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Physical Science in Microgravity within the Thematic Group Fundamental and Applied Microgravity / *Sciences physiques en microgravité au sein du GDR Micropesanteur Fondamentale et Appliquée*

# On species separation in $n$-component mixture under microgravity

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**Abstract.** Recently, we proved that it was possible to significantly increase the importance of the species separation for binary mixtures, under microgravity, using forced convection obtained by a uniform translational displacement of the horizontal isothermal walls of the cell maintained at $T_h$ and $T_c$ respectively, with $\Delta T = T_h - T_c$.

The present work is an extension of the study performed by Mojtabi (2020) with various mixtures, from binary to $n$-component mixtures. An application with a ternary mixture was presented. The mixture of tetralin, isobutyl benzene, $n$-dodecane with respectively 0.8–0.1–0.1 mass fractions was studied experimentally in weightlessness.

**Keywords.** Thermo-diffusion, Species separation, Soret effect, Microgravity, Forced convection, Multicomponent mixtures.

## 1. Introduction

In the gravity field or under microgravity, pure thermo-diffusion leads to very weak species separation. To increase the species separation in the presence of gravity, many authors use thermo-gravitational diffusion in vertical or inclined columns (TGC) [1–4]. The flow velocity strongly depends on the temperature difference, $\Delta T$, imposed between the two walls facing each other, and also on the distance, $H$, between the walls. An optimum species separation cannot be obtained in relation to $\Delta T$ and $H$ simultaneously. We can obtain an optimum which is only a function of $H$ for a fixed $\Delta T$ or as a function of $\Delta T$ for a fixed $H$, Mojtabi [5].

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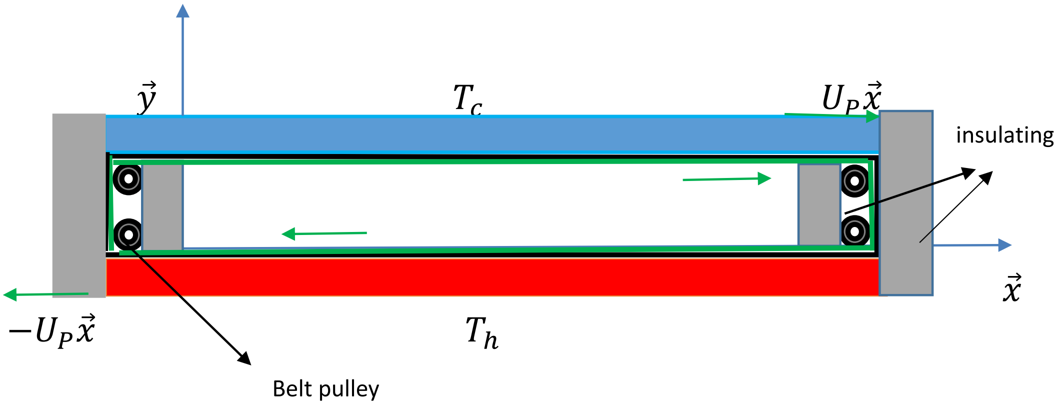


**Figure 1.** Schematic diagram of the rectangular cavity.

Studies on ternary mixtures are more recent. Experiments were conducted recently in the International Space Station (ISS) to measure the thermodiffusion coefficients of the ternary mixture tetralin, isobutyl benzene and $n$-dodecane [6, 7].

Mutschler and Mojtabi [8] studied numerically and theoretically the Soret driven convection in a horizontal porous layer saturated by $n$-components, with an application to a ternary hydrocarbon mixture composed of tetralin, isobutyl benzene, $n$-dodecane.

Recently, Mojtabi [9] showed that it is possible to significantly increase the importance of species separation for binary mixtures, in microgravity, using forced convection obtained by a uniform translational displacement of the isothermal walls maintained at $T_h$ and $T_c$ respectively, with $\Delta T = T_h - T_c$. In this new configuration, the species separation is several orders of magnitude greater than the one obtained in thermo-gravitational columns (TGC). The author verified that it is possible to carry out experiments, in microgravity, in order to measure directly the thermodiffusion coefficients of a binary mixture.

