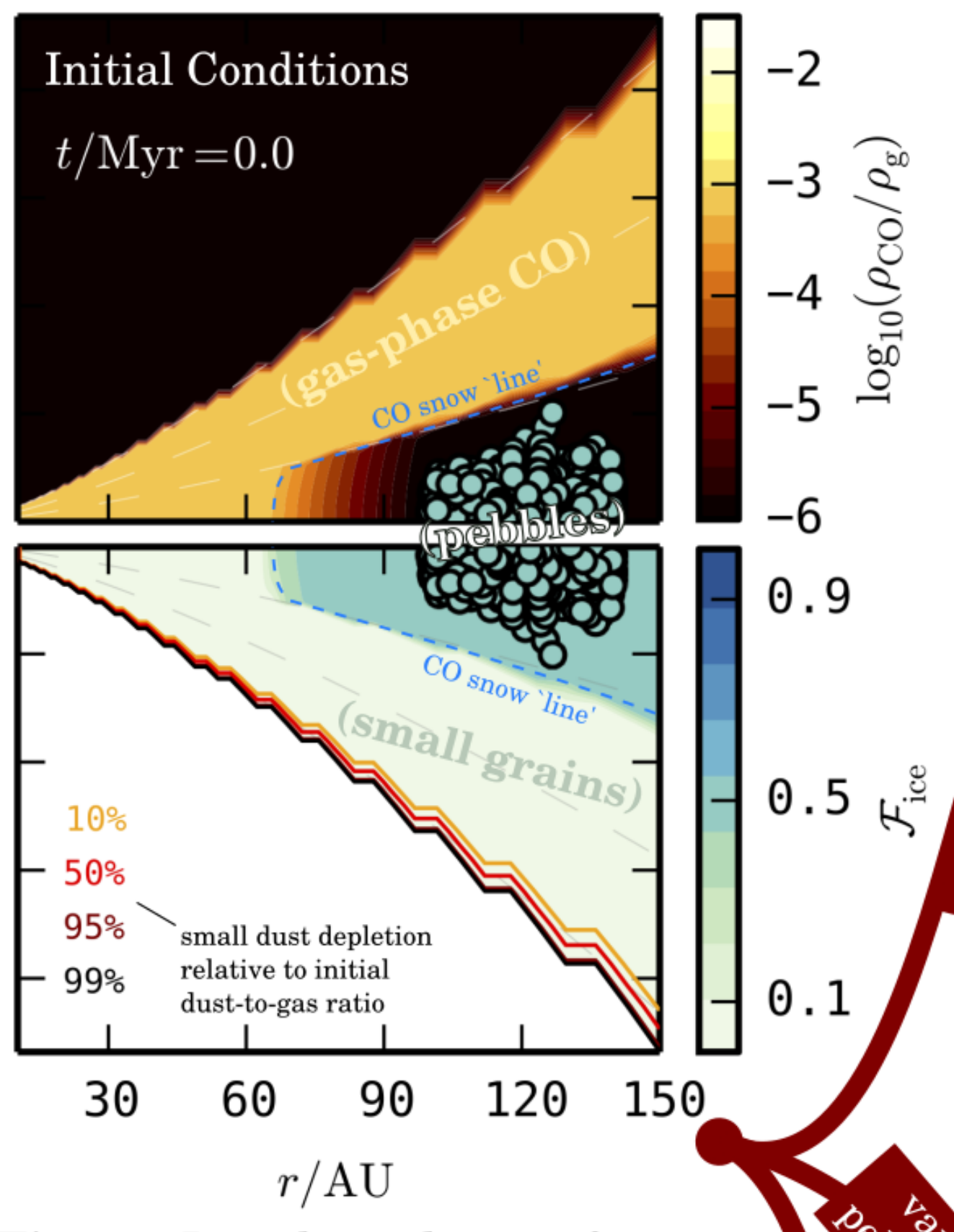
