



Boussinesq approximation, convection

Boussinesq approximations, and beyond, in a tall thermo-gravitational column

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Received 6 December 2006; accepted after revision 25 May 2007

Abstract

This article focuses on the main aspects of the non-Boussinesq treatment that is required for analyzing the simplest flow regimes occurring in a tall thermo-gravitational column, when the Soret coefficient S_T is considered as depending upon temperature and composition, $S_T(T, C)$. As a main result, the *horizontal* dynamics is mainly governed by the Soret *thermal* sensitivity, and the species *vertical* separation by its *compositional* one. **To cite this article:** G. Labrosse, C. R. Mecanique 335 (2007).

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R sum 

Approximations de Boussinesq et au del , en tr s haute colonne thermo-gravitationnelle. Cet article pr sente les points essentiels d'un traitement non-Boussinesq n cessaire pour une analyse th orique des  coulements de base dans une colonne thermo-gravitationnelle, o  le coefficient de Soret S_T d pend de la temp rature et de la composition, $S_T(T, C)$. Le r sultat principal est que la structure *horizontale* est contr l e par la d pendance *thermique* de S_T , alors que la d pendance *compositionnelle* de S_T fixe la structure de la stratification *compositionnelle* verticale. **Pour citer cet article :** G. Labrosse, C. R. Mecanique 335 (2007).

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Keywords: Fluid mechanics; Boussinesq approximations; Thermo-gravitational column

Mots-cl s : M canique des fluides ; Approximations de Boussinesq ; Colonne thermo-gravitationnelle

Version fran aise abr g e

La colonne thermo-gravitationnelle est connue depuis les ann es 1930 pour sa capacit    s parer, partiellement ou presque totalement, le m lange binaire qu'elle contient. Cette s paration est induite par la convection thermo-solutale coupl e   la thermo-diffusion, elle-m me souvent appel e « effet Soret ». La s paration est obtenue sous la forme d'une stratification verticale compositionnelle, avec un tr s faible gradient car il est contr l  par le coefficient de Soret, S_T , dont la valeur est tr s petite. Des colonnes extr mement hautes peuvent alors conduire   des s parations

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compositionnelles presque complètes, les deux extrémités, haute et basse, de la colonne contenant chacune l'un des composants du mélange.

L'analyse théorique de l'hydrodynamique de cette configuration s'est d'abord faite de façon assez simplifiée ([3]) pour calculer le pouvoir de séparation isotopique de ces colonnes. Elles sont utilisées de nos jours comme système de mesure des coefficients de Soret, en fixant les paramètres de fonctionnement de sorte que la thermique soit essentiellement contrôlée par la diffusion. Bien connaître l'hydrodynamique correspondante est ainsi devenu essentiel. Ici intervient la première difficulté. Il est expérimentalement établi que le coefficient de Soret dépend de la température T et de la composition C du mélange, $S_T \equiv S_T(T, C)$. Comment modéliser cette dépendance ? Quel effet peut-elle avoir sur les régimes de convection, et sur la séparation compositionnelle ? Comment aussi, et c'est la deuxième difficulté, traiter analytiquement le problème dans le cas où les colonnes sont assez hautes pour permettre une séparation compositionnelle importante et, donc, faire jouer la dépendance compositionnelle du coefficient de Soret ? Ces questions ouvrent un vaste champ d'analyse dont seule une toute petite partie a été faite ([8]) : l'identification des régimes stationnaires d'écoulements de base. Il faudrait ensuite étudier leur stabilité pour pouvoir interpréter l'ensemble des résultats expérimentaux.

Cet article présente les points essentiels de l'analyse théorique qui peut se faire pour des colonnes très allongées dans lesquelles la thermique est de nature diffusive. Les écoulements sont supposés bi-dimensionnels et établis parallèlement aux parois verticales dans une grande partie de la colonne. Tout ceci correspond bien aux observations expérimentales.

La première étape consiste à choisir un modèle de dépendance analytique du coefficient de Soret avec la température et la composition. A cet effet, il est tenu compte d'un constat expérimental montrant que les dépendances thermiques des paramètres physiques sont généralement très lentes, tant que l'on reste loin du point critique, et monotones. Par contre, les dépendances compositionnelles peuvent être très variées, non monotones par exemple. D'où le choix de la relation (4) comme modèle pour $S_T(T, C)$. Ceci ouvre la possibilité d'effectuer une analyse en « modes normaux », c'est-à-dire de considérer des « cas purs » de mélanges pour lesquels la dépendance de S_T se réduit à la relation (5).

