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Computational evaluation of micro-scale and macro-scale error sources in a thermodiffusive cell

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ABSTRACT

Computational fluid dynamics simulations have been made to understand the effect of various types of error sources in the experiments that can influence the thermodiffusion process. Specifically, errors due to emissive boundaries (due to improper thermal insulation), micro-scale gravitational force (static gravity), micro-vibrations acting on the fluid and small fluctuations in temperature profile along the constant temperature boundaries, on the thermodiffusive separation in a ternary hydrocarbon mixture that is subjected to a unidirectional thermal gradient, have been investigated. It has been found that the emissive boundaries and the static micro-accelerations have a dominant negative influence on the thermodiffusive separation. On the other hand, harmonic micro-accelerations have anywhere between four to thirty times smaller influence on the thermodiffusive separation, than the other types of error sources. This is because the errors are introduced in both directions due to the oscillating profile of the acceleration, thereby canceling each other.

1. Introduction

Thermodiffusion or the Soret effect is a coupled mass and heat transport phenomenon in which there is a segregation of the components of a mixture under the influence of a non-uniform thermal field. It is believed to play an influential role in many natural processes and applications such as ocean salinity, convection in stars, biological processes, morphological stability of the solidification front in crystal growth processes, semiconductor fabrication, isotope separation, nuclear reactor design, etc. In natural oil reservoirs, component stratification occurs due to a combined influence of thermodiffusion and sedimentation [15]. Understanding this requires a precise knowledge of the thermodiffusion process and this has led to extensive scientific research activity, theoretical as well as experimental.

Due to the complex inter-particle interactions in this hydrodynamic phenomenon, most of the research is still done on binary [11,12,2,3,14,8] and ternary mixtures [10,9,1,29]. The continued experimental research has led to the development of many experimental apparatus to study thermodiffusion [25].

For increased accuracies, studies of this purely diffusive phenomenon are also undertaken on space platforms such as the International Space Station that promise reduced gravity environments, minimizing convective disturbances. The success in such investigations has been demonstrated in several works in the literature [19,20,28,27,23]. Specifically, researchers have found larger diffusive separations in space due to the absence of buoyancy driven convections that can enhance the mixing process thereby interfering with the small thermodiffusive separations.

From the perspective of the oil industry, to understand the stratification of crude oil, the role of thermodiffusion has to be more thoroughly investigated. This includes collection of more experimental data by studying various hydrocarbon mixtures. Keeping this in mind, under the framework of the Canadian Space Agency and European Space Agency's physical science's program, thermodiffusion experiments on seven different compositions of a ternary hydrocarbon mixture containing n-dodecane (nC_{12}), Isobutylbenzene (IBB) and 1,2,3,4-tetrahydronaphthalene (THN) is currently being performed in the Selectable Optical Diagnostic Instrument (SODI) facility on the International Space Station (ISS). SODI is a high accuracy setup on the ISS that promises precise thermal control and high quality optical diagnostics for a variety of fluids. Its use in studying thermodiffusion in ternary hydrocarbon mixtures of the type considered here is expected to yield a good understanding of the thermodiffusion process.

These three hydrocarbons have been chosen because, a mixture of these components is a model that is representative of crude oil composition. The experiments are to be performed by subjecting each mixture to a unidirectional temperature gradient of 10 K. This is done by maintaining one wall of the chamber at 293 K and the opposite wall at 303 K. Further, in the planned experiments,

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the initial temperature and pressure of the mixtures are 298 K and 1 atm, respectively.

While reduced gravity experiments promise higher accuracy, the experiments are prone to the following errors that must be carefully investigated: (1) *Inaccuracy of the applied thermal gradient*: despite the highest precautions, radiative loss from the boundaries or non-uniform heating of the boundaries can result in inaccurate thermal gradients that can in turn influence the thermodiffusion process. (2) *Static and harmonic micro-accelerations*: objects on the space platforms like the ISS experience vibrations due to the operation of on-board devices, crew activity, firing of thrusters to uplift the ISS, etc. Such vibrations can induce deleterious effects on the small concentration gradients that are achieved via thermodiffusive processes.

The objective of this work is to perform a detailed study on the effects of such macro-scale and micro-scale error sources in the experiments on the thermodiffusive separation. Such an understanding can enable the investigators to explain the experimental data in relation to the operating conditions on the ISS more accurately. In particular, using computational fluid dynamics simulations, a systematic study of one of the experimental mixtures has been made. Specifically the following sources of errors in the experiments have been closely investigated:

1 Different levels of emissivity of the boundary walls that are orthogonal to the domain boundaries maintained at a fixed temperature.
2 Different levels of static micro-gravity that exist in the presence of vibrations.
3 Harmonic micro-accelerations that exist in the presence of vibrations.
4 Non-uniform heating of the constant temperature walls.