The present work is an extension of the study performed by Mojtabi [9] with various mixtures, from binary to $n$-component mixtures. An application with a ternary mixture was presented. The mixture of tetralin, isobutyl benzene, $n$-dodecane with respectively 0.8–0.1–0.1 mass fractions was studied experimentally in weightlessness. The geometry is a rectangular cavity. An analytical solution was obtained using the parallel flow approximation. The parameters leading to the optimal species separation for tetralin and $n$-dodecane were calculated. The analytical results were corroborated by direct numerical simulations (Comsol Multiphysics software).

## 2. Mathematical formulation

We considered a rectangular cavity of large aspect ratio $B = L/H$, where $H$ is the thickness of the cavity along the $y$ axis and $L$ is the length along the $x$ axis. The cavity is filled with a multicomponent mixture of density $\rho$ and dynamic viscosity $\mu$. The two walls $x = 0$ and $x = L$ are adiabatic and impermeable. The two other walls $y = 0$ and $y = H$ are kept at constant and uniform temperature $T_h$ and $T_c$ respectively and move at two opposite but constant imposed velocities $(-U_P\vec{e}_x, U_P\vec{e}_x)$ (see Figure 1).

The Boussinesq approximation is assumed to be valid. Thus, the thermo-physical properties of the multicomponent mixture are constant, except for the density in the buoyancy term, which varies linearly with the temperature and the mass fraction of $(n-1)$ components of the fluid mixture:

$$\rho = \rho_0 \left( 1 - \beta_T (T - T_0) - \sum_{k=1}^{n-1} \beta_{C_k} (C_k - C_{0k}) \right), \tag{1}$$

where $\beta_T$ and $\beta_{C_k}$ are respectively the thermal expansion coefficient of the mixture and the mass expansion coefficients of $(n-1)$ components of mass fraction $C_k$ with $k = 1, n-1$. The mass flux density vector of each constituent is defined as follows:

$$\vec{J}_k = -\rho_0 \sum_{j=1}^{n-1} (D_{kj} \nabla C_j + D'_{T,k} \nabla T), \quad k = 1, n-1. \tag{2}$$

The parameters $D_{kj}$ is the mass diffusion coefficient of species $k$ in species $j$ and $D'_{T,k}$ the thermodiffusion coefficients of species $k$. They are defined as follows:

$$D'_{T,k} = F(C_k) D_{T,k}.$$

The functions $F(C_k)$ verify: $F(C_k = 0) = 0$ and $F(C_k = 1) = 0$.

We assumed that the variations of the mass fraction in the vicinity of $C_{0k}$ remain small:

$$F(C_k) \approx F(C_{0k}).$$

Most of the authors use the hypothesis: $F(C_{0k}) = C_{0k}(1 - C_{0k})$ where $C_{0k}$ is the mass fraction of species $k$ at the initial state of the mixture.

The dimensional equations governing the forced convection flow of a multi-component fluid, in microgravity, are given by:

$$\begin{cases} \nabla \cdot \vec{V} = 0 \\ \rho_0 \left( \dfrac{\partial}{\partial t} \vec{V} + \vec{V} \cdot \nabla \vec{V} \right) = -\nabla P + \mu \nabla^2 \vec{V} \\ \dfrac{\partial T}{\partial t} + \vec{V} \cdot \nabla T = \alpha \nabla^2 T \\ \dfrac{\partial C_k}{\partial t} + \vec{V} \cdot \nabla C_k = \displaystyle\sum_{j=1}^{j=n-1} (D_{kj} \nabla^2 C_j + \nabla \cdot (D'_{T,k} \nabla T)) \quad \text{with } k = 1, n-1, \end{cases} \tag{3}$$

where $\vec{V}$ is the velocity field, inside the rectangular cavity, induced by the walls $y = 0$ and $y = H$ moving at constant velocity $-U_P \vec{e}_x$ and $U_P \vec{e}_x$ respectively, where $\alpha$ is the thermal diffusivity and $\mu$ is the dynamic viscosity of the $n$-components fluid.