L'analyse de la dynamique distingue les deux directions, horizontale (coordonnée x) et verticale (coordonnée z). Dans la direction horizontale, la thermo-diffusion agit autour d'une composition moyenne $\widehat{C}_k(z)$ définie par la relation (13). Les approximations usuelles de Boussinesq conviennent pour cette partie du traitement. Mais ce n'est plus le cas pour l'analyse de la dynamique dans la direction verticale, comme l'indique la relation (16). Cependant, grâce au fait que le coefficient de Soret est de très petite valeur (le paramètre ϵ_k défini par la relation (7)), un découplage s'introduit, au premier ordre en ϵ_k , entre les deux parties, horizontale et verticale, de la dynamique. La dynamique horizontale se résout directement, avec toutefois des nombres adimensionnels qui dérivent lentement avec z . Et la dynamique verticale se résume à la relation différentielle (14) qui gouverne $\widehat{C}_k(z)$, donc la stratification compositionnelle. On constate ainsi que la structure horizontale des écoulements de base est contrôlée par la dépendance thermique de S_T , alors que la dépendance compositionnelle de S_T fixe la structure de la stratification compositionnelle verticale.

La dérive verticale lente de la dynamique horizontale fait que cette configuration (très haute colonne thermo-gravitationnelle) est certainement d'une dynamique de stabilité très riche à analyser. L'expérimentation numérique de situations réalistes est probablement difficile à mettre en œuvre, et coûteuse en temps calcul, de même que la recherche expérimentale systématique des seuils de stabilité sera certainement de longue haleine.

1. Introduction

Thermal convection in binary mixtures is known, for several decades now, as offering very specific behavior (see [1] and [2], for example).

The thermo-gravitational column is one of the typical illustrative configurations. Initially designed, more than 60 years ago, for the isotopic separation ([3,4]), the column (see its 2D cross-section sketched in Fig. 1) is mainly used, nowadays, as a measuring device of the binary mixture Soret coefficient, see [5–7] for instance.

In this simple system, the thermal convection which is primarily driven by an horizontal thermal gradient imposed in presence of gravity, \vec{g} , is used, coupled with thermo-diffusion, for carrying out a compositional separation, by accumulation-depletion of the species in the vertical extremities of the column. An initially homogeneous binary mixture can thus be separated into its solutal components, partially or almost completely, depending on whether the vertical extension is moderately or extremely large compared to the distance separating the active vertical walls,

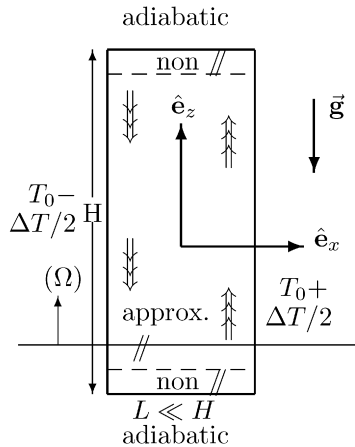


Fig. 1. Two-dimensional model of the thermo-gravitational column.
 Fig. 1. Modèle bi-dimensionnel de la colonne thermo-gravitationnelle.

those which are maintained at fixed temperature. The 2D approximation suits well the usual experimental working parameters, chosen so that the flow regime be mainly controlled by thermal diffusion and, therefore, steady.

A first theoretical analysis ([3]) was proposed, essentially dedicated to evaluating the separation power of the device, and based upon several simplifications, such as absence of solutal buoyancy, and constant Soret coefficient.

A recently published analysis ([8]) has significantly improved our knowledge of the possible steady basic states, still controlled by thermal diffusion. Indeed, first, this work takes into account the solutal buoyancy coming from thermo-diffusion, and, on the other hand, it allows the Soret coefficient, S_T , to depend upon temperature T and mass fraction C , $S_T = S_T(T, C)$.

