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Diffusivity of heavy elements in Jupiter and Saturn

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ABSTRACT

Recent work has suggested that gas giant planets such as Jupiter and Saturn may not consist of a small number of fully convective and chemically homogenous layers as has been conventionally assumed, but instead may be chemically inhomogeneous with convective redistribution of elements limited by semiconvection. Constructing accurate planetary models which include semiconvective processes requires accurate estimates of the diffusion constants of minority chemical species in planetary fluids, which have not previously been available. In this work we use ab initio density functional molecular dynamics simulations to simulate the diffusion of heavy elements (specifically carbon, silicon, iron) in hydrogen–helium mixtures at conditions corresponding to giant planet deep interiors. We find diffusivities at the high end of the previously proposed range, and estimate that semiconvective processes may be able to redistribute a substantial fraction of Jupiter's core mass within the planet's age.

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1. Introduction

Conventional models of the interiors of gas giant planets (Chabrier et al., 1992; Saumon and Guillot, 2004; Militzer and Hubbard, 2008; Militzer et al., 2008; Nettelmann et al., 2008, 2012) have considered their interiors to be simple and homogeneous, consisting of a (optional) dense core of rock and ice surrounded by one or two layers of homogenous and fully convective hydrogen–helium fluid with a small amount of heavier elements. Convection is a fast process compared to planetary lifetime, ensuring that a fully convective interior layer will remain chemically homogeneous. A convective layer will also follow an adiabatic temperature profile with the temperature increasing predictably with pressure. In recent years, however, there has been a growing understanding that giant planet interiors may not be as homogeneous, or as convective, as previously thought. Two important thermodynamic processes may create an inhomogeneous distribution of elements in a planetary interior. The first is sedimentation: if a layer exists in which all components are not mutually fully soluble this results in phase separation and a rain-out of the heavier component towards deeper layers; this process is believed to occur and Jupiter and Saturn for helium (Stevenson and Salpeter, 1977; Morales et al., 2009) and neon (Wilson and Militzer, 2010). The second process is core erosion: if the heavy elements of a gas giant's initial dense rock-ice core are soluble in the surrounding hydrogen–helium layers then a high density solvated layer will be created at the bottom of the H–He fluid region which cannot necessarily be redistributed quickly by convection. Simulations now predict all likely core components ice (Wilson and Militzer, 2012a), MgO (Wilson and Militzer, 2012b), SiO$_2$ (Gonzalez-Cataldo et al., 2014) and Fe (Wahl et al., 2013) to be highly soluble in fluid hydrogen at giant planet core mantle boundary conditions. The existence of core erosion within Jupiter and Saturn may create an ongoing source injecting chemical inhomogeneity at the bottom of the hydrogen–helium layer.

The existence of a chemical density gradient which increases with depth will inhibit convection if the buoyancy of the warmer but compositionally denser material down below is insufficient to loft it above the higher, less dense material (Ledoux et al., 1961). In such a situation, a subcase of the effect more generally known as double diffusive convection or semiconvection, well known in oceanography and stellar interiors, will occur, resulting in a semi-convective steady state in which convective layers of constant composition are separated by thin diffusive layers with a rapid compositional and thermal gradient. Semiconvection leads to three important effects: a rate of redistribution of mass from the core to the upper layers which is slow even on billion year timescales, a slower rate of cooling in the interior than would be predicted from a fully convective model, and a super-adiabatic temperature profile in which the temperatures of the interior layers are higher than would occur in a fully convective planet. The role of these effects, in particular the inhomogeneity of the mass distribution, must be understood in order to properly interpret the gravitational moment data to be measured by the Juno orbiter, due to arrive at Jupiter in 2016.

Inclusion of compositional inhomogeneity in planetary models complicates the business of modelling considerably, and only a few previous models over the past few decades have been made to model the effect of double diffusive behaviour on planetary interiors. The evolution of the heavy element distribution of a gas giant with an eroding core was first considered by Stevenson (1982) and later by Guillot et al. (2004). More recently, Leconte and Chabrier (2012, 2013) constructed detailed interior models of the structure and evolution of planetary interiors with layered double diffusive convection. A key ingredient into all these models is the diffusivity or diffusion constant D of the heavy elements within the envelope as a function of temperature and pressure. Stevenson and Salpeter (1977) in 1977 estimated the diffusivity of hydrogen in hydrogen based on the hard sphere model of Vadovic and Colver (1971), and estimated the self-diffusion constant of hydrogen in the atomic regime as:

$$D_{\mathrm{H}} \approx 3.0 \times 10^{-3} \rho^{-2/3} T_4^{3/2} \ \mathrm{cm^2 \ s^{-1}} \tag{1}$$

where ρ is the density in $\mathrm{g \ cm^{-3}}$ and T_4 is the temperature in units of 10^4 K and of helium as approximately half that value.

$$D_{\mathrm{He}} \approx 1.5 \times 10^{-3} \rho^{-2/3} T_4^{3/2} \ \mathrm{cm^2 \ s^{-1}} \tag{2}$$