The corresponding dimensional boundary conditions are:

$$\begin{cases} x = 0, L\colon\ \vec{V} = 0; \dfrac{\partial T}{\partial x} = 0, \displaystyle\sum_{j=1}^{j=n-1} D_{kj} \dfrac{\partial C_j}{\partial x} = 0, k = 1, n-1 \quad \forall y \in [0, H] \\ y = 0, H\colon\ \vec{V} = -Up\vec{e}_x, Up\vec{e}_x, T = T_h, T_c; \displaystyle\sum_{j=1}^{j=n-1} D_{kj} \dfrac{\partial C_j}{\partial y} + D'_{T,k} \dfrac{\partial T}{\partial y} = 0, \quad k = 1, n-1\ \forall x \in [0, L]. \end{cases} \tag{4}$$

## 3. Analytical solution in the case of shallow cavity

In the case of a shallow cavity $B \gg 1$ the parallel flow approximation, used by many previous authors [10], is considered. The streamlines are all parallel to the $x$ axis throughout the cavity except for the vicinity of the insulated walls $x = 0$ and $x = L$, which gives:

$$\vec{V}_b = U_b(y) \vec{e}_x. \tag{5}$$

The temperature and mass fraction profiles can then be written as the sum of a term defining a linear variation along $x$ and another term giving the distribution along $y$:

$$\begin{cases} T_b = bx + g(y) \\ C_{bk} = m_k x + f_k(y) \quad \forall k = 1, n-1. \end{cases} \tag{6}$$

The constants $b$ and $m_k$ represent the temperature and mass fraction gradients along the $x$ direction respectively. The constant $b$ is zero due to constant temperatures imposed on the walls $y = 0,\ H$. By replacing in the system of Equations (3), the velocity, the temperature and the mass fractions by their expression in the Equations (5) and (6) we obtain the following simplified equations

$$\begin{cases} \dfrac{\partial^3 U_b}{\partial y^3} = 0 \\ \dfrac{\partial^2 T_b}{\partial y^2} = 0 \\ m_k U_b - \displaystyle\sum_{j=1}^{j=n-1} (D_{kj}\nabla^2 C_{bj} + \nabla \cdot (D'_{T,k} \nabla T_b)) = 0. \end{cases} \tag{7}$$

For weak separations, the last equation of the system (7) is written:

$$m_k U_b - \sum_{j=1}^{j=n-1} (D_{kj}\nabla^2 C_{bj} + C_{k0}(1 - C_{k0}) D_{T,k} \nabla^2 T_b) = 0. \tag{8}$$

By using the boundary conditions (4), we deduce the expressions of the temperature field and the velocity field:

$$\begin{cases} T_b = T_C - \dfrac{(T_H - T_C)y}{H} \\ U_b = \dfrac{U_P(2y - H)}{H}. \end{cases} \tag{9}$$

We obtained for the mass fraction the following result in matrix form:

$$\begin{aligned} [C_{bk}] = {} & [m_k]x - \left(\int \left(\int U_p \, \mathrm{d}y\right) \mathrm{d}y\right) [D_{kj}]^{-1} [m_j] \\ & + [D_{kj}]^{-1} \left[ D_{T,j}(T_H - T_C) C_{j0}(1 - C_{j0}) \left( \frac{y}{D_{kj}H} + \frac{1}{2D_{kj}} \right) \right] + C_{k0}, \quad k = 1, n-1. \end{aligned} \tag{10}$$

The different mass fraction gradients were obtained assuming that the mass flux associated with each components $k$ through any cross-section of the rectangular cavity perpendicular to the $x$-axis is equal to zero:

$$\int_0^H \left( U_b C_{bk} - \left( [D_{kj}] \frac{\partial C_{bj}}{\partial x} + \left[ D_{T,k} C_{k0}(1 - C_{k0}) \frac{\partial T_b}{\partial x} \right] \right) \right] \mathrm{d}y = 0, \quad k = 1, n-1. \tag{11}$$