This latter consideration is not gratuitous given the experimental evidence supplied, for instance, in [9–14,5]. It is in particular shown in [8] that the S_T compositional sensitivity plays the major role in constituting the species vertical stratification (see Section 4.2 below), and also that its slope can be a misleading sensor of the S_T thermal sensitivity when the mean temperature T_0 is such that $S_T(T_0, C) \simeq 0$, as in the oceanic concentration solution of sodium chloride in water about 12.09 °C ([10]).

The former hypothesis, that solutal buoyancy has to be taken into account, is essential. The Soret coefficient has indeed small values, much smaller for molecular solutions, $|S_T| \simeq (10^{-3}–10^{-2}) \text{ K}^{-1}$, than for colloidal mixtures, $|S_T| \simeq (0.03–0.5) \text{ K}^{-1}$. But the solutal buoyancy depends upon the relative importance of the solutal and thermal expansions, this being measured through the so-called separation ratio parameter defined by

$$\Psi = \frac{\frac{\partial \rho}{\partial C} |\vec{\nabla} C|}{\frac{\partial \rho}{\partial T} |\vec{\nabla} T|}$$

Also, even small values of Ψ can significantly influence the dynamics of a thermal free convection system. The Rayleigh–Bénard configuration with binary fluid is a good illustration of the major effect the presence of solutal buoyancy has on the stability behaviour of the layer (see [1]).

Introducing both the thermal and compositional Soret coefficient sensitivities led to phenomenologically separate the T and C modelling of S_T , and also, correlatively, thanks to the smallness of $|S_T|$, to separate the horizontal and vertical dynamics of the thermo-diffusive regimes, simplifying thereby the non-Boussinesq treatment of the balance equations. The detailed physical and analytical treatment of this configuration is published in [8]. The present paper merely aims at supplying the main steps and results.

2. The two-dimensional thermo-gravitational column

A binary mixture, of mean mass fraction C_0 , fills in a closed planar slender slot, Fig. 1, of height H much larger than L , its horizontal size. Constant temperatures are uniformly imposed on the vertical rigid walls, with for instance $T_0 - \Delta T/2$ and $T_0 + \Delta T/2$ respectively on the left and right walls, T_0 being the mean temperature. The horizontal

rigid boundaries are adiabatic and impervious. From the chosen working experimental parameters, the flow, mainly governed by thermal diffusion and steady, can be, to a very good approximation, taken as parallel to the active (vertical) walls in the major part of the cavity, obviously excluding the extremities where the flow has to close over itself.

What occurs in these extremities is essential for the separation process. There, the flow crosses the iso-thermal and iso-compositional lines leading to a convective accumulation-depletion of heat and species in the fluid particles. This part of the flow is thus responsible for the creation of the compositional vertical gradient. A thermal vertical gradient is also generated in this way, but it can be considered as negligible with respect to the imposed horizontal gradient provided the Rayleigh number be not too large ([15]). This part of the flow is not analytically tractable.

3. General approach

Let us first define a reference hydrostatic state ($\vec{v} = 0, \rho_0, p_0, T_0, C_0$), where the density ρ_0 is

$$\rho_0 = \rho(p_0, T_0, C_0) \tag{1}$$

and the pressure p_0 verifies

$$\vec{\nabla} p_0 = \rho_0 \vec{g} \tag{2}$$

The quantities T_0 and C_0 are constant, corresponding to the initial-state thermo-compositional configuration, while, by (1), (2), ρ_0 and p_0 are vertically stratified via a state equation which needs not be specified here. The state of interest, the dynamic state, is defined by (\vec{v}, ρ, p, T, C) with

$$\rho = \rho_0 + \delta\rho, \quad p = p_0 + \delta p, \quad T = T_0 + \delta T, \quad C = C_0 + \delta C$$

By (2) one has

$$-\vec{\nabla} p + \rho \vec{g} = -\vec{\nabla}(\delta p) + (\delta\rho) \vec{g}$$

The key point of the thermo-gravitational column dynamics with respect to what occurs in any thermo-solutal problem is that the range ΔC of variation of the mass fraction in the column is not controlled by the experimentalist, but by the flow dynamics. It is known from [3] and [8] that ΔC can be almost 1, that is the solutal separation can be almost complete, if the column aspect ratio $A = \frac{H}{L}$ is much larger than some typical aspect ratio A_s which increases as S_T^{-1} . The ratio $\frac{\Delta C}{C_0}$ turns out then to be non-bounded, implying the presence of non-Boussinesq effects, and also requiring to take into account the C -sensitivity of S_T .

