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Semi-convective layer formation

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Abstract. Semi-convective mixing, as an example of double-diffusive convection, is of general importance in multi-component fluid mixing processes. In astrophysics it occurs when the mean molecular weight gradient caused by a mixture of light material on top of heavier one counteracts the convective instability caused by a temperature gradient. Direct numerical simulations of double-diffusive fluid flows in a realistic stellar or planetary parameter space are currently non-feasible. Hence, a model describing incompressible semi-convection was developed, which allows to investigate semi-convective layer formation. A detailed parameter study with varying Rayleigh number and stability parameter has been performed for the giant planet case. We conclude that semi-convective layering may not play that important role as suggested in earlier works for the planetary case.

1. Introduction

Various situations are found in nature and in engineering problems where an unstably stratified fluid column is partially stabilized by a counteracting gradient. The double-diffusive instability (DD) belongs to these scenarios. As the name suggests, two different diffusivities are needed to describe this instability: the diffusivity κ_T of a fast diffusing component, e.g. temperature T, and the diffusivity κ_S of, say, a slowly diffusing solute such as salt in water or a component of a gas with different mean molecular weight than the other component(s) of the gas (such as helium in comparison to hydrogen in a gas mixture such as that one found in many stars). The ratio of both diffusivities is known as the Lewis number Le and for the cases of interest here, $\mathrm{Le} = \kappa_S/\kappa_T \ll 1$. Apart from the diffusivities the stratification is an important component of DD. Situations where the temperature stratification is unstable against small perturbations and the solute stabilises the convective buoyancy force are known as the *diffusive regime*. In astrophysics this case is known as *semi-convection*. On the other hand, if the solute is unstably stratified and the temperature gradient is positive in the vertical direction, so-called *salt-fingers* can occur. Consequently, both instabilities are determined mainly by the ratio of the thermal and the solute Brunt-Väisälä frequencies N_T^2 and N_S^2. The stability ratio R_ρ compares the impact of the solute stratification on the thermal buoyancy. The diffusive regime is thereby defined as $R_\rho = -N_S^2/N_T^2$, the salt-finger regime as $R_\rho = -N_T^2/N_S^2$. In spite of this classification the value of R_ρ related to unity is important: $R_\rho > 1$ implies that the stratification is much more stable than in the opposite case of $R_\rho < 1$. In particular, the parameter space of $1 < R_\rho < \mathrm{Le}^{-0.5}$

is characterized by layering processes which lead to so-called *staircases*. These staircases are well mixed layers separated by sharp interfaces with large gradients of T and S. The common challenge of modelling layered DD processes is to calculate the thermal and the solute flux over these interfaces. The fluxes in turn are needed to calculate the effective diffusivities, which can be used to estimate merging timescales and hence further evolutionary properties (mixing times, overshooting) of the star. The investigated numerical model is based on a modified experimental setup inspired by Turner [15]. The purpose of the numerical study is to investigate evolutionary aspects of the formation of the staircases and their spatial evolution.

1.1. DD in astrophysics

The challenging stellar parameter regime of $\mathrm{Pr}, \mathrm{Le} \ll 1$ makes it impossible to investigate the realistic stellar fluid flow with direct numerical simulations. Merryfield [7] performed the first simulations for $\mathrm{Pr} = 0.1$ and $\mathrm{Le} = 0.04$ for a setup otherwise akin to the convective core boundary of massive stars. He found coherent structures, but layer formation was missing, which was explained with a too low numerical resolution. Biello [2] investigated semi-convection in the same parameter space. He improved Merryfield's model setup and observed layering. Bascoul [1] found semi-convective layering for both regimes, the astrophysical one and the geophysical one. He simulated an expanding core by applying a time-dependent flux boundary condition at the bottom. Zaussinger et al. [16], [17] compared compressible and incompressible semi-convection experiments and confirmed Spruit's estimates for a parameter space accessible to direct numerical simulation ($0.01 \leqslant \mathrm{Le} \leqslant \mathrm{Pr} \leqslant 7$ with Ra up to about 10^6). Kupka et al. [10] recently published results concerning comparisons of semi-convection in oceans and in stars. Even extrapolations from the oceanographic to the stellar parameter space have been presented. Moll and Garaud [4] recently published a new model for double diffusive mixing, based on an extensive series of 3D simulations. As a result a modified power law for estimating the thermal and solute fluxes was derived. Layered semi-convection has been investigated by Chabrier and Baraffe [3] for the giant planet case, where the Prandtl- and the Lewis number are surprisingly high. The present study is oriented towards investigating their approximations.