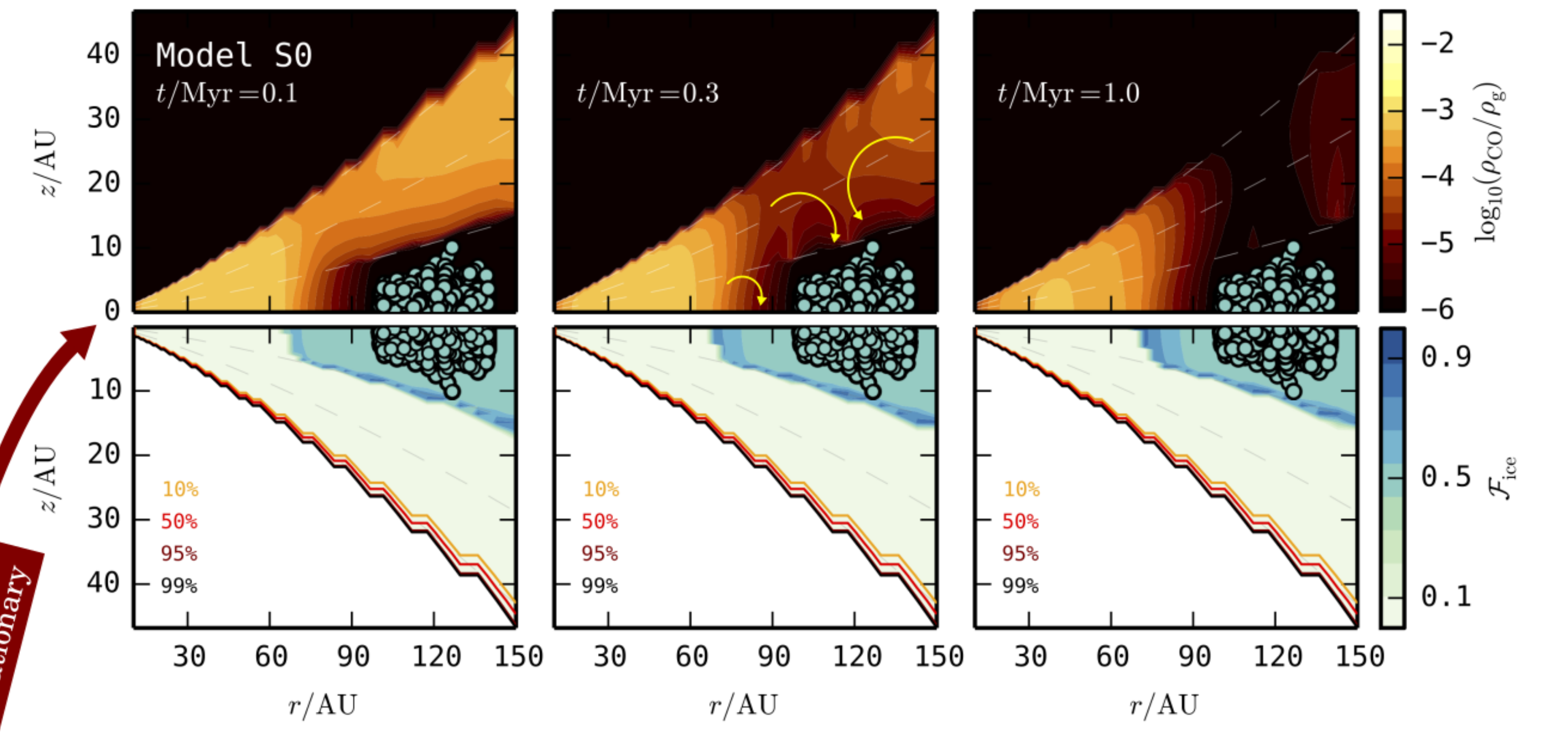