The primary effect, thermo-diffusion, leads to a first species separation along the thermal gradient, that is, horizontally. The separation amplitude, noted $\Delta_H C$, is supplied by the solutal flux density,

$$\vec{j} = -\rho(T, C)D(T, C)[\vec{\nabla} C + C(1 - C)S_T(T, C)\vec{\nabla} T] \tag{3}$$

where, by thermodynamics, the solute diffusivity $D(T, C)$ is positive, whereas S_T can have either sign. In diffusive thermal regime, $\vec{\nabla} T$ is constant and horizontal, and $\Delta_H C$ is of the order of

$$|\Delta_H C| \simeq C_0(1 - C_0)|S_T(T_0, C_0)\Delta T| \ll C_0$$

therefore small by $|S_T(T_0, C_0)\Delta T|$. But, accessing to a realistic estimate of ΔC in the whole column requires now to look at the convection dynamics, and, therefore to write a model for $S_T(T, C)$.

The phenomenological model adopted for $S_T(T, C)$ leans on an experimental constatation. The thermal sensitivity of this coefficient is mild, monotonic, whereas its mass fraction sensitivity, over $C \in]0, 1[$, can be whatever, monotonic, or not. This is, by the way, not specific to $S_T(T, C)$. For instance, the water–alcohol dynamical viscosity exhibits a strong dependence upon C (see [16] for instance). This suggests writing the following phenomenological decomposition:

$$S_T(T, C) = \sum_{k=0, \text{ integer}}^{\infty} \tilde{S}_{T,k} \left(\frac{T - T_0}{\Delta T/2} \right)^k \mathcal{S}_k(C) \tag{4}$$

in which $\tilde{S}_{T,k}$ is a positive partial Soret coefficient (in K^{-1}), constant, and $\mathcal{S}_k(C)$ an $\mathcal{O}(1)$ dimensionless function.

Then, a normal-mode like analysis can be carried out, by considering pure cases, those where $S_T(T, C)$ contains only one k term in (4),

$$S_T(T, C) = \tilde{S}_{T,k} \Theta^k \mathcal{S}_k(C), \quad \text{integer } k \quad (5)$$

where

$$\Theta = \frac{T - T_0}{\Delta T/2} \in [-1, 1]$$

is the reduced temperature. In thermal diffusion regime, the only one here considered, it reads

$$\Theta = \frac{x}{L/2} \quad (6)$$

Identifying the specific effects of each k contribution, for a couple of typical $\mathcal{S}_k(C)$ functions, leads to a deep understanding of the base behaviors of the hydrodynamics in thermo-gravitational column.

4. Survey of the separation dynamics

Understanding the separation dynamics is essential for carrying out the analytical handling of the balance equations, based in particular upon the forthcoming relations (13). Here are recalled results coming from [8].

4.1. Horizontal separation

4.1.1. In absence of gravity

Let us first consider, as a guide, the hypothetical case where gravity is totally suppressed, that is where convection has disappeared. The fluid is in a hydrostatic state, characterized by the absence of species flux because all the boundaries are impervious, that is $\mathbf{j} = 0$. Using the relations (3), (5), (6) then supplies the hydrostatic-state solute distribution, noted $\bar{C}_k(x)$, in function of the reduced temperature. Indeed, starting from the following equivalent writing of (3),

$$d\bar{C}_k = -\epsilon_k \bar{C}_k (1 - \bar{C}_k) \mathcal{S}_k(\bar{C}_k) d(\Theta^{k+1}), \quad \epsilon_k = \frac{\tilde{S}_{T,k} \Delta T}{k+1} \frac{1}{2} \ll 1 \quad (7)$$

where the quoted condition, $\epsilon_k \ll 1$, is easily satisfied in the experiments (both S_T and ΔT are small), and requiring that the solution keeps C_0 as horizontal average of the mass fraction, that is

$$\int_{-1}^1 (\bar{C}_k(\Theta) - C_0) d\Theta = 0 \quad (8)$$

one can analytically write the $\bar{C}_k(\Theta)$ field provided $\mathcal{S}_k(C)$ be given. In fact, \bar{C}_k is fairly well approximated by its first order in ϵ_k . It reads

$$\bar{C}_k(\Theta) = C_0 - \epsilon_k C_0 (1 - C_0) \mathcal{S}_k(C_0) \left(\Theta^{k+1} - \frac{\delta_{k,2q+1}}{k+2} \right) \quad (9)$$

