SF2A 2014
J. Ballet, F. Bournaud, F. Martins, R. Monier and C. Reylé (eds)

A 2D DUST CHEMISTRY OF THE INNER SOLAR NEBULA

F.C. Pignatale[1,2], K. Liffman[3], S.T. Maddison[2] and G. Brooks[2]

Abstract. The chemical composition of the dust in the inner layers of protoplanetary discs is unknown since infrared observation only probe the chemistry of the thin surface layer of discs. Given that planets formation occurs in the midplane, direct important information from the bulk chemistry of the disc is missing, and modelling is required. We compute for the first time the 2D chemical distribution of condensates in the inner Solar Nebula using a thermodynamic equilibrium model, and derive timescales for vertical settling and radial migration of the dust to predict the chemical evolution of the dust. We find two enstatite-rich zones within 1 AU from the protosun: a band ∼0.1 AU thick in the upper layer of the disc interior to 0.8 AU, and in the disc midplane out to ∼0.4 AU.

Our results are consistent with infrared observation of protoplanetary disc which show emission of enstatite-rich dust arising from the inner warmer surface of the disc. The inner midplane of the disc is a chemically diverse zone in which enstatite-rich dust coexists with sulfides and unprocessed material. Our finding of two enstatite-rich zones in the disc supports recent evidence that Mercury and enstatite chondrites shared a bulk material with similar composition.

The derived timescales for vertical settling suggest that dust can be chemically sorted in the hotter, inner surface of the disc leading to fractionated Mg-Fe-poor gas which can produce enstatite-rich dust. We suggest that the migration of enstatite-rich grains toward the midplane and-or condensation after gas fractionation may account for the formation of the bulk material which then formed the EL (low-Fe) chondrites.

Keywords: Protoplanetary discs, Solar Nebula, chemistry, planets, meteorites

1 Introduction

Infrared observations only probe the chemistry of the surface of protoplanetary discs (Henning & Meeus 2011), and thus direct information of the dust chemistry in the midplane, where planets formation occurs, is missing. 1D radial condensation sequences modelled to resemble the midplane of discs provided a general agreement with the derived bulk chemical composition of the Solar System planets, with refractory material and silicates in the inner region (Yoneda & Grossman 1995; Gail 1998), but cannot account for the global chemistry of a multilayered disc, where temperature and pressure are a function of both radius and height above the midplane. Furthermore, 1D condensation sequences fail to reproduce the complex chemistry of meteorites. Moreover, dynamical processes, such as dust vertical settling and radial migration (Barrière-Fouchet et al. 2005) and the dead zone (Gammie 1996), play an important role in mixing the dust and determining its distribution within the discs, and thus they need to be taken in account.

In order to address these limitations, we compute for the first time the two dimensional chemical distribution of condensates in the inner Solar Nebula using a thermodynamic equilibrium model, and derive timescales for vertical settling and radial migration of the dust to predict the chemical evolution of the condensates. With mapping the 2D dust chemistry in the disc, we also aim to provide the necessary chemical background for future complex studies on dust and gas interaction and dynamics.

[1] Université de Lyon, Lyon, F-69003, France; Université Lyon 1, Observatoire de Lyon, 9 avenue Charles André, Saint-Genis Laval, F-69230, France; CNRS, UMR 5574, Centre de Recherche Astrophysique de Lyon; Ecole Normale Supérieure de Lyon, F-69007, France. e-mail: `francesco.pignatale@univ-lyon1.fr`