2. Governing Equations

The double-diffusive system is described by four non-linear equations for the incompressible case. The scaled set of equations are based on the Boussinesq approximation, where the underlying equations are the mass conservation, the Navier-Stokes equation, the solute equation and the temperature equation. The density is assumed to be constant, apart from the buoyancy term. This approximation is justified since we consider small layers (in terms of the vertical extent), moderate flow speeds (compared to the sound speed) and small fluctuations of the dynamical variables around their (constant) background state.

$$\begin{aligned} \nabla \cdot \vec{u} &= 0 \\ \frac{\mathrm{D}\,\tilde{\mathrm{u}}}{\mathrm{D}\,\mathrm{t}} &= -\frac{1}{\rho_0}\nabla p + \nu \Delta \vec{u} + \rho \vec{g} \\ \frac{\mathrm{D}\,\mathrm{T}}{\mathrm{D}\,\mathrm{t}} &= \kappa_T \Delta T \\ \frac{\mathrm{D}\,\mathrm{S}}{\mathrm{D}\,\mathrm{t}} &= \kappa_S \Delta S \end{aligned} \tag{1}$$

Here we use the subsequent scaling denoted by *, which follows the idea that semi-convective processes happens on the thermal time scale,

$$\begin{aligned} \mathrm{t} &= t^* \cdot \frac{H^2}{\kappa_T} \\ \mathrm{u} &= u^* \cdot \frac{\kappa_T}{H} \\ \mathrm{p} &= p^* \cdot \frac{\rho_0 \kappa_T \nu}{H^2} \\ \mathrm{T} &= T_0 + \Delta T T^* \\ \mathrm{S} &= S_0 + \Delta S S^*. \end{aligned} \tag{2}$$

The buoyancy is modelled in terms of the extended Boussinesq approximation. The density, normalized to a background density $\rho_0 = 1$, hence is given by

$$\rho = 1 - \alpha(\mathrm{T} - \mathrm{T}_0) + \beta(\mathrm{S} - \mathrm{S}_0) \tag{3}$$

We follow standard notation, where the velocity is denoted by $\vec{u}(\vec{x}, t) = (u(\vec{x}, t), v(\vec{x}, t), w(\vec{x}, t))$, and $T(\vec{x}, t)$ is the (potential) temperature with units chosen to scale between 0 and 1, $S(\vec{x}, t)$ is the solute concentration scaled in similar manner such that S is between 0 and 1, and $p(\vec{x}, t)$ is the pressure. The height H, the thermal diffusion coefficient κ_T, the solute diffusion coefficient κ_S, the background density ρ_0, the kinematic viscosity ν, the vertical temperature contrast ΔT, the vertical saline contrast ΔS, the thermal expansion coefficient α, the saline expansion coefficient β and the gravitational acceleration g_z are needed to describe the double diffusive system. The dimensionless set of equations is obtained by applying the mentioned scaling (2),

$$\begin{aligned} \nabla \cdot \vec{u} &= 0 \\ \mathrm{Pr}^{-1} \frac{\mathrm{D\,\tilde{u}}}{\mathrm{D\,t}} &= -\nabla p + \Delta \vec{u} - \mathrm{Ra_T} \cdot T + \mathrm{Ra_S} \cdot S \\ \frac{\mathrm{D\,T}}{\mathrm{D\,t}} &= \Delta T \\ \frac{\mathrm{D\,S}}{\mathrm{D\,t}} &= \mathrm{Le}\Delta \mathrm{S} \end{aligned} \tag{4}$$