$\delta_{k,q}$ being the Kronecker symbol, and q a positive integer. Hence the amplitude of the mass fraction *horizontal* separation,

$$\frac{\Delta_H \bar{C}_k}{2} = \bar{C}_k(\Theta = 1) - \bar{C}_k(\Theta = 0) = -\epsilon_k C_0 (1 - C_0) \mathcal{S}_k(C_0) \quad (10)$$

from which $\bar{\Gamma}_k(\Theta)$, the reduced mass fraction field, is defined

$$\bar{C}_k(\Theta) = C_0 + \frac{\Delta_H \bar{C}_k}{2} \bar{\Gamma}_k(\Theta) \quad (11)$$

Eqs. (9)–(11) supply the $\mathcal{O}(\epsilon_k)$ mass fraction hydrostatic distribution. The horizontal variation is described by the reduced field $\bar{\Gamma}_k(x)$, and $\frac{\Delta_H \bar{C}_k}{2}$ is evaluated from $\mathcal{S}_k(C)$ taken at the *horizontally averaged value* of C which thermodiffusion acts about, C_0 here.

This result is now used, extended, in the real case where convection occurs within the cavity.

4.1.2. With gravity

In presence of convection, now, a mass fraction *vertical* stratification sets in, and, at any height z , thermodiffusion acts about an horizontal average noted $\widehat{C}_k(z)$. The corresponding scale $\frac{\Delta_H C_k}{2}$ thus becomes z -dependent, and mimics (10), namely

$$\frac{\Delta_H C_k}{2} = -\epsilon_k \widehat{C}_k(z) [1 - \widehat{C}_k(z)] S_k(\widehat{C}_k(z)), \quad \left\| \frac{\Delta_H C_k}{2} \right\| \leq \frac{|\epsilon_k|}{4} \tag{12}$$

where $\|f\|$ stands for the amplitude reached by f in its domain of variation,

$$\|f\| = [\max - \min]_{(x,z) \in ([-\frac{L}{2}, \frac{L}{2}], [-\frac{H}{2}, \frac{H}{2}])} f(x, z)$$

The resulting mass fraction field can then be decomposed, following (11), and the reduced field distribution $\Gamma_k(x)$ introduced, all that according to

$$C_k(x, z) = \widehat{C}_k(z) + \delta C_k(x, z), \quad \delta C_k(x, z) = \frac{\Delta_H C_k}{2} \Gamma_k(x), \quad \|\delta C_k(x, z)\| \ll \widehat{C}_k(z) \tag{13}$$

with, by definition (see (8)),

$$\int_{-L/2}^{L/2} \delta C_k(x, z) dx = 0$$

At first order in ϵ_k , the field $\Gamma_k(x)$ turns out to be governed by an *horizontal* advection-diffusion balance, simplified according to the specific Boussinesq approximation treatment which is presented in Section 5.

4.2. Vertical separation

Convection generates a species vertical stratification whose slope is shown (see relations (24), (25) below) to be also scaled with $\Delta_H C_k$, up to a multiplicative constant \widehat{K}_k bounded according to $|\widehat{K}_k| \leq 0.5$. Then this vertical stratification is governed by

$$\frac{d\widehat{C}_k}{\widehat{C}_k(1 - \widehat{C}_k) S_k(\widehat{C}_k)} = -\widehat{K}_k \epsilon_k d\left(\frac{z}{L/2}\right), \quad \int_{-H/L}^{H/L} (\widehat{C}_k - C_0) d\left(\frac{z}{L/2}\right) = 0 \tag{14}$$

This relation clearly shows the control that $S_k(C)$ exerts on the vertical stratification structure. From (14) it also becomes obvious that

$$\Delta_V C \equiv |C_{\text{top}} - C_{\text{bottom}}|$$

can be of order 1 provided $H \gg L$, in fact provided the aspect ratio exceeds some characteristic aspect ratio A_s ,

$$\frac{H}{L} \gg A_s = \mathcal{O}(\epsilon_k^{-1}) \tag{15}$$

This last requirement is necessary but not sufficient. It is indeed shown in [8] that the species separation cannot be complete, that is over the $[0, 1]$ range, if $S_k(C)$ has zeroes with C . The separation can only be complete in the C -interval which contains C_0 and is delimited by two successive zeroes of $C(1 - C)S_k(C)$.