[2] Swinburne University of Technology, Melbourne, Australia

[3] CSIRO, Melbourne, Australia

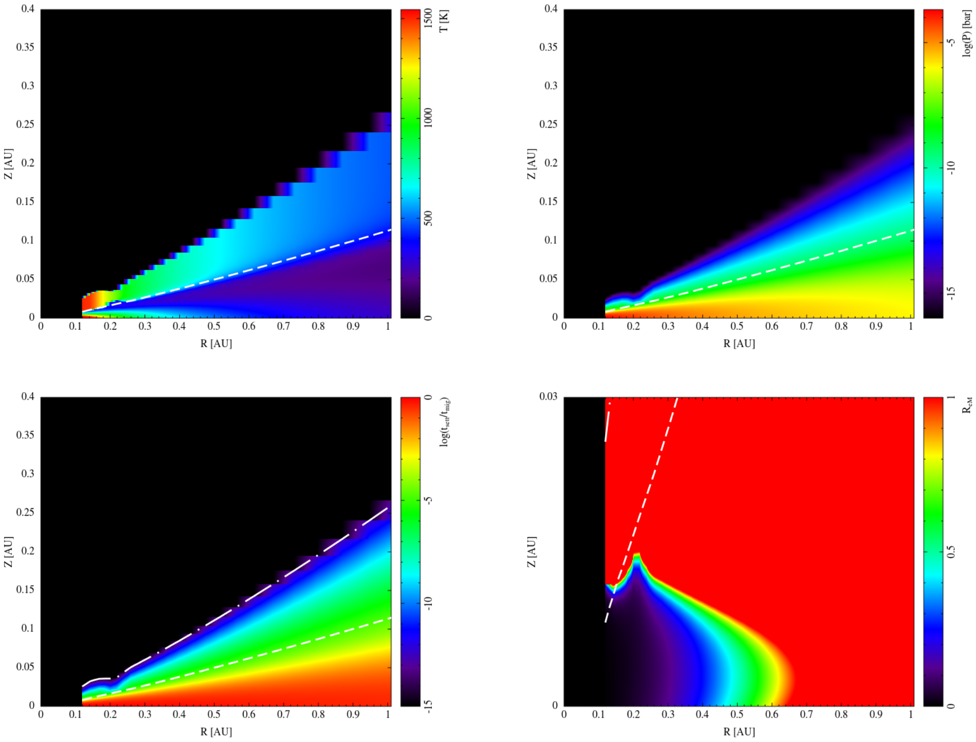

Fig. 1. Top row: temperature distribution (left), and pressure distribution (right) of the disc (D'Alessio et al. 1998). The dashed line represents the disc optically thin limit, the dot-dash line defines the disc contour. Bottom row: τ_{set}/τ_{mig} (left), and calculated Re_{M} (right) (note the change of scale in the z-axis).

2 Model

The temperature and pressure distribution within the disc, $T(R, Z)$ and $P(R, Z)$ are determined using the 2D disc model of D'Alessio et al. (1998, 1999) (Fig. 1). We chose a star-disc system with $M_* = 1\,\mathrm{M}_\odot$, $\dot{M} = 10^{-8}\,\mathrm{M}_\odot\mathrm{yr}^{-1}$, and $\alpha = 0.01$, assuming a 1 Myr old star.

We derive the 2D distribution of condensates by determining the thermodynamic equilibrium of an initial gas mixture, given a set of temperatures and pressures, using the Gibbs free energy minimization technique (DeHoff 1993). We utilize the FactSage software package (Bale et al. 2002, 2009), which uses the minimization method described by Eriksson & Hack (1990) and Eriksson & Konigsberger (1995). The initial gas mixture is composed of the 15 most abundant elements of the solar photosphere from Asplund et al. (2009), with their abundances normalized to 100 kmol. We assume that the gas is initially homogeneous throughout the disc and we perform equilibrium calculations using (T, P) at each location (R, Z) in the disc. The list of possible compounds that can condense comprise 170 gases and 317 solids. We use the ideal solution for modelling the phase behaviour in this region of the disc.

In the midplane, the stellar radiation is strong enough to heat the disc over 1000 K. Thus, for this disc, equilibrium is a reasonable assumption for the surface out to 0.8 AU and in the midplane within 0.4 AU. The optically thick zone of the disc beyond 0.4 AU, where the temperature decreases dramatically, will not be considered in our discussions.

We follow the approach of Liffman & Brown (1996) and Liffman & Toscano (2000) to derive the timescale of dust vertical settling (τ_{set}) within our disc model. τ_{set} is proportional to $1/a_p\rho_p$ where a_p is the dust grain radius, ρ_p is the dust grain density. The dust radial migration timescale (τ_{mig}) for a particle at distance R from the star is obtained by Hartmann (2000), and it is function of the average kinematic viscosity, and the inner boundary of the disc. For these calculations the value of the dust density, ρ_p, is chosen to represent the average density of silicates, 3 g cm^{-1}, and $a_p = 0.1\mu$m, which is the average size of forsterite grains as modelled by infrared observation (Bouwman et al. 2008). R_{in} is set to 0.1 AU.

