Proceedings of CHT-17
ICHMT International Symposium on Advances in Computational Heat Transfer

May 28-June 1, 2017, Napoli, Italy

CHT-17-xxx

Further considerations about double-diffusive convection in ternary systems DCMIX1 type

Rafael Jurado*§, Diana Dubert*, M. José Simón**, Jordi Pallarés**, Fina Gavaldà*, Xavier Ruiz*,***
*Dept. Química Física i Inorganica, Universitat Rovira i Virgili. Tarragona, Spain
**Dept. d'Enginyeria Mecànica, Universitat Rovira i Virgili. Tarragona, Spain
***Institut d'Estudis Espacials de Catalunya. Barcelona, Spain
§Correspondence author. Email: rafael.jurado@urv.cat

Following the considerations reported in a recent paper about double diffusive convection in ternary mixtures of 1,2,3,4-tetrahydronaphtaline, THN, isobutylbenzene (IBB) and n-dodecane, nC_{12}, (DCMIX1 type), at room temperature [1]. The present work will try to complete the problem considering another two different starting profiles of concentration used experimentally in the determination of the four molecular diffusion coefficients of this kind of transparent ternary mixtures. The first profile, a linear function, is related with the purely diffusive step of a thermodiffusion experiment inside a Soret cell, a typical arrangement commonly used in the International Space Station for the quantitative determination of the thermodiffusion coefficients of different transparent ternary mixtures at low temperature [2]. The second profile, an initial constant one, is characteristic of the Open Ended Capillary Tube, OECT, technique used on Earth experiments [3].

To avoid convective masking, experimentalists try to work, in all cases, under purely diffusive conditions. However in ternary systems the unavoidable competition between the two driving forces generated by the concentration gradients of both independent components could generate flow instabilities which, in turn, could be translated in appreciable perturbations in the experimental determination of the matrix elements of the molecular diffusion coefficients. These instabilities, depending on the initial conditions and the values of the set of diffusion coefficients considered, are detected and classified using as criterion the sign characteristics of the first and second derivatives of the density with respect to the direction of the gravity vector.

The mathematical procedures used here to detect potential instabilities are based on the following steps, i) obtaining of the analytical solutions of both independent species accomplishing the unsteady one-dimensional pure diffusive problem, ii) transformation of these profiles in density profiles by means of a set of calibration coefficients, iii) calculation of the first and second derivative using, as usual, centred differences and iv) evaluation of the sign characteristics of these profiles. Finally, the potential instabilities are in deep analysed using 3D numerical simulations of the flow established in the different experimental arrangements, diffusive cells and capillary tubes.

[1] J. Pallarés, Jna. Gavaldà, X. Ruiz, *Solutal natural convection flows in ternary mixtures,* International Journal of Heat and Mass transfer
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.10.063
[2] A. Ahadi, M. Z. Saghir, *The microgravity DSC-DCMIX1 mission onboard ISS: Experiment description and results on the measurement of the Soret coefficients for isobutylbenzene, dodecane, tetralin ternary hydrocarbons mixtures,* Experimental Thermal and Fluid Science 74 (2016) 296–307.
[3] Q. Galand, S. Van Vaerenbergh, *Contribution to the benchmark for ternary mixtures: Measurement of diffusion and Soret coefficients of ternary system tetrahydronaphtalene-isobutylbenzene-n-dodecane with mass fractions 80-10-10 at 25 C°.* The European Physical Journal E 38 (2015) 26.