4.3. (T, C)-sensitivity and (horizontal, vertical) separations

It is thus interesting to note that, at $\mathcal{O}(\epsilon_k)$, the (T, C) -sensitivities of S_T play each one a particular role. Through (14), the C -sensitivity controls the vertical stratification, and makes the horizontal dynamics, governed by the T -sensitivity, drifting along the vertical.

5. Non-Boussinesq dynamics

The overall analytical treatment of the problem is presented here, which leads to the aforementioned conclusions and also to the analytical identification of the steady base states which are allowed in thermal diffusion regime. Complements can be found in [8].

5.1. Density state equation approximation

The linear approximation of the density state equation proceeds as follows, making first a decomposition of the density about its horizontally averaged value, $\widehat{\rho}_k(z)$,

$$\rho(T, C) = \widehat{\rho}_k(z) + \delta\rho_k(x, z), \quad \widehat{\rho}_k(z) = \rho(T_0, \widehat{C}_k(z))$$

then linearizing the departure $\delta\rho_k(x, z)$ about T_0 and $\widehat{C}_k(z)$,

$$\delta\rho_k(x, z) = \left. \frac{\partial\rho}{\partial T} \right|_{T_0, \widehat{C}_k(z)} (T - T_0) + \left. \frac{\partial\rho}{\partial C} \right|_{T_0, \widehat{C}_k(z)} \delta C_k(x, z)$$

and finally introducing expansion coefficients which depend upon z ,

$$\alpha_T(T_0, \widehat{C}_k(z)) = -\left. \frac{1}{\widehat{\rho}_k(z)} \frac{\partial\rho}{\partial T} \right|_{T_0, \widehat{C}_k(z)}, \quad \alpha_C(T_0, \widehat{C}_k(z)) = \left. \frac{1}{\widehat{\rho}_k(z)} \frac{\partial\rho}{\partial C} \right|_{T_0, \widehat{C}_k(z)}$$

5.2. Conductivities and diffusion approximation

The solute and momentum conductivities, respectively D and μ , as well as the momentum diffusivity ν , are considered as constant along the horizontal, and taken as slowly drifting along the vertical, according to

$$D = D(T_0, \widehat{C}_k(z)), \quad \mu = \mu(T_0, \widehat{C}_k(z)), \quad \nu = \frac{\mu}{\rho(T_0, \widehat{C}_k(z))}$$

As regards the diffusion term, generically written for any quantity a whose corresponding conductivity is noted $\lambda(T, C)$, it can be decomposed as follows:

$$\vec{\nabla} \cdot (\lambda(T, C) \vec{\nabla} a) \simeq \lambda(T_0, \widehat{C}_k(z)) \frac{\partial^2 a}{\partial x^2} + \frac{\partial}{\partial z} \left(\lambda(T_0, \widehat{C}_k(z)) \frac{\partial a}{\partial z} \right) \quad (16)$$

At first order in ϵ_k , the last term is negligible, and one has

$$\vec{\nabla} \cdot (\lambda(T, C) \vec{\nabla} a) \simeq \lambda(T_0, \widehat{C}_k(z)) \frac{\partial^2 a}{\partial x^2} \quad (17)$$

5.3. Balance equations

Three balance equations are considered, and approximated at the leading order in the following three parameters, $\alpha_T \Delta T \ll \Delta T/T_0 \ll 1$, L/H and $|\epsilon_k|$. The momentum balance is written taking into account the parallel flow approximation, $\vec{v} = W(x) \hat{e}_z$. Making use of (17), it simply reads

$$\frac{dp}{dz} = -\rho g + \mu \frac{d^2 W}{dx^2} \quad (18)$$

For the species balance, an overall mass balance is performed in the part (Ω) of the cavity (Fig. 1) which goes down from the top boundary until an horizontal plane located at an arbitrary height z lying within the parallel flow region. Since the walls are impervious, the transport of solute only occurs across the lower boundary of (Ω), through which the net vertical convective supply must be balanced, in steady regime, by a vertical diffusion, that is

$$\int_{(\Omega)} \vec{\nabla} \cdot (\rho(x, z) \vec{v} C + \vec{j}) d\Omega = 0$$

