Constraining how giant planets influence planet formation through self-consistent chemical and dynamic models

Overview

Despite the confirmed detections of over 6,000 exoplanets[1], how planets form and what sets their composition is still unclear. As the ISM collapses to form a new star, left over dust and gas from star formation creates a protoplanetary disk (PPD) around the young star. Over the course of 1-10 Myr, the gas disk dissipates leaving behind planets formed from the solid grains, their ice mantles, and gravitationally bound gas. While these disks and planets can be observed separately, the actual process of planet formation is hidden from view, occurring in the relatively cold and dense midplane of the PPD. We must rely on simulations to connect these stages of planetary growth and to answer the questions of *when* and *where* do planets form and *what* sets the composition of these planets.

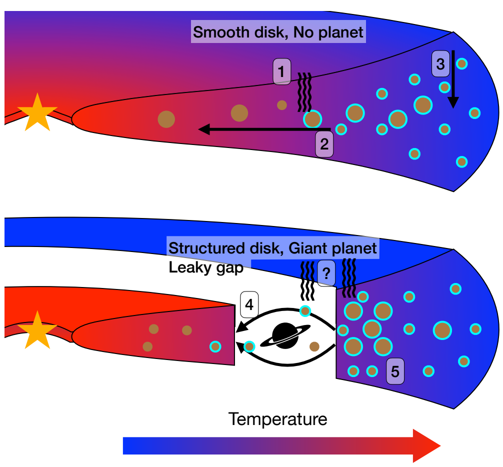

Figure 1: Cartoon cross-section of a smooth disk (left) and one containing a planet-induced gap (right). Various physical processes affecting the dust are numbered: 1) sublimation of ice, 2) inward radial drift, 3) dust growth and settling, 4) filtering of small dust past the planet, and 5) dust pile-up exterior to the planet. It is currently unclear how this dust pile-up and filtering may affect the composition of planets forming within the disk.

To answer these questions, we must consider planet formation as an ongoing processes. Observations of PPDs have shown that substructures – rings, gaps, spirals, and asymmetries – are common in many disks [1]. While these gaps in PPDs may be carved out by giant planets, they also fundamentally change the environment of the disk *throughout the formation of the giant planet*. In addition to the typical coagulation, settling, and drift of solid grains that is expected in smooth disks, these planet-induced substructures can have drastic consequences for the resulting size, distribution, and composition of these dust grains throughout the disk (Fig 1). During giant planet formation, these planets are expected to alter not only their own growth environment, but also gas and dust composition throughout the entire disk. How do these grains go on to form additional planets? How does a planet impact its own chemical environment in the disk? **What are the key chemical and dynamic feedback mechanisms of planet formation?**

Understanding how giant planet formation impacts subsequent planet formation, as well as its own formation environment, is necessary for connecting disk and planet compositions and constraining the current population of giant planets in observed disks. This requires connecting both the dynamics and chemistry of disks to accurately model how one effects the other. Throughout my PhD I have pioneered the this research, creating new modeling techniques to tackle these difficult problems [17, 18]. As a 51 Pegasi b fellow, I will continue this work to better understand the chemical consequences of planet formation in an evolving disk and what this means for the planets that form within.

[1] https://exoplanetarchive.ipac.caltech.edu

1. Dust evolution and processing in leaky disks

The first project I propose will be the first of its kind to combine dust growth and mixing across the gap in 3D. These results will help to drastically reduce the parameter space for planets in gaps in observed PPDs, or if results do not match they may be evidence to rule out planets entirely. While dust growth and coagulation has been done in 1 and 2D using prescribed relative velocities, **this has never been approached using a full 3D simulation**. This 3D approach not only accounts for the 3D flow created by planets, but the use of Monte Carlo tracer particles also allows for simultaneous modeling of ice processing, providing for the first time a self-consistent constraint on expected volatile delivery past giant planets. These results are necessary to interpret not only the solar system record but also to interpret observations of PPDs and the exoplanet systems that form within.

As giant planets form within disks, they naturally create ring and gap substructures in the dust via gravitational interactions with the surrounding gas, concentrating dust exterior to the planet's orbit [6, 13]. In cold regions of the disk, these grains are covered by ice mantles containing volatile molecules, including H_2O, HCN, CO_2, and any products of these ices that may be formed through astrochemical processes. Understanding the transport and evolution of this dust is required for accurate modeling of the PPD chemical environment. Recently, models of these dust traps have shown that instead of preventing the inward drift of all solids, small solids may filter past the planet from the outer disk (exterior of the orbit of the planet) to the inner disk (interior to the orbit) [15]. While these leaky disks have been modeled in 1 and 2D, in Van Clepper et al. (2025), I modeled the 3D structure of the disk, accounting for prominent vertical flows away from the midplane created by the accreting planet. **I showed that this 3D structure has important implications for the expected sizes of solids capable of leaking past embedded planets of different masses**. Naturally, the question of arises: *How much material is expected to filter past the planet in leaky disks?* To answer this, dust growth and fragmentation must be considered to constrain the population of surviving small dust capable of passing the planet.