Fig. 4: Initial conditions for *t*=0. showing the different components in our model. *Top panel:* Gas-phase CO is present in the inner disk and atmosphere. In the midplane, pressure & temperature are such that CO molecules freeze out in the outer disk. A disk of pebbles is present in the outer disk. *Bottom panel:* Small grains are everywhere; but their ice-content ($\mathcal{F}_{ice}$) is larger in regions where CO has frozen out.

TABLE 1
Summary of model runs.

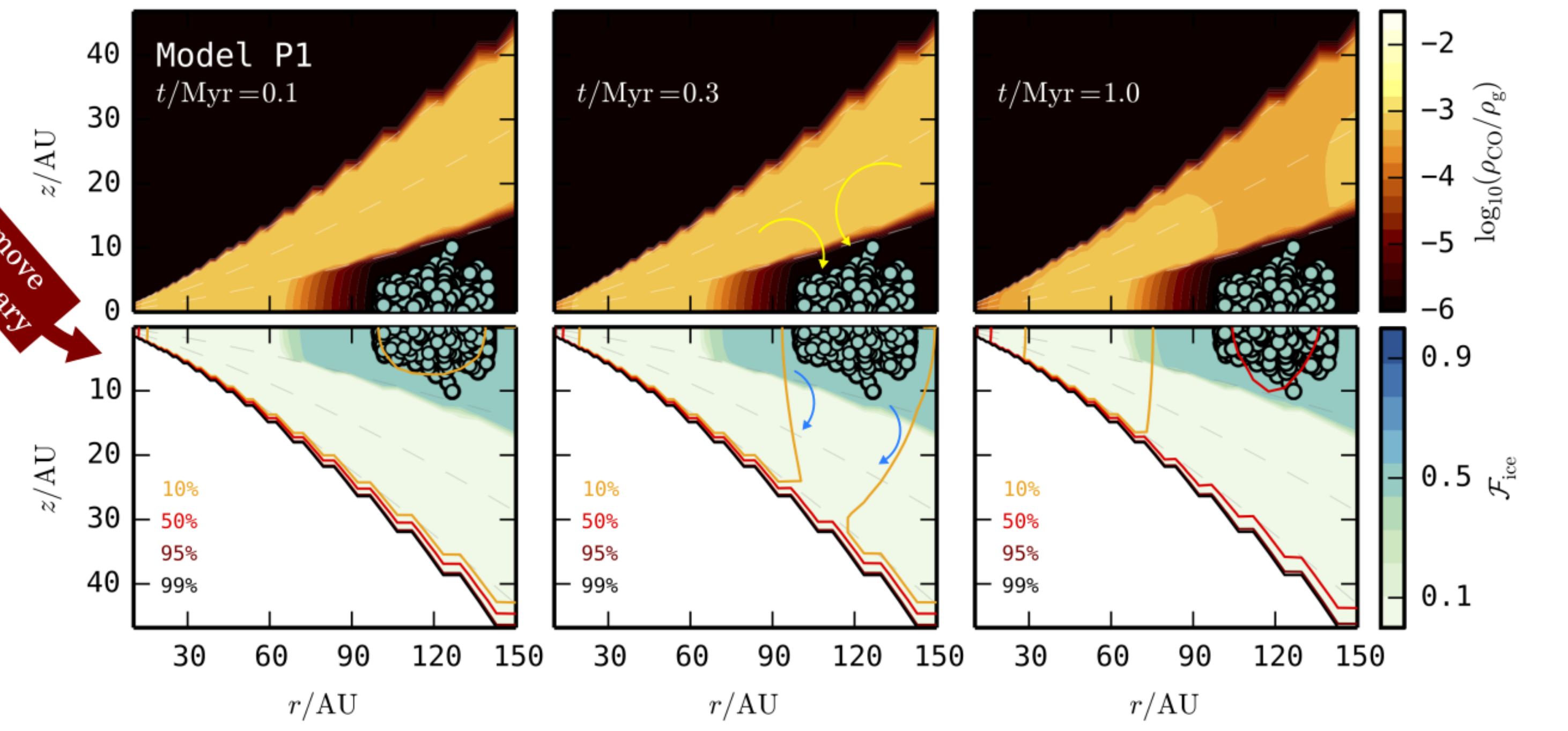
Model ID →	S0	P1	C0
Vapor diffusion	✓	✓	✓
Freeze-out/sublimation	✓	✓	✓
Small dust dynamics	×	✓	✓
Pebble sweep-up	×	✓	✓
Pebble dynamics	×	×	✓
(Gas accretion	×	×	×)
C_d^0 (initial small-dust-to-gas ratio)	10^{-3}	-	-
α (dimensionless turbulence strength)	10^{-3}	-	-
s_p $(t=0)$ (pebble size)	mm	-	-
f_p $(t=0)$ (pebble-to-gas surf. density)	10^{-2}	-	-