Its leading part reads

$$\int_{-L/2}^{L/2} W(x)C(x, z) dx = D \frac{d}{dz} \left(\int_{-L/2}^{L/2} C(x, z) dx \right) \tag{19}$$

A local mass balance can also be written,

$$\rho(x, z)W(x) \frac{\partial C}{\partial z} = \frac{\partial}{\partial z} \left(\rho(x, z)D \frac{\partial C}{\partial z} \right) - \frac{\partial j_x(x, z)}{\partial x}$$

where j_x is the species flux density horizontal component, from \vec{j} given by (3). Taking $\rho \simeq \widehat{\rho}_k(z)$, and realizing that the vertical contribution of the right hand side is $\mathcal{O}(\epsilon_k^2)$ whereas the other terms are of first order in this parameter, lead to approximate this relation by

$$\widehat{\rho}_k(z)W(x) \frac{d\widehat{C}_k}{dz} = - \frac{\partial j_x(x, z)}{\partial x} \tag{20}$$

The *dimensionless* formulation of these balance equations is based on $L/2$, $\Delta_H C_k$ and V_{scale} , as length, mass fraction and velocity scales respectively, with

$$V_{\text{scale}}(z) = \alpha_T(z) \frac{\Delta T}{2} g \frac{(L/2)^2}{\nu(z)}$$

The scales $\Delta_H C_k$ (see (13)) and V_{scale} , as well as all the numbers to come, drift very slowly with z . Combining the previously mentioned Boussinesq/non-Boussinesq treatments together with the $\mathcal{O}(\epsilon_k)$ approximation, and introducing these scales lead one to separate the (x, z) -dependencies. The resulting dimensionless equations will thus consist of purely horizontal differential problems controlled by parameters slowly drifting with z .

Let

$$\vec{v} = W_k(x)\hat{e}_z$$

be the dimensionless velocity describing the parallel flow within the column, associated with $\Gamma_k(x)$ the dimensionless mass fraction field, already introduced by (13).

Introducing the scales into (18) supplies the following dimensionless momentum balance:

$$\left(\frac{dp}{dz} + \frac{2}{\alpha_T \Delta T} \right) = \Theta(x) + \Psi_k \Gamma_k(x) + \frac{d^2 W_k}{dx^2} = \Pi \tag{21}$$

where the constant Π is the dynamical pressure vertical gradient, and

$$\Psi_k \equiv \Psi_k(T_0, \widehat{C}_k(z)) = - \frac{\alpha_C \Delta_H C_k}{\alpha_T \Delta T} \tag{22}$$

is the partial separation ratio at height z . No-slip conditions are imposed on the vertical walls,

$$W_k(x = \pm 1) = 0 \tag{23}$$

Exploiting (19) leads to two important results. The species vertical stratification slope also scales with $\Delta_H C_k$,

$$\frac{d\widehat{C}_k(z)}{dz} = \Delta_H C_k \frac{d\widehat{\Gamma}(z)}{dz} \tag{24}$$

where $\frac{d\widehat{\Gamma}(z)}{dz}$ can easily be shown as being constant, according to

$$\frac{d\widehat{\Gamma}(z)}{dz} = \frac{Pe}{2} \int_{-1}^1 W_k(x)\Gamma_k(x) dx = \text{constant} = \widehat{K}_k \tag{25}$$

Pe being the compositional Péclet number,

$$Pe = Pe(T_0, \widehat{C}_k(z)) = V_{\text{scale}} \frac{L/2}{D}$$

At last, Eq. (20) leads to

$$\frac{d\Gamma_k}{dx} = -Pe \widehat{K}_k \Phi_k(x) + (k+1)x^k \quad (26)$$

with $\Phi_k(x)$ defined by

$$W_k(x) = -\frac{d\Phi_k(x)}{dx}, \quad \Phi_k(x = \pm 1) = 0 \quad (27)$$

its boundary values being equal in order to satisfy $\int_{-1}^1 W_k(x) dx = 0$.