For a ternary mixture, in the general case ($D_{kj} \neq 0,\ j \neq k = 1,2$) we deduced:

$$\begin{cases} m_1 = \dfrac{5[FC_1\,((HU_P)^2 + 30(D_{22}^2 + D_{21}D_{12})D_{T1} - 30FC_2 D_{12}(D_{11} + D_{22})D_{T2}](T_H - T_C)U_P}{(HU_P)^2[(HU_P)^2 + 30(D_{11}^2 + 2D_{21}D_{12} + D_{22}^2)] + 900(D_{11}D_{22} - D_{21}D_{12})^2} \\ m_2 = \dfrac{5[FC_2\,((HU_P)^2 + 30(D_{11}^2 + D_{12}D_{21})D_{T2} - 30FC_1(D_{21}(D_{11} + D_{22})D_{T1})](T_H - T_C)U_P}{(HU_P)^2[(HU_P)^2 + 30(D_{11}^2 + 2D_{21}D_{12} + D_{22}^2)] + 900(D_{11}D_{22} - D_{21}D_{12})^2}, \end{cases} \tag{12}$$

where: $FC_k = C_{k0}(1 - C_{k0})$, for $k = 1,2$.

In the case where the cross-diffusion coefficients $D_{ij} (i \neq j)$ are negligible compared to $D_{ii}$, we obtained:

$$\begin{cases} m_1 = \dfrac{5FC_1 D_{T1}(T_H - T_C)U_P}{(HU_P)^2 + 30D_{11}^2} \\ m_2 = \dfrac{5FC_2 D_{T2}(T_H - T_C)U_P}{(HU_P)^2 + 30D_{22}^2}. \end{cases} \tag{13}$$

In the case of $n$ components under the previous approximation, we found the following general results for $k = 1, n-1$:

$$m_k = \frac{5C_{k0}(1 - C_{k0})D_{Tk}(T_H - T_C)U_P}{(HU_P)^2 + 30D_{kk}^2} \tag{14}$$

and

$$C_{bk} = m_k x - \frac{m_k U_P \left[\frac{y^3}{3H} - \frac{y^2}{2} + \frac{H^2 - 6DL}{12}\right]}{D_{kk}} + \frac{D_{Tk}(T_H - T_C)C_{k0}(1 - C_{k0})\left(\frac{y}{H} + \frac{1}{2}\right)}{D_{kk}} + C_{k0}. \tag{15}$$

## 4. Optimization of the species separation

The species separation of the component $k$, $S_k = m_k L$ is defined as the difference in mass fraction of the component $k$ between the two ends of the cell, $x = 0$ and $x = L$, with $m_k$ obtained in Equation (14). For a given $n$-component mixture, the mass diffusion coefficient $D_{kk}$, the thermodiffusion coefficient $D_{Tk}$ and the initial mass fraction of the denser component $C_{k0}$, for the component $k$, are known. The analysis of Equation (14) shows that the species separation decreases as the thickness, $H$, of the cavity increases. Moreover, the species separation, $S_k$, increases when the temperature difference $(T_H - T_C)$ increases. Then, only one independent control parameter remains, namely the velocity $U_p$ imposed on the wall $y = 0$ and $-U_p$ imposed on the wall $y = H$. The optimum separation $S_k$ is obtained solving equation:

$$\frac{\partial m_k}{\partial U_p} = 0. \tag{16}$$

The resolution of the algebraic equation (16) leads to:

$$U_{Pk\text{Opt}} = \pm\sqrt{30} D_{kk}/H. \tag{17}$$

The optimal velocity $U_{Pk\text{Opt}}$, with respect to the parameter $U_p$, depends only of the mass diffusion coefficient $D_{kk}$ and the distance $H$. So, if the mass diffusivity of the component $k$ is known, the experiments can be conducted with this optimal velocity. Replacing $U_p$ by $U_{Pk\text{Opt}}$ in Equation (14) leads to the expression of the maximum mass fraction gradient:

$$m_{k\text{Opt}} = \frac{\sqrt{30} C_{k0}(1 - C_{k0})D_{Tk}(T_H - T_C)}{12HD_{kk}}. \tag{18}$$

Equation (18) can also be written in the following form:

$$m_{k\text{Opt}} = \frac{\sqrt{30} C_{k0}(1 - C_{k0})S_{Tk}(T_H - T_C)}{12H}, \tag{19}$$

where $S_{Tk} = D_{Tk}/D_{kk}$ is the Soret coefficient of the component $k$ of the mixture.