after having introduced the thermal Rayleigh number

$$\mathrm{Ra_T} = \frac{\alpha g \Delta T H^4}{\kappa_T \nu},$$

the solute Rayleigh number

$$\mathrm{Ra_S} = \frac{\beta g \Delta S H^4}{\kappa_T \nu},$$

the Prandtl number $\mathrm{Pr} = \frac{\nu}{\kappa_T}$, the Lewis number $\mathrm{Le} = \frac{\kappa_S}{\kappa_T}$ and the stability parameter $R_\rho = \frac{\mathrm{Ra_S}}{\mathrm{Ra_T}}$. The material derivative is defined as $D/D\,t = \partial/\partial\,t + \vec{u} \cdot \nabla$. We have dropped the scaling indicator * here for better readability.

The height of the domain is set to $1 < H < 5$ and the thermal diffusion time scale $\tau = \frac{H^2}{\kappa_T}$ defines one unit of time. Especially the correct height of the box is difficult to find, since the expected height of the single layers vary in time. However, a rough estimate gives $H_{\mathrm{layer}} = R_\rho^{-1}$ for a macroscopic and well developed layer. Consequently, the dynamical behaviour of double diffusive convection is described by the four dimensional space spanned by $(\mathrm{Pr}, \mathrm{Le}, \mathrm{Ra_T}, \mathrm{R}_\rho)$. The boundaries are assumed to be impermeable for the temperature (top: $T = 0$, bottom: $T = H$) and the solute (top: $S = 0$, bottom: $S = H$). This ensures a thermal and a solute diffusive flux of $\frac{\Delta T}{H} = \frac{\Delta S}{H} = 1$. Impenetrable, stress free boundary conditions are set for the velocity, hence $\frac{\partial v}{\partial z} = 0$ and $u = 0$ with z denoting the vertical direction. The horizontal boundary conditions

are periodic. We define the standard box by setting $H = 1$, $\Delta T = 1$ and $\Delta S = 1$. In order to use higher boxes with, e.g., the scaling factors aH and $a\Delta T$ as well as $a\Delta S$, the Rayleigh number as function of the height needs to be rescaled by

$$\mathrm{Ra[aH]} = \mathrm{Ra_{ref}} \cdot \mathrm{a}^4. \tag{5}$$

The reference Rayleigh number $\mathrm{Ra_{ref}}$ refers always to a box with height $H = 1$ and gradients in temperature and the solute as defined. However, it is very convenient to compare different box geometries with $\mathrm{Ra_{ref}}$. The simulation time changes accordingly $(aH)^2$.

2.1. Numerical setup

The governing equations are solved numerically with the ANTARES software suite, which treats advective terms with a 5th-order WENO type scheme on a rectangular grid. A comprehensive overview on the numerical details of this code is presented in Muthsam et al. [9] and Zaussinger and Spruit [16]. The interior domain consists of several layers 'peeled off' from the boundary of the underlaying convective zone. Hence a non-uniform grid is not needed. The main focus in choosing the grid size lies on the resolution of the solute boundary layers, which are the steepest. Not resolving them is a major limitation and hence would alter extrapolations in the numerically non-feasible stellar case significantly. Consequently, the thermal and the solute boundary layers are resolved with at least three points to guarantee correctly calculated fluxes. The minimum resolution can easily be estimated with the thermal Rayleigh number, by estimating the thermal boundary layer thickness δ_T,

$$\frac{\delta_T}{H} \approx \sqrt[4]{\frac{1}{\mathrm{Ra_T} \cdot \mathrm{Pr}}} \tag{6}$$

and by using

$$\delta_S = \sqrt{\mathrm{Le}}\,\delta_T, \tag{7}$$

the solute boundary thickness is calculated in turn. The layer formation itself is triggered by a linear temperature and solute gradient, and a small perturbation in the solute.