Eq. (26) and the second part of (21) govern the horizontal dynamics. They are coupled by the separation ratio Ψ_k . Eliminating $\Phi(x)$ between (21) and (26) yields the following dimensionless differential equation ($k \leq 3$),

$$\frac{d^4 \mathcal{E}(x)}{dx^4} = Ra_{C,k} \mathcal{E}(x) \quad (28)$$

where

$$\mathcal{E}(x) = \frac{d\Gamma_k}{dx} + \frac{1}{\Psi_k} \quad (29)$$

expresses the x -derivative of the dimensionless buoyancy, i.e. the reduced buoyant torque. Equation (28) has to be completed with boundary conditions. By (26) together with (23), (27) one gets

$$\left. \frac{d\Gamma_k}{dx} \right|_{(x=\pm 1)} = (\pm 1)^k (k+1), \quad \left. \frac{d^2 \Gamma_k}{dx^2} \right|_{(x=\pm 1)} = (\pm 1)^{k-1} k(k+1) \quad (30)$$

The parameter involved in (28) is the compositional Rayleigh number

$$Ra_{C,k} = -(\widehat{K}_k \Psi_k) Pe \equiv \left(\alpha_C \frac{d\widehat{C}_k}{dz} \right) g \frac{(L/2)^3}{\nu D} \quad (31)$$

Based on the mass fraction dimensionless *vertical* slope, it also slowly drifts with z , and can have either sign.

Thus, the dimensionless horizontal dynamics is fully described by the relation set (28)–(30). It is monitored by two numbers, Ψ_k and $Ra_{C,k}$, both slowly drifting with z since they follow, through the C -dependence of the physical properties, the species vertical stratification of slope given by (14).

6. Conclusions

Analyzing the dynamics of the flow generated by Soret-induced thermo-solutal convection in very tall thermo-gravitational column reveals itself to be difficult, even considering that the flow is two-dimensional, develops in the regime of thermal diffusion and is mainly parallel to the active vertical walls. The convectively created vertical species stratification, although of very small slope, imposes that one takes into account a vertical drift of all the material properties, and also to introduce a compositional sensitivity of the Soret coefficient. However, the Soret coefficient (S_T) and the imposed temperature difference (ΔT) being very small, the analysis is greatly simplified if it is carried out at the first order in $\epsilon_k \simeq S_T \Delta T$, a parameter introduced in (7) whose values are effectively very small. It is worth noting that this parameter ϵ_k defines (see the relation (15)) the order of magnitude of a very large characteristic aspect ratio A_s , such that, for $\frac{H}{L} \gg A_s$, the species separation can start becoming complete in the meaning given at the end of Section 4.2.

Then a specific non-Boussinesq approach allows one to uncouple the horizontal and vertical behaviors of the thermo-gravitational column hydrodynamics, and to treat the realistic case where the Soret coefficient depends upon temperature and mass fraction. Its temperature sensitivity governs the horizontal dynamics, while the species vertical stratification is determined by the Soret coefficient compositional dependence. The slow vertical drift (within the parallel flow region) of the horizontal flow structure (see Eqs. (28)–(30)) simply results from the drift of the compositional Rayleigh number (defined by (31)) and of the separation ratio (defined by (22)). This might well lead, not only in very tall columns, to localized instabilities.

The steady base states allowed in such thermo-gravitational column can thus be analytically determined as solutions of the relations (28)–(30). They are given and analyzed in detail in [8]. Their stability is not known, so far.

It would be worth confronting these results with experiments, in particular to pinpoint the peculiar influence the Soret compositional dependence can have on the species vertical stratification structure. This is an ambitious task.

One could also appeal to numerical approaches for solving the non-Boussinesq balance equations, together with the introduction of realistic temperature and compositional dependence of the material properties, and of the Soret coefficient. This is also an ambitious task, even in 2D. Solving the Boussinesq coupled balance equations does not present particular difficulties when the fluid is a binary mixture, but to treat configurations with very large aspect ratios is expensive. Alternative numerical methods could be used, such as Molecular Dynamics methods, [17], or Lattice Boltzmann methods. This former approach is still rudimentary as regards thermal convection in binary fluid, [18]. Are these alternative methods capable of treating the non-Boussinesq balance equations ?

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