In Stevenson (1982), the diffusivity of heavier elements was considered in the context of core erosion, and estimated of this value being on the order of 10^{-3} to $10^{-4} \ \mathrm{cm^2 \ s^{-1}}$ were used to estimate that only a few percent of the initial cores of Jupiter and Saturn could have been redistributed over the planetary lifetime. Guillot et al. (2004), using the same assumed values of D but a different model, estimated that core erosion could redistribute up to 19 M_{Earth} of an initial 30 M_{Earth} core in Jupiter but just 2 M_{Earth} of a similar-sized initial core in Saturn. Guillot et al. (2004) estimate that the efficiency of core erosion is roughly proportional to $\chi \approx \sqrt{D/K}$ where K is the thermal diffusivity, with:

$$\dot{m}_{core} = \frac{\chi}{\bar{\omega}} \frac{RL_1(t)}{GM} \tag{3}$$

where $\dot{m}_{core}$ is the rate of core mass change, $\bar{\omega}$ is a geometric factor close to 0.3, and $L_1(t)$ is the planet's intrinsic luminosity in the first convective shell.

Recently, French et al. (2012) have computed a number of physical and transport properties of hydrogen–helium mixtures at conditions along the Jupiter adiabat including the diffusion coefficients of hydrogen and helium in hydrogen–helium mixtures using density functional molecular dynamics (DFT-MD) simulations, however the diffusion of elements heavier than helium has not yet been determined via any ab initio model, and the order of magnitude estimate of Stevenson (1982) over thirty years ago have been used in all subsequent works. Given the importance of semiconvection in future inhomogeneous models of giant planet interiors, we believe that the determination of accurate diffusion constants for common planetary heavy elements via ab initio molecular dynamics is overdue.

In this work, we use DFT-MD simulations to compute the diffusion constants of three of the most prevalent heavy elements in gas giant interiors: carbon, silicon and iron. As well as being the fourth, eighth and sixth most common elements in the Solar System respectively, these are representative of the light, medium and heavy components of the $Z > 3$ Solar System components. We compute diffusion coefficients of these elements in H–He mixtures across a range of densities from 1.0 to 4.5 $\mathrm{g \ cm^{-3}}$ corresponding to pressures of 1.5–40 Mbar, and temperatures from 10,000 to 20,000 K. These conditions more or less span the metallic hydrogen regime which makes up the lower 60% or so of Jupiter's interior and where double diffusive convection effects may be expected

to be most important. The problem of diffusion in the *molecular* hydrogen regime is not considered in this work.

2. Methods

2.1. Computation of diffusion constants

Diffusion coefficients are a dynamical property and can only be extracted from a dynamical simulation of the material in question. Molecular dynamics works by the propagation of the trajectories of a system of simulated atoms forwards in time by computation of interatomic forces and the integration of Newton's equations of motion.

There are two common ways to estimate a diffusion coefficient from a molecular dynamics trajectory. The first is based on displacements, and holds that the diffusion coefficient is related to the time derivative of the mean square displacement of each atom from its initial position:

$$D = \frac{d}{dt} \frac{1}{6} \frac{\langle \sum_i \mathbf{x_i}^2 \rangle}{N} \tag{4}$$

where $\mathbf{x_i}$ is the displacement of the ith atom from its position at some arbitrary zero time. The second, which we will primarily use in this work, is based on the velocities, and holds that the diffusion constant is related to the time integral of the velocity autocorrelation function:

$$D = \frac{1}{3} \int_0^\infty \langle \mathbf{v_i}(\mathbf{0}) \cdot \mathbf{v_i}(\mathbf{t}) \rangle dt \tag{5}$$

where $\mathbf{v_i}(\mathbf{t})$ is the velocity of the ith atom at time t. In practice this integral can and should be truncated after a reasonably short amount of time as the system loses all memory of previous velocities quite rapidly. The average is taken over all atoms i of a given type and a number of starting points $t = 0$. Some care must be taken in truncating the time integration for the velocity autocorrelation function, as in practice extending this integration past the point at which the initial autocorrelation has died away will only lead to the accumulation of noise. From careful inspection of autocorrelation functions we determined that five hundred timesteps (100 fs) was sufficient to encompass the signal without excessive noise across the studied range of elements, densities and temperatures.

2.2. Details of electronic structure calculations

All simulations in this work were undertaken using the VASP DFT package (Kresse and Furthmüller, 1996). Each simulation used a cubic cell with periodic boundary conditions containing 116 hydrogen and 12 helium atoms resulting in a mixture with a helium mass percentage ($Y = 29\%$) close to that of the protosolar nebula (28%) (Bahcall et al., 2001). To this mixture was (optionally) added a single C, Si or Fe atom. Atomic trajectories were propagated by Born–Oppenheimer molecular dynamics using a timestep of 0.2 fs. Temperatures were controlled using a Nosé thermostat. Each trajectory was run for between 20,000 and 40,000 timesteps to obtain adequate statistics. Kohn–Sham wavefunctions were represented in a plane-wave basis set with a cutoff of 1000 eV and $(2 \times 2 \times 2)$ k-points in the Brillouin Zone, using the exchange–correlation potential of Perdew et al. (1996), and pseudopotentials of the PAW type (Blochl, 1994).