2.2. Model parameters and box geometry

The four dimensional parameter space spanned by the quantities $(\mathrm{Pr}, \mathrm{Le}, \mathrm{Ra_T}, R_\rho)$ is too large to be covered by numerical simulations without excessive computational expenses. The astrophysically relevant restriction of $\mathrm{Le} < \mathrm{Pr}$ reduces the computational amount significantly. This is reflected by the Schmidt number, $\mathrm{Sc} = \frac{\nu}{\kappa_S}$, which is typically in the oder of $\mathrm{Sc} \approx 100$. In the following the 'loosely' astrophysical (giant planet) based case of $\mathrm{Pr} = 1$ and $\mathrm{Le} = 0.01$ is investigated in more detail.

Since layer formation needs a certain amount of convective cells, the aspect ratio is an important factor. Based on a couple of initial tests, the aspect ratio is set to 2, which results in a typical box geometry of height $H = 5$ and width $L = 10$. This leads to thermal Rayleigh numbers of $\mathrm{Ra_T} > 10^7$, where the smallest scales are resolved by a standard Smagorinsky subgrid model. In order to reduce confusion all values are given in terms of the reference height $H = 1$ and have to be scaled according to equation (5).

3. The giant planet case with $\mathrm{Pr} = 1$ and $\mathrm{Le} = 0.01$

This case represents values, which are comparable to a giant gas planet with $10^{-2} < \mathrm{Pr} < 1$ and $\mathrm{Le} = 10^{-2}$. The study is covered by 72 numerical simulations, where the parameter space is spanned by the Rayleigh number and the stability parameter (see table 1). The dynamical changes have typically occurred within $\tau = 0.1$, which reduces the computational costs significantly. The numerical time step is of the order of $\Delta\tau = 10^{-6}$ and gives a computational

	R_ρ					
Ra_{ref}	1	$1.1-1.3$	1.4	1.5	1.6	$1.7-3.5$
$5.0\cdot10^3$	C	LU	D	D	D	D
$1.0\cdot10^4$	C	LU	L4	D	D	D
$1.5\cdot10^4$	C	LU	L5	D	D	D
$2.0\cdot10^4$	C	LU	L6	L6	D	D
$5.0\cdot10^4$	C	LU	L6	L7	D	D
$1.0\cdot10^5$	C	LU	L6	L8	D	D
$2.0\cdot10^5$	C	LU	L7	L9	D	D

Table 1. Semi-convective regimes for varying $\mathrm{Ra_{ref}}$ and R_ρ after $\tau = 0.05$. No layering, full overturns (C), layers unstable with tendency to full overturning (LU), diffusive or conductive (D) and layered regime with number X of staircases (LX).

effort of two days on 36 processors for each simulation. However, this is very cheap compared to other setups. High resolution 3D simulations with more than 400 points in each direction are very expensive, especially, when non-linearities begin to dominate the processes and thus lead to restrictive, advection dominated time steps. Since the stability parameter is less then the predicted maximum value of $R_{\max} = \mathrm{Le}^{-0.5} = 10$, layer formation is expected in $1 < R_\rho < R_{\max}$.