Thus, the optimum value of the mass fraction gradient (Equation (19)) depends only on the thermal gradient in the $y$ direction, $(T_H - T_C)/H$, once the initial mass fraction $C_{k0}$, $k = 1, n-1$ and the Soret coefficient $S_{Tk}$ are known. Equations (17) and (19) show that it possible to access

**Table 1.** Thermophysical properties of tetralin, isobutyl benzene, $n$-dodecane with respectively mass fraction 0.8–0.1–0.1 at 25 °C [11].

| $D_{11}$ ($10^{-10}$ m$^2$·s$^{-1}$) | $D_{12}$ | $D_{21}$ | $D_{22}$ | $D_{T1}$ ($10^{-10}$ m$^2$·(s·K)$^{-1}$) | $D_{T2}$ |
|---|---|---|---|---|---|
| 5.96 | 0.15 | 1.1 | 6.79 | 0.0065 | −0.0049 |

the indirect measurement of the Soret coefficient $S_{Tk}$ by measuring the optimal mass fraction gradient $m_{k\,\mathrm{Opt}}$:

$$S_{Tk} = 12Hm_{k\,\mathrm{Opt}}/\sqrt{30}C_{k0}(1-C_{k0})(T_H-T_C). \tag{20}$$

To measure $m_{k\,\mathrm{Opt}}$, it is necessary that the walls be set in motion with the optimal velocity $U_{Pk\,\mathrm{Opt}}$. The determination of the optimal velocity requires the mass diffusivity $D_{kk}$ of the component $k$.

In the following paragraph, we showed that it is also possible to measure of the mass diffusion coefficient $D_{kk}$ using Equation (14). To do so, it is sufficient to carry out two experiments, one with a velocity $U_{P1}$ and the other with different velocity $U_{P2}$ for the same cell of thickness $H$ subjected to the same temperature difference $\Delta T = T_H - T_C$.

We obtained:

$$m_{ki} = \frac{5C_{k0}(1-C_{k0})D_{Tk}(T_H-T_C)U_{Pi}}{(HU_{Pi})^2+30D_{kk}^2} \tag{21}$$

with $i = 1, 2$. The ratio $m_{k1}/m_{k2}$ leads to:

$$m_{k1}/m_{k2} = U_{P1}((HU_{P2})^2+30D_{kk}^2)/U_{P2}((HU_{P1})^2+30D_{kk}^2). \tag{22}$$

From Equation (22) we can deduce the mass diffusion coefficient $D_{kk}$ after measuring the mass fraction gradients $m_{k1}$ and $m_{k2}$ obtained from two fixed wall velocities $U_{P1}$ and $U_{P2}$ respectively. We obtained:

$$D_{kk}^2 = U_{P1}U_{P2}(U_{P1}m_{k1}-U_{P2}m_{k2})H^2/30(U_{P1}m_{k2}-U_{P2}m_{k1}). \tag{23}$$

## 5. Application to the species separation of a tetralin, isobutyl benzene, *n*-dodecane with respectively 0.8–0.1–0.1 mass fractions

### 5.1. *Species separation under weightlessness conditions*

To illustrate the analytical results obtained in this study, we only considered the experimental values of the thermophysics parameters of tetralin, isobutyl benzene, $n$-dodecane with respectively 0.8–0.1–0.1 mass fractions studied experimentally in weightlessness [11].

The thermophysical properties of this ternary solution at the mean temperature 25 °C are presented in Table 1.

Using the values presented in Table 1 for a cavity of thickness $H = 2\times10^{-3}$ m, the optimum value of the velocity and the mass fraction gradient following the $x$ axis for the component 1 namely tetralin and the component 2 namely isobutyl benzene were obtained as a function of the thermal gradient following the $y$ axis, $\Delta T$.

$$\begin{cases} U_{Pk\,\mathrm{Opt}} = \pm\dfrac{\sqrt{30}D_{kk}}{H} \\ m_{k\,\mathrm{Opt}} = \dfrac{\sqrt{30}C_{k0}(1-C_{k0})D_{Tk}(T_H-T_C)}{12HD_{kk}}. \end{cases} \tag{24}$$