For the numerical computations, an in-house Fortran-based CFD code [5] that solves a complete set of governing equations coupled with the diffusion and thermodiffusion models has been employed. In the ensuing paragraphs, subsequent to the description of the problem formulation, the associated governing equations and the numerical scheme, a mesh resolution analysis is presented for this study. The computational cases corresponding to this investigation are outlined in Section 4 and the outcome of the simulations along with the analysis of the results are presented in Section 5. Finally, in Section 6, the conclusions drawn from this study are summarized.

2. Problem formulation and basic equations

The schematic of the computational domain is shown in Fig. 1. For the CFD simulations, a two-dimensional area of size 1 cm × 0.5 cm that is filled with the ternary mixture of nC_{12}-IBB-THN at a mean temperature and pressure of 298 K and 1 atm, respectively, is considered. A thermal gradient of 10 K is applied across the longer walls by maintaining the $y = 0.5$ cm boundary (hot wall) at 303 K and the $y = 0$ cm boundary (cold wall) at 293 K.

2.1. Governing equations

To understand the separation and flow behavior in the domain, a complete set of the governing equations comprising of the mass, species, momentum, and energy equations were solved. The principle of mass conservation is applied by assuming a weakly compressible flow, where density variations are due to fluctuations in local temperature and concentration. The resulting continuity equation is represented as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0. \tag{1}$$

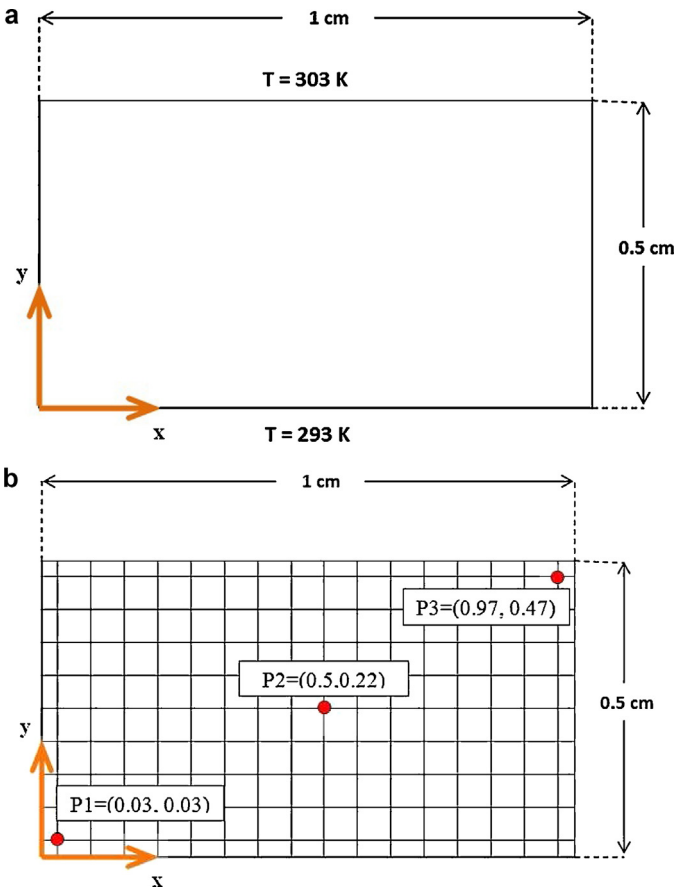

Fig. 1. (a) Schematic of the computational domain that is simulated and (b) the corresponding mesh along with the points at which transient analysis has been made.

In the above equation, t is the time and ρ is the density of the mixture. The velocity components in the x and y directions are represented by u and v, respectively.

The mixture investigated does not involve any chemical reactions. Hence, the mass conservation applies not only to the entire mixture but also to the individual constituents of the mixture. In this study, for the first two species in the mixture ($i = 1, 2$), the following equation is applied

$$\left(\frac{\partial}{\partial t}(\rho c_i) + \frac{\partial}{\partial x}(\rho u c_i) + \frac{\partial}{\partial y}(\rho v c_i)\right) = \frac{\partial}{\partial x}\left(\rho\left(D_{i1}\frac{\partial c_1}{\partial x} + D_{i2}\frac{\partial c_2}{\partial x} + D_{T,i}\frac{\partial T}{\partial x}\right)\right) + \frac{\partial}{\partial y}\left(\rho\left(D_{i1}\frac{\partial c_1}{\partial y} + D_{i2}\frac{\partial c_2}{\partial y} + D_{T,i}\frac{\partial T}{\partial y}\right)\right), \tag{2}$$

and the species conservation at every location in the domain is completed with the following additional equation:

$$\sum_i c_i = 1. \tag{3}$$

In the above equations, c_i is the mole fraction of respective species and T is the temperature of the mixture at the location (x, y) at a particular time, t.

In Eq. (2), D_{ii} and D_{ij} represent the main term and the cross term diffusion coefficients. The thermodiffusion coefficient of the ith species is $D_{T,i}$. The CFD code used in this study incorporates models based on the principles of non-equilibrium thermodynamics for

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