

## **Coupled Fluid Transport Through Vapor-Gap Membranes for Use in Cleaning Contaminated Liquids**

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Contaminated liquids can be cleaned by membrane distillation using so-called vapor-gap membranes [1]. When a temperature difference is applied to a membrane with hydrophobic walls, clean vapor will pass the membrane, but the contaminated liquid will not. This occurs by evaporation on one side and condensation on the other side, thereby producing clean fluid transport across the vapor gap [1].

Conventional descriptions of transport in vapor-gap membranes account for the temperature difference by considering the equilibrium vapor pressure difference inside the membrane as the driving force for the mass flux. However, for a precise control of the flow, it is important to distinguish between independent and dependent driving forces. For a quantitative description it is furthermore essential to account for coupling between heat and mass transfer, as mass can also be transported by a temperature gradient, the so-called Soret effect [2]. It has been common to neglect this interaction of fluxes, but we know from other studies that the coupling between heat and mass transport at interfaces is significant [3].

In this work we present the non-equilibrium thermodynamic theory for heterogeneous systems, which describes the coupled transport processes across the vapor-gap membrane, along with non-equilibrium molecular dynamics simulations to illustrate equations. We present a computational proof of concept, and elucidate the mechanism of the temperature driven transport at isobaric as well as non-isobaric conditions. We compute the transfer coefficients and show that a Soret-Equilibrium exists for transport across a vapor-gap membrane.

### References:

[1] Meindersma et al., "Desalination and water recycling by air gap membrane distillation," *Desalination*, 2006.

[2] Platten, "The soret effect: a review of recent experimental results," *J.Appl.Mech.*, 2006.

[3] Wilhelmson et al., "Coherent description of transport across the water inter-face: From nanodroplets to climate models," *Phys.Rev.E*, 2016.