only vapor moves
solids are stationary



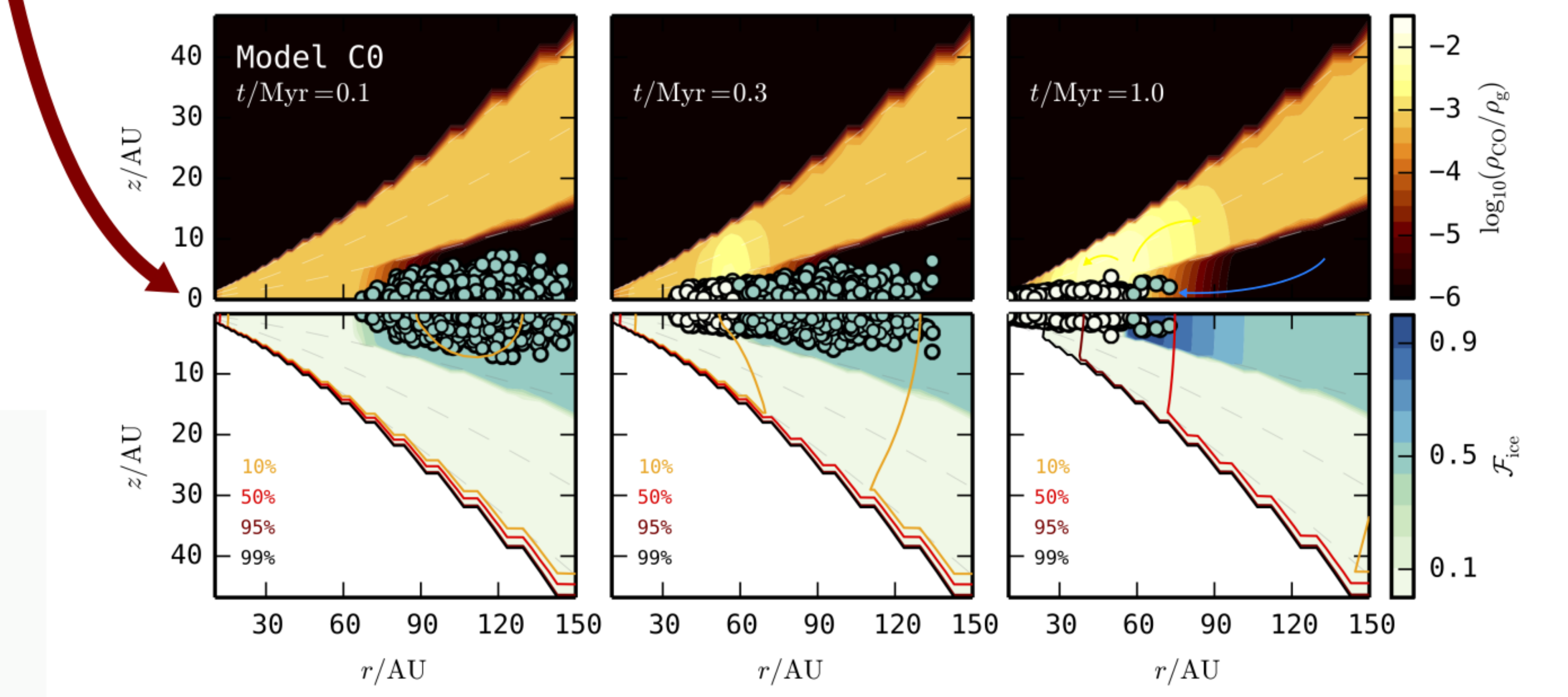
Model S0: When solids are not allowed to move, turbulent transport of vapor followed by rapid freeze-out (the `cold finger' effect [8,10]) removes CO molecules from the disk atmosphere. A geometrically thin layer of ice-rich small grains forms below the surface snowline, and no new ice is added to the larger pebbles deeper down in the disk.

vapor & dust move
pebbles are stationary



Model P1: When small grains are allowed to move, the depletion seen in model S0 practically disappears as ice-rich dust dust particles replenish the CO vapor in the astmosphere. However, small grains are accreted by the pebbles in the midplane, resulting in some removal of small grains & CO vapor after 1 Myr. In this case, the depletion traces the location of the pebble disk.