For $\Delta T = 10$, we obtained:

$$\begin{cases} U_{P1\,\mathrm{Opt}} = \pm\dfrac{\sqrt{30}D_{11}}{H} = \pm5.96\dfrac{10^{-7}\sqrt{30}}{2} = \pm1.63\times10^{-6}\ \mathrm{m/s} \\ m_{1\,\mathrm{Opt}} = 0.597\ \mathrm{m}^{-1} \end{cases} \tag{25}$$

and

$$\begin{cases} U_{P2\,\mathrm{Opt}} = \pm\dfrac{\sqrt{30}D_{22}}{H} = \pm 6.79\dfrac{10^{-7}\sqrt{30}}{2} = \pm 1.86\times 10^{-6}\ \mathrm{m/s} \\ \qquad\qquad m_{2\,\mathrm{Opt}} = -0.222\ \mathrm{m}^{-1}. \end{cases} \tag{26}$$

Considering the low optimal velocity $U_{Pk\,\mathrm{Opt}}$ obtained, the time required to reach the stationary state of species separation would be around ten hours. The main interest here is given by Equation (24) which specifies that the measurement of the optimal mass fraction gradient $m_{k\,\mathrm{Opt}}$ allows access to the determination of the thermodiffusion coefficient $D_{Tk}$.

If the cross-diffusion coefficients $D_{ij}$ $(i \neq j)$ are non-zero, the analytical expression leading to the optimal velocity is the solution of an algebraic equation of the 6th degree. We obtained this velocity using the values in Table 1.

$$\begin{cases} U_{P1\,\mathrm{Opt}} = \pm 1.61\times 10^{-6}\ \mathrm{m/s} \\ \quad m_{1\,\mathrm{Opt}} = 0.605\ \mathrm{m}^{-1} \end{cases} \tag{27}$$

$$\begin{cases} U_{P2\,\mathrm{Opt}} = \pm 1.37\times 10^{-6}\ \mathrm{m/s} \\ \quad m_{2\,\mathrm{Opt}} = -0.329\ \mathrm{m}^{-1}. \end{cases} \tag{28}$$

### 5.2. *Comparison with the species separation inside a vertical thermogravitation column under gravity conditions*

The theoretical study of the thermogravitational separation process of $n$-component mixture inside a vertical column, under gravity conditions, was the subject of a communication at the French Mechanical congress in 2017 [12]. This study focused on a bi-dimensional vertical thermogravitational column. The analytical study was based on the parallel flow approximation and the theory was developed by Furry Jones and Onsager. Using these hypotheses, the velocity, the mass-fraction of each component and the temperature at the stationary state were calculated. Knowing the different flowfields in the column, the separation of each component in the mixture was determinated. Analytical expressions of the separation and transport coefficients were obtained. The results obtained were in good agreement with the thermo-diffusion coefficients found in the literature. In the case where the cross-diffusion effect can be neglected, it is possible to obtain a formula that allows us to calculate the coefficients of thermo-diffusion $D_{Tk}$ knowing the term $D_{kk}$, explicitly, from the measurements of the different mass fraction gradients $m_k^c$:

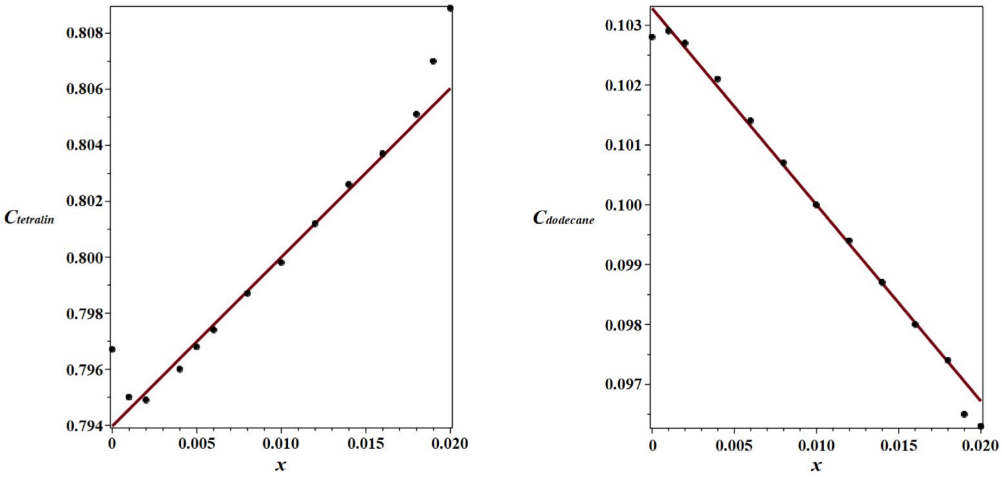
$$m_k^c = \frac{504H^2 g D_{Tk}\nu\beta_T(T_H - T_C)^2}{H^6(g\beta_T(T_H - T_C))^2 + 362880\nu^2 D_{kk}^2}. \tag{29}$$