To solve for the extent of the dead zone we calculate the magnetic Reynolds number, Re_{M}, at each location

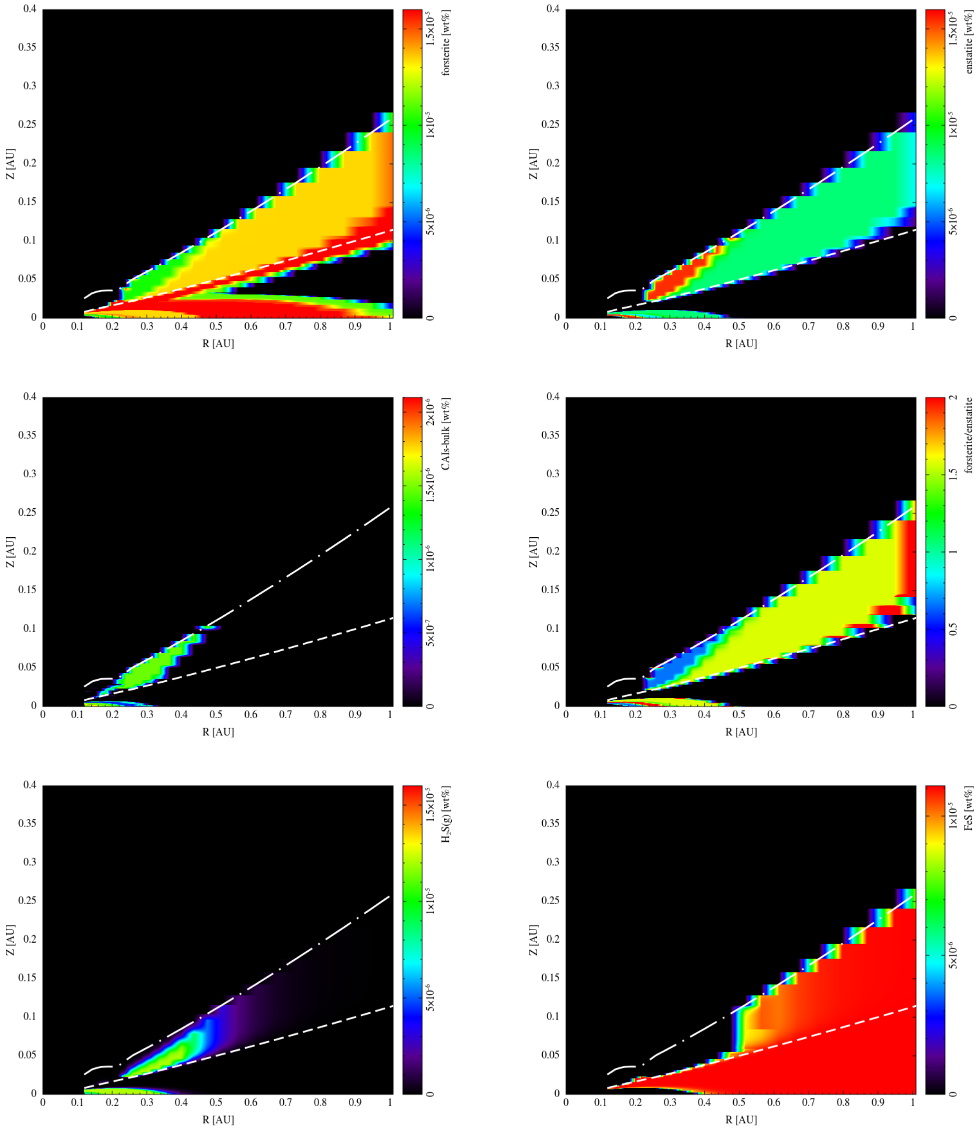

Fig. 2. Top row: forsterite (left) and enstatite (right) distribution. Mid row: CAIs-bulk components (left) and forsterite-to-enstatite (fo/en) ratio (right). Bottom row: H_2S(g) (left) and FeS (right) distribution. Note the change of scales in the color bar. Dashed line, limit under which the disc becomes optically thick. Dashed-dot line, disc contour.

in the disc following Gammie (1996). The magneto-rotational instability, which drives accretion in the disc, will be suppressed if $Re_{\mathrm{M}} \leq 1$ (Gammie 1996). In Fig.1 we report the τ_{set}/τ_{mig} ratio (bottom-left) and Re_{M} (bottom-right) in all the region of our disc.

3 Results and discussion

Figure 2 (top row), shows the 2D distribution of forsterite (Mg_2SiO_4) and enstatite ($MgSiO_3$), and (middle row) the location in which the calcium-aluminium bulk components* (CAI-bulk) condense and the forsterite-to-enstatite (fo/en) ratio. In the bottom row we report the H_2S(g) and FeS distribution.