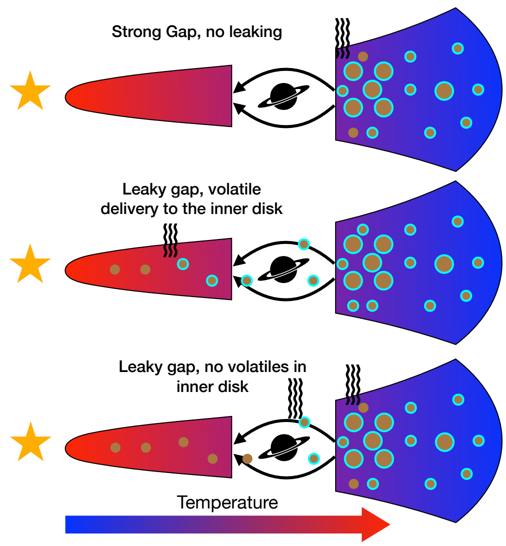

Figure 2: Different grain and ice processing pathways in a disk containing a giant planet. The theoretical work I propose here will aim to identify under what conditions we should consider mixing of dust and their volatiles, and provide context for the observations of warm volatiles in some disks.

The extent of this radial mixing of solids and their volatile ices is currently unclear. Observations of PPDs have shown that, typically, smooth disks show warm water emission from the inner disk, while structured disks tend to have less water in the inner disk, pointing to efficient trapping of water ice-rich grains in the outer disk [2, 7]. The solar system, similarly shows evidence for a separation of two major reservoirs, often interpreted to be physically separated by the Jovian embryo [8]. This separation cannot have been absolute, however, as isotopic analysis of various meteorite parent bodies in addition to the Earth show that some amount of this inner and outer solar system material must have mixed [16]. Similarly the disk PDS 70, which is known to host two planets, shows warm water emission and evidence from continuum dust emission that point to a leaky gap [12, 14]. Additionally, the AGE-PRO survey showed that the dust evolution for disks of varying ages is best modeled using leaky gaps, potentially informing us of the planets forming within [9].

I will us a combination of 3D hydrodynamic, radiative transfer, and Monte Carlo particle tracking models, to constrain the disk and planet conditions under which both grains and the volatile ices present on their mantles are expected to pass a growing planet as both the planet and disk evolve in a self-consistent manner. Because I will consider the grain transport and processing at the same time, I will be able to determine not just when grains are transported across the planetary gap, but also how, where, and when different ice species may desorb off the grain (Fig 2). Using with both ALMA and JWST measurements, which can tell us the composition of both the cold and hot regions of the disk respectively, I will be able to directly connect molecular line emission to dust evolution and transport in the disk for the first time. This work will be the first of its kind to self-consistently model the transport of grains through gaps while accounting for the 3D accretion of gas onto the embedded planet, allowing for a new framework to understand the phenomenon of "leaky disks" and their implications for planetary formation.

2. Chemical consequences of planet-induced substructures

Dust evolution sets the conditions for chemistry in the disk, controlling not only grain surface chemistry – such as adsorption, (photo)desorption, and hydrogenation – but also the temperature and irradiation in the disk. Because of this, **understanding the small grain distribution in the disk, both radially and vertically, is necessary for accurate modeling of the chemical environment of the disk.** As I previously showed in Van Clepper et al. (2022), dust growth and settling to the midplane not only removes volatile ice from the gas, but also increases the local radiation field, accelerating UV driven chemistry. It is natural, then, to ask: *How do planet induced substructures affect chemistry throughout the disk, and how does this affect the composition of subsequent forming planets?* Öberg et al. [11] showed that not only are substructures in dust common, but emission from molecular line tracers in the gas also show ring and gap substructures. While there are various possible explanations for these substructures, there appears to be no consistent correlation with continuum substructures nor expected snowline locations across disks [10].

Given this, it is clear that the dust and gas are interacting in currently unexplained ways to produce these observable chemical signatures. While we know that disks are constantly evolving, dynamic environments, this is rarely reflected in chemical models. Although considering dust and chemical evolution simultaneously is challenging, my experience modeling the connections between dust evolution and chemistry [17] and the dust dynamics in structured disks [18] prepares me to tackle this issue to provide a self-consistent framework for combined dust and chemical evolution.

As my second project, I propose to combine my 3D dust simulations from project 1 with chemical models to self-consistently model the gas and dust evolution in disk containing a giant planet. In Van Clepper et al. (2022) I developed a coupled chemistry and dust growth model, which simultaneously tracked the gas phase and solid composition of small dust and pebbles. Here, I will expand this methodology to 2D (in the $R-Z$ plane), which can be used to track the chemical evolution of the disk with an evolving dust structure, accounting for the vertical and radial transport of solids and gas. This will allow for a comprehensive study to determine not only how and when dust emission may align with continuum emission, but also how these observable signatures may inform us of the planetary compositions within.