It can be noticed that, from Equation (29), we find the classical relation giving the expression of the mass fraction gradient $m_{\mathrm{col}}$ in the case of binary solutions:

$$m_{\mathrm{col}} = \frac{504H^2 g D_T\nu\beta_T(T_H - T_C)^2}{H^6(g\beta_T(T_H - T_C))^2 + 362880\nu^2 D^2}. \tag{30}$$

Larrañaga *et al.* [13] determined the separation of each constituent of the ternary mixture tetralin, isobutylbenzene and $n$-dodecane in mass fraction (0.8–0.1–0.1). From the values of the mass fractions measured, these authors determined the values of the coefficients of thermodiffusion $D_{Tk}$ of each component $k$. The mass fraction gradient $m_1^c$ and $m_2^c$ in the $z$ direction for the vertical thermogravitational column and for a cavity with the same thickness $H = 2\times 10^{-3}$ m submitted of the same temperature difference $(T_H - T_C) = 10$ are respectively:

$$m_1^c = 0.00721\ \mathrm{m}^{-1} \quad \text{and} \quad m_2^c = 0.00544\ \mathrm{m}^{-1}. \tag{31}$$



(a) (b)

**Figure 2.** (a) Mass fraction of the tetralin and (b) mass fraction of the $n$-dodecane as a function of $x$ for $y = H/2 = 1$ mm, for a cavity of $L = 20$ mm and $H = 2$ mm (analytical results — numerical solution •).

Thus, the mass fraction gradient $m_{1\,\mathrm{Opt}} = 0.597\ \mathrm{m}^{-1}$ obtained in microgravity is 82.8 times greater than $m_1^c = 0.00721\ \mathrm{m}^{-1}$. The mass fraction gradient $m_{2\,\mathrm{Opt}} = -0.222\ \mathrm{m}^{-1}$ obtained in microgravity is 40.84 times greater than $m_2^c = 0.00544\ \mathrm{m}^{-1}$.

## 6. 2D numerical simulations

The dimensional system (3) associated to boundary conditions (4) was solved numerically using a finite element code, Comsol Multiphysics, with rectangular mesh. The time-dependent solver and the set of equations (incompressible Navier–Stokes, energy equation and two conservation equations of chemical species, one for the tetralin and the other one for the $n$-dodecane) in transient form were used. The condition of conservation of the average mass fraction in the cavity was imposed for each iteration. Direct numerical simulations were performed for cavities of the same thickness $H = 2 \times 10^{-3}$ m and various lengths $L = 2 \times 10^{-2}$ m and $5 \times 10^{-2}$ m, which correspond to aspect ratios of 10 and 25 respectively. We considered quadrangle spatial resolutions from 20–200 up to 30–700. The analytical calculations led to $m_{1\,\mathrm{Opt}} = 0.605\ \mathrm{m}^{-1}$ and $m_{2\,\mathrm{Opt}} = -0.329\ \mathrm{m}^{-1}$ for the tetralin and the $n$-dodecane respectively and the direct numerical simulations to $m_{1\,\mathrm{num}} = 0.590\ \mathrm{m}^{-1}$ and $m_{2\,\mathrm{num}} = -0.324\ \mathrm{m}^{-1}$. The numerical values obtained for $m_{1\,\mathrm{num}}$ and $m_{2\,\mathrm{num}}$ are in good agreement with the analytical values, except for the neighborhood of $x = 0$ and $x = L$. The reason for this is that our analytical solution assumes a fluid layer of very large extension along $x$ and does not take into account the return flow of the fluid at $x = 0$ and from $x = L$.

