Understanding Thermophoresis using non-Fickian diffusion current

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Thermophoresis and thermodiffusion are yet-to-be-understood phenomena that are also extremely important for applications. The current theoretical approach to understanding thermophoresis is based on two competing physical mechanisms of transport. One of these is the Fickian diffusion current, and the other is the solvation current originating in the solvation layer around a particle in the fluid. The quantity or parameter that characterises the process of thermophoresis is the Soret coefficient, determined with respect to a static non-equilibrium steady state. The Soret coefficient crosses zero at an intermediate temperature when a thermophilic-to-thermophobic (or vice versa) transition has been experimentally observed. Here arises an important fact: the temperature at which the thermophilic-thermophobic transition occurs is an extremum of the steady-state particle concentration undergoing thermophoresis. This means that, as the Fickian diffusion current crosses zero, the other current, the solvation current, must also pass through zero at the same temperature. Both currents should reverse direction relative to the temperature gradient at this temperature. The solvation mechanism, as yet understood, must be able to account for this direction reversal as a general process, but it has not. This fact raises the question: Is the model being used built on a correct hypothesis?

A general mechanism can account for this reversal of current when one considers the so-called 'solvation current' to have two distinct parts, governed by independent physics. One part of it is the current arising from the solvation mechanism; the other is an indispensable component of the diffusion current when diffusion is coordinate-dependent, the non-Fickian part.

In this talk, we will show that the above-mentioned three-current mechanism can readily be used to construct models that account for experimentally obtained Soret coefficient curves for thermophoresis events in which such a transition occurs [1]. We will argue that, in general, this competition among three currents serves as a basis for modelling thermophoresis and thermodiffusion. However, there may exist various model classes based on these three current scenarios, given the vast complexity of such systems.

Reference:

[1] A model of thermophoresis of colloidal proteins in water using non-Fickian diffusion currents, Mayank Sharma, Angad Singh and A. Bhattacharyay, arXiv:2602.13328v2.