vapor, dust, and
pebbles all move

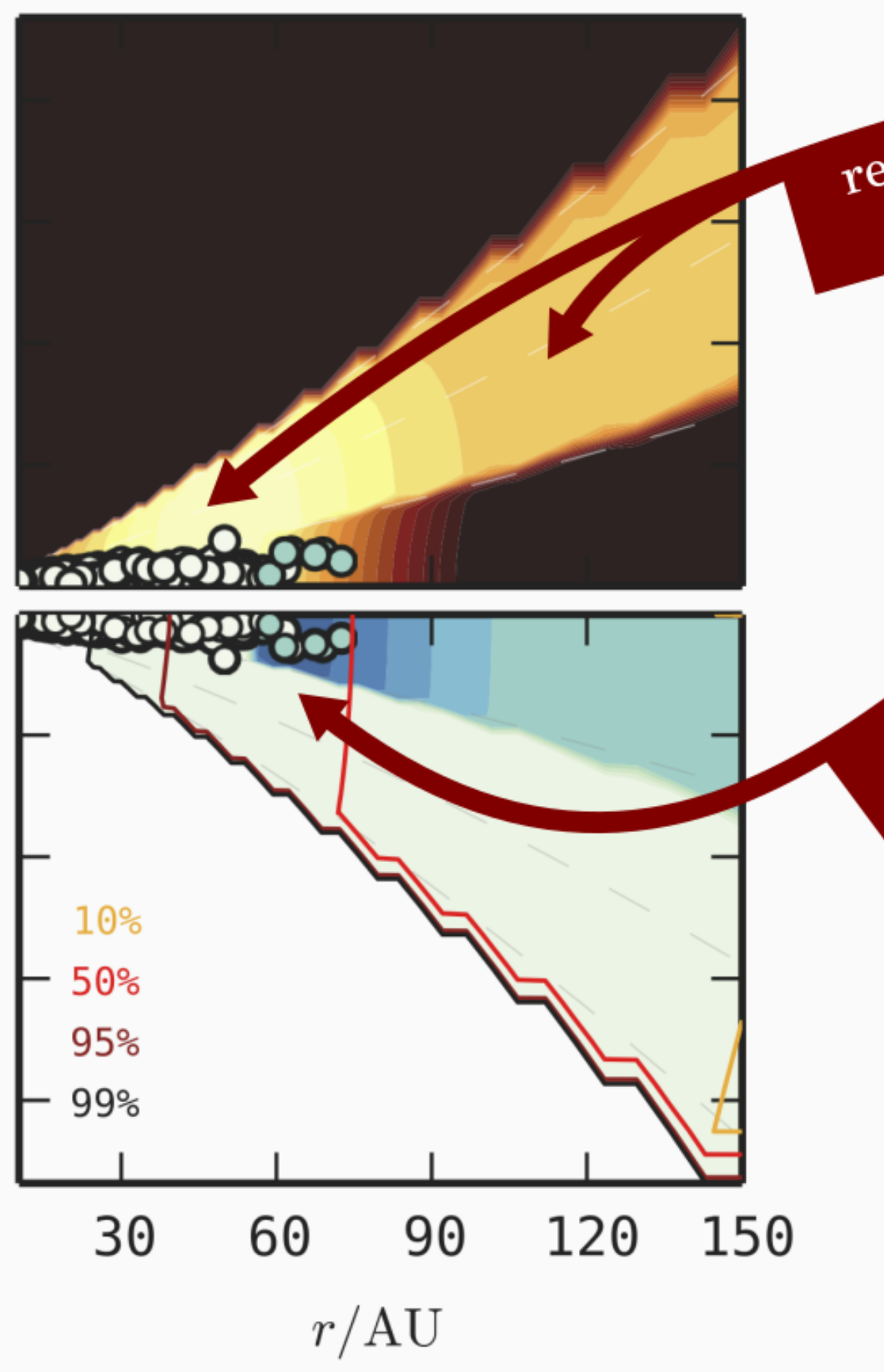


Model C0: When pebbles are allowed to drift/migrate radially, the story changes again. The pebbles are not around for long enough to act as a sink for CO in the outer disk. Instead, they drift through the midplane snowline and release new CO vapor in the inner disk, which subsequently diffuses in all directions. Outward mixing and freeze-out dramatically increases the ice-content of the small grains just outside the midplane snowline.

Conclusions/outlook

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., 11].

By creating synthetic images of our model predictions, and connecting them to a suite of independent but connected observables (e.g., the radial extent of the millimeter emmision, strenght of CO lines at different temperatures, etc.), we will be able to constrain the efficiency of various transport mechanisms and extract key parameters such as the dust-to-gas ratio, pebble sizes and concentration, and turbulence strength.



resolved CO emission

size of the pebble disk

In the future, we plan to add more volatile species (e.g., water, organics) and include more complex gas-phase chemistry. By simulating a region that spans multiple snowlines, we will be able to construct 2D maps of the C/O ratio (for the gas and for solids of different sizes) as a function of time.

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