Current chemical models of planet formation tend to assume a single bump and gap (if any substructure), and a static disk, with chemistry taking place over the disk lifetime with no evolution of the dust or planet-induced features. As a result, it is impossible to account for the dynamic and evolving nature of the disk, including transport of dust and gas and how the growth and fragmentation of dust grains can affect the gas phase chemistry of the disk. **One consequence of current approaches of disk modeling is the difficulty in differentiating between chemical and dynamic effects.** For example, pebble drift may transport ices throughout the disk, leading to an excess in emission near snowlines where sublimation occurs. If, however, these molecular tracers are processed either in the gas or on the grain surface, then the signal of this sublimation may be hidden. Additionally, the turbulent transport of grains through the disk can expose ice mantles to high temperature and radiation environments, leading to ice processing on grains during short excursions to surface regions of the disk [4, 5, 19]. These effects will result in unique signatures of *dynamic* chemical processes in disks that are impossible to predict using standard, equilibrium chemical models.

The combined 2D chemical and dynamic models proposed here will, for the first time, be able to disentangle chemical and dynamic effects in evolving disks. These models will have important implications for understanding the radial distribution of molecular tracers, with the goal of understanding under what conditions continuum and molecular line substructures should be correlated. The 2D nature of the proposed models will also provide insight to the vertical structure of disks, with self-consistent dust and thermal evolution, providing a theoretical framework for connecting observations from the disk surface to midplane compositions. Finally, these new combined chemical and dynamic models will explain how the disk responds to a growing planet chemically, in addition to the widely observed dynamic consequences of planet formation.

3. Planetary inheritance of disk chemistry

While it is typically believed that planets reflect the composition of the disk they formed within, planet formation is an ongoing process with dynamic and chemical consequences, as explored in projects 1 and 2. Given that planets can drastically alter the disk environment, **do giant planets reflect the conditions of the disk, or does the planet significantly alter its own composition through the act of accretion?**

Observations show that disks tend to be carbon rich, with hydrocarbon emission indicating C/O>1 in some disks. Giant planet atmospheres, on the other hand, tend to have C/O closer to stellar values [3]. To address this inconsistency, I will combine the dynamic and chemical models of projects 1 and 2 to self-consistently model the evolution of not only the disk, but the planets that form within. In a recently submitted paper currently in review [19], I proposed a novel mechanism by which fragmentation in the pressure bump can lead to dust lofting and sublimation of ice, which can then be accreted onto the growing planetary embryo. If volatile ice is sublimated from the grains via desorption as a result of this process, then this may lead to a natural transfer of volatiles from the disk to the planetary atmosphere, leaving behind refractory carbon in the disk explaining these observations.

This is a promising avenue of research, highlighting the dynamic environment of planet formation and the need to better understand how active accretion onto the planet affects

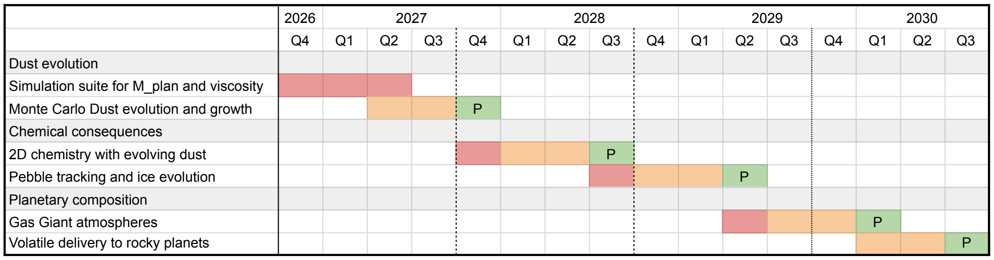

Figure 3: Proposed timeline for projects during my 51 Peg b fellowship. Expected publications are highlighted in green.

the composition of the accreted gas. This effect must be explored in more detail and in a self-consistent manner to constrain under what conditions we might expect this volatile enhancement in giant planets. Understanding this formation mechanism will allow us to better constrain planet formation environments and locations in disks, connecting the observed exoplanets to their formation histories and evolutionary pathways.

Combined with work from projects 1 and 2 modeling the transport of material across the gap will also allow for the study of volatile delivery to planets interior to planetary gaps. As discussed earlier, isotopic evidence from the Earth indicates a mixture of material from the inner and outer disk [16]. Through the combination of chemistry and dynamic models during planet formation, I will be able to link not only planet and disk compositions, but also compositions between planets within the same system.

Expected Research Impact

It is clear from observations that disks are dynamic environments, with actively forming planets leading to important dynamic effects in the surrounding gas and dust. While disk observations point to "leaky gaps," what this means for the composition of planets, both the giant planets in the gap and other planets in the disk, is unclear. I expect these projects to result in a number of publications during my fellowship (Fig 3), including the development of new models and software to advance the field. With the research presented here I will be at the forefront of this new research avenue and provide a fill key knowledge gaps on the connection between disks and the planets that form within in a comprehensive manner.

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