The mass fraction $C_{\mathrm{tetralin}}$ and $C_{\mathrm{dodecane}}$ as a function of $x$ for $y = H/2 = 1$ mm (Figure 2a) and (Figure 2b) for $L = 20$ mm show a very good agreement between the analytical calculations (red line) and the direct numerical simulation results (dark points).

The streamlines, iso-mass fraction lines and mass fraction field (in colour) for $\Delta T = 20$, $L = 50$ mm, $H = 2$ mm are presented in Figure 3 ($n$-dodecane) and Figure 4 (tetralin).

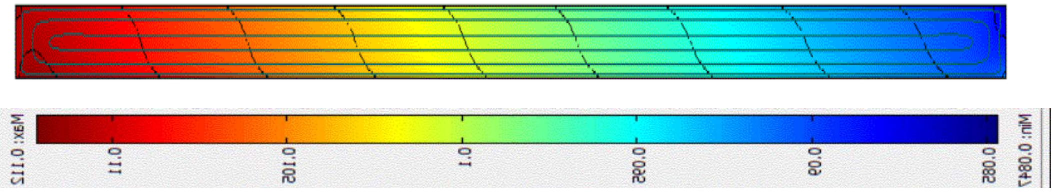


**Figure 3.** Streamlines, iso-mass fraction lines and mass fraction field (in colour) for $n$-dodecane and for $\Delta T = 20$, $L = 50$ mm, $H = 2$ mm.

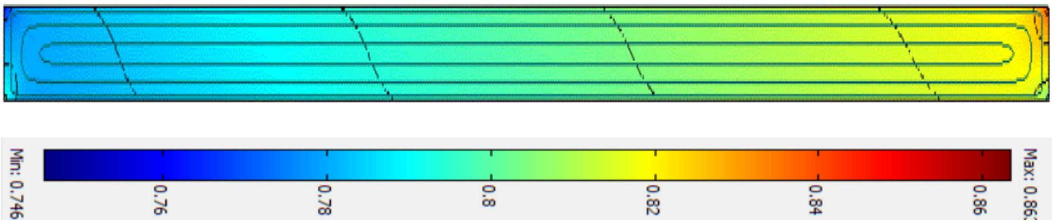


**Figure 4.** Streamlines, iso-mass fraction lines and mass fraction field (in colour) for tetralin and for $\Delta T = 20$, $L = 50$ mm, $H = 2$ mm.

## 7. Conclusion

In the vertical thermogravitation columns previously used in terrestrial applications to increase the species separation, the velocity of the flow depends on the temperature gradient imposed $(T_H - T_C)$ and its thickness $H$. However, for these columns, it was shown that there is no optimum of species separation according to these two independent parameters $(T_H - T_C)$ and $H$, [14]. For a given value of $(T_H - T_C)$ the separation is optimal for a very small thickness of the column $H < 1$ mm. Similarly, for fixed $H$, if we increase the value of $(T_H - T_C)$ to increase the separation, we increase the velocity of the flow which reduces the species separation. In microgravity, the temperature difference $(T_H - T_C)$ does not induce convective motion. The flow in the cell was obtained using a rectangular cavity with two opposite isothermal walls ($T_H$ and $T_C$) of great length, moving with equal optimal velocities in opposite directions, $U_{Pk\mathrm{Opt}}$ and $-U_{Pk\mathrm{Opt}}$. The velocities of these two walls are independent of $(T_H - T_C)$. We can increase $(T_H - T_C)$ to increase the separation without modifying the velocity. We showed that the species separation in microgravity with $U_{P\mathrm{Opt}}$ is several orders of magnitude greater than the one obtained in a vertical thermogravitation column of same geometrical dimensions and submitted to the same temperature difference. These results, previously obtained in binary mixtures, were extended to multi-component mixtures with a detailed study on ternary tetralin, isobutyl benzene and $n$-dodecane with respectively 0.8–0.1–0.1 mass fractions. To obtain the coefficients of thermodiffusion $D_{Tk}$ associated with each of the components of the mixture, the experiments must be carried out with the optimal velocity associated with the species considered $U_{Pk\mathrm{Opt}}$.

## Conflicts of interest

Authors have no conflict of interest to declare.

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