We find that stable enstatite is limited to two well-defined zones within the disc: a band ~0.1 AU thick

*These include hibonite ($CaAl_{12}O_{19}$), gehlenite ($Ca_2Al_2SiO_7$), akermanite ($Ca_2MgSi_2O_7$), Mg-spinel ($MgAl_2O_4$), grossite ($CaAl_4O_7$) and anorthite ($CaAl_2Si_2O_8$).

in the upper layer of the disc interior to 1 AU, and in the disc midplane out to ∼0.4 AU. Forsterite is more abundant in a wider zone in the outer upper layer of the disc and the stability zone in the midplane reaches 1 AU. However, as previously stated, the zone beyond 0.4 AU falls in the non-equilibrium zone.

There are also two stability zones in the inner 1 AU of the disc where CAI-bulk components are present: one in the upper layer of the disc between $0.2 \leq \mathrm{R(AU)} \leq 0.5$ and another 0.01 AU thick zone in the midplane between the inner boundary of the disc and 0.3 AU. A "cloud" of H_2S(g) is stable between 0.25 and 0.5 AU below the surface of the disc, and a thick zone of stability out to 0.4 AU is present in the midplane.

Regions in which $fo/en \leq 1$ are present in both the surface and midplane of the disc. The average grain composition where $fo/en \leq 1$ is forsterite (Mg_2SiO_4) 20.2 wt%, enstatite ($MgSiO_3$) 29.6 wt%, metals ($Fe{-}Ni$) 47.2 wt%, diopside ($CaMgSi_2O_6$) 1.3 wt%, others 1.7 wt%. No sulfides condensed in this region.

Disc surface. On the surface of the disc, the main silicates are all distributed in the optically thin region (Fig.2). Infrared observations of the upper layers of protoplanetary discs show a spatial variation of the forsterite and enstatite distribution, with more enstatite in the warm inner regions than in the cooler outer regions where forsterite dominates (Kessler-Silacci et al. 2006; Bouwman et al. 2008; Meeus et al. 2009). The reason for this distribution remains uncertain. To account for the forsterite observed in the outer regions of discs several theories have been proposed: thermal annealing of enstatite from heating shocks (Fabian et al. 2000; Harker & Desch 2002) or an efficient radial grain transport mechanism which distributes the forsterite formed via condensation in the inner zones of the disc toward the cooler regions (van Boekel et al. 2004; Juhász et al. 2012).

Our 2D distribution of enstatite-rich dust is in good agreement with observations. Furthermore, the enstatite-rich dust can constitute the bulk material from which forsterite can form due to secondary processes. We see forsterite-rich dust naturally distributed in the outer surface of the disc. However, equilibrium calculations in this low temperature region might fail to predict the real dust composition because of kinetics barriers.

Disc midplane. Looking at our 2D distribution, the limitations of 1D condensation sequences clearly emerges. The midplane region of the disc within 0.4 AU is not chemically radially sorted as 1D calculations predict. It is a zone in which high-temperature material, enstatite-rich dust, sulfides and unprocessed dust can coexist. The presence of the dead zone in the midplane might prevent this mixture from migrating inwards. Since grain growth in this zone of the disc is very efficient, with grains reaching cm-size in a few thousand years (Laibe et al. 2008), enstatite-rich planetesimals may form in short timescales. Our results are compatible with recent observations and analysis from the Messenger X-Ray Spectrometer which suggest that the surface of the Mercury comprises Mg-rich minerals like enstatite and it is enriched in sulfur (Weider et al. 2012).

Dust dynamics. The derived vertical settling timescales of the dust on the surface of our disc suggests that condensed dust can quickly migrate towards the midplane and accumulate at the boundary of the dead zone. Thus, enstatite-rich grains can traverse the sulfides-rich regions and can experience secondary alterations during transient events such as outburst and shocks (Lehmann et al. 1995).

Furthermore, since vertical settling is function of the composition and the size of the grains, vertical chemical sorting of dust can also occur in the surface of our disc. Iron-rich and silicate-rich grains, which condense in the inner hotter surface of the disc, can leave their location of formation, not reacting with the surrounding gas and thus producing fractionated gas with Mg/Si and Fe/Si ratios lower than the initial solar with values close to the low-Fe enstatite chondrites (EL), rare objects with pure enstatite as the main pyroxene compound (Weisberg & Kimura 2012). A further condensation of gas with low Mg/Si leads to enstatite-rich dust (Ferrarotti & Gail 2001).

We suggest that the migration of enstatite-rich grains toward the midplane and-or condensation after gas-fractionation may account for the formation of the bulk material which constitute the EL chondrites.