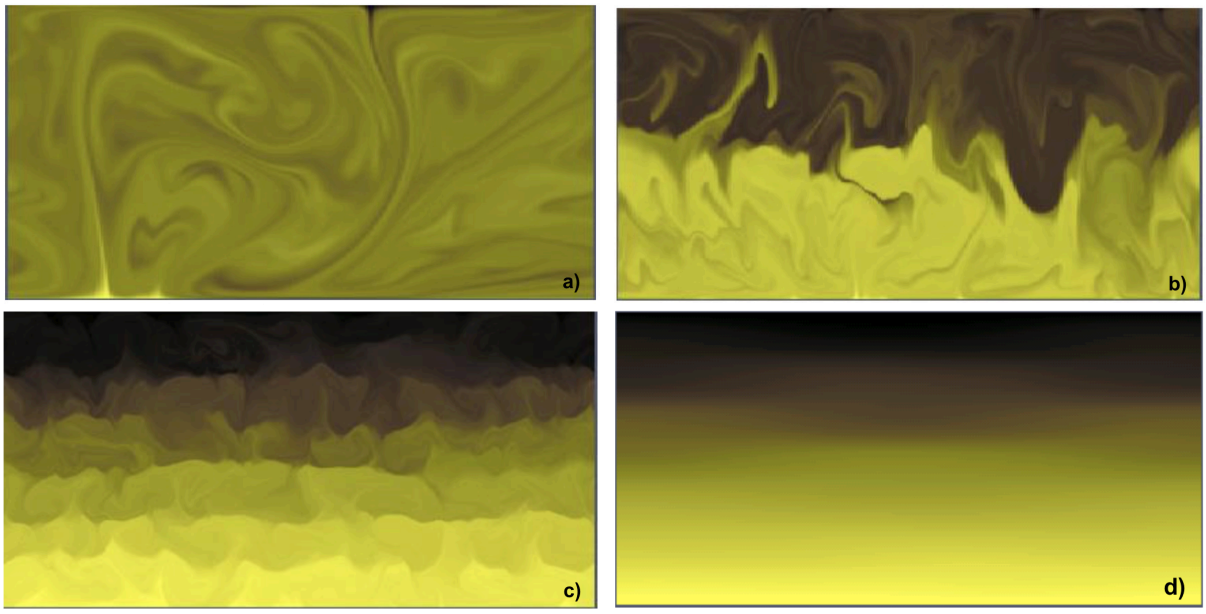

Figure 1. Solute (yellow high content, black low content) for varying stability parameters. $Ra_T = 3\cdot10^7$, $Pr = 1$, $Le = 0.01$: a) $R_\rho = 1$ fully convective, b) $R_\rho = 1.3$ unstable layering, c) $R_\rho = 1.4$ stable layering, d) $R_\rho = 3$ conductive.

Chabrier and Baraffe [3] and Zaussinger et al. [16], [17] estimated $10^5 - 10^6$ layers per pressure scale height H_p after a short initial layer formation period of some weeks. However, this number of layers has not to be simulated, since most relevant fluid dynamical processes can be investigated with 4–7 stairs. The layered convective regime is embedded between the fully convective regime, $R_\rho \lessapprox 1$, and the very stable conductive regime, $R_{\rho,\max} \gtrapprox 10$. The existence of this upper stability limit $R_{\rho,\max}$ is known from, e.g., Stevenson [14] and in the astrophysical context from Spruit [13].

However, the actual range of layered convection for the presented values of Rayleigh numbers is fairly small, $1.4 < R_\rho < 1.5$, which coincides with theoretical estimates from Mirouh [8] and Leconte [12] that a minimum stability parameter $R_{\rho,\min}$ separates the layered regime from the turbulent diffusive state. We found this value for $R_{\rho,\min} \approx 1.5$ (see figure 1c). The stability change from layered convection to turbulent diffusive convection is very sharp and needs to be investigated by numerical simulations for each new set of parameters. Since the super adiabatic gradient in the interior of a giant gas planet like Jupiter is extremely small, $\nabla - \nabla_{\rm ad} \approx 10^{-8}$ (see [3]), it has to be a happy coincidence that ∇_μ ranges exactly between $10^{-8} - 10^{-7}$ to trigger layering over the whole pressure scale height H_p in the small layering windows. This leads to the assumption that layering is a rare phenomenon and rather local than global. We found that the amount of layers increase with the Rayleigh number and is only limited by the vertical extent of the box and by $R_{\rho,\max}$. Since merging processes between convective cells destabilise the stack, the layered regime is only a short-term phenomenon. Merging effects and local entrainment decompose the stack, which leads to the question, how important the (temporal) layered semi-convective state is for the planetary evolution. A detailed study on time scales is currently in preparation.

4. Conclusion

Realistic numerical simulations of double diffusive stacks are a formidable task, since the small diffusivities and especially the extreme gap between the convective and the evolutionary time scale of the giant planet have to be covered. It seems to be impossible to simulate a whole pressure scale height with all scales resolved. But this is not necessary, since extrapolations from numerically feasible parameters and theoretical assumptions give enough tools to investigate the astrophysically relevant regime. The results show that the geophysical relevant parameter space can be applied to the astrophysical case, even when some properties like different time scales or the heights are numerically challenging.

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