4 Conclusions

In this work we derived for the first time the 2D condensates distribution in the inner Solar Nebula. We found two enstatite-rich zones: in the inner upper layer and in the inner midplane of the disc. The inner midplane is a chemically diverse zone in which high temperature crystalline material, enstatite-rich dust and unprocesses material can coexist and be trapped in the dead zone. Our results are compatible with infrared observation and recent discovery on the Mercury's enstatite-rich composition.

We presented a simplified model whereby dust efficiently settles toward the midplane, experiencing secondary alteration and fractionating the gas. These processes can account for the bulk material which formed rare objects like enstatite chondrites. Our finding of two enstatite-rich zone in the disc supports recent evidence that Mercury and enstatite chondrites shared a bulk material with similar composition.

This work was supported by the Swinburne University Postgraduate Research Awards (FCP) and CSIRO Astrophysics and Space Science (KL). FCP is grateful to the LABEX Lyon Institute of Origins (ANR-10-LABX-0066) of the Université de Lyon for its financial support within the program "Investissements d'Avenir" (ANR-11-IDEX-0007) of the French government operated by the National Research Agency (ANR). The authors wish to thank Paola D'Alessio for providing the detailed structure of the disc model and Jean-François Gonzalez for helping with the visualization of the data.

References

Asplund, M., Grevesse, N., Sauval, A. J., & Scott, P. 2009, ARA&A, 47, 481

Bale, C., Belisle, E., Chartrand, P., et al. 2009, CALPHAD, 33, 295

Bale, C., Chartrand, P., Decterov, S., Eriksson, C., & et. al. 2002, CALPHAD, 2, 189

Barrière-Fouchet, L., Gonzalez, J.-F., Murray, J. R., Humble, R. J., & Maddison, S. T. 2005, A&A, 443, 185

Bouwman, J., Henning, T., Hillenbrand, L. A., & et al. 2008, ApJ, 683, 479

D'Alessio, P., Calvet, N., Hartmann, L., Lizano, S., & Cantó, J. 1999, ApJ, 527, 893

D'Alessio, P., Cantö, J., Calvet, N., & Lizano, S. 1998, ApJ, 500, 411

DeHoff, R. 1993, Thermodynamics in Materials Science (McGraw-Hill International Editions)

Eriksson, C. & Hack, K. 1990, Metall. Trans., 21

Eriksson, C. & Konigsberger, E. 1995, CALPHAD, 19, 207

Fabian, D., Jager, C., Henning, T., Dorschne, J., & Mutschke, H. 2000, in ESA Special Publication, Vol. 456, ISO Beyond the Peaks: The 2nd ISO Workshop on Analytical Spectroscopy, ed. A. Salama, M. F. Kessler, K. Leech, & B. Schulz, 347

Ferrarotti, A. S. & Gail, H. 2001, A&A, 371, 133

Gail, H.-P. 1998, A&A, 332, 1099

Gammie, C. F. 1996, ApJ, 457, 355

Harker, D. E. & Desch, S. J. 2002, Apjl, 565, L109

Hartmann, L. 2000, Accretion processes in star formation, Vol. 32 (Cambridge University Press)

Henning, T. & Meeus, G. 2011, Dust Processing and Mineralogy in Protoplanetary Accretion Disks, ed. P. J. V. Garcia, 114–148

Juhász, A., Dullemond, C. P., van Boekel, R., et al. 2012, ApJ, 744, 118

Kessler-Silacci, J., Augereau, J.-C., Dullemond, C. P., & et al. 2006, ApJ, 639, 275

Laibe, G., Gonzalez, J.-F., Fouchet, L., & Maddison, S. T. 2008, A&A, 487, 265

Lehmann, T., Reipurth, B., & Brandner, W. 1995, A&A, 300, L9

Liffman, K. & Brown, M. J. I. 1996, in Chondrules and the Protoplanetary Disk, 285–302

Liffman, K. & Toscano, M. 2000, Icarus, 143, 106

Meeus, G., Juhász, A., Henning, T., & et al. 2009, A&A, 497, 379

van Boekel, R., Min, M., Leinert, C., et al. 2004, Nature, 432, 479

Weider, S. Z., Nittler, L. R., Starr, R. D., et al. 2012, Journal of Geophysical Research (Planets), 117, 0

Weisberg, M. K. & Kimura, M. 2012, Chemie der Erde, 72, 101

Yoneda, S. & Grossman, L. 1995, Geochim. Cosmochim. Acta, 59, 3413