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Evaporation – Condensation Dynamics Affecting Vapor Transport in Partially Saturated Porous Media - Models and Experiments

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Introduction

- Diffusion of condensable vapor in the presence of liquid in porous media may be enhanced relative to diffusion of inert gas and potentially exceed diffusion flux rates in free air
- This enhanced vapor diffusion may be attributed to the capillary and thermally assisted liquid flow as postulated by Philip and deVries (PdV) [1957] (see **Figure 1**)
- The objectives of our work are:
  - To model kinetics of evaporation - condensation and the process potential for enhancement
  - To quantify thermal and capillary - assisted vapor transport enhancement across liquid bridges in model pores (single and 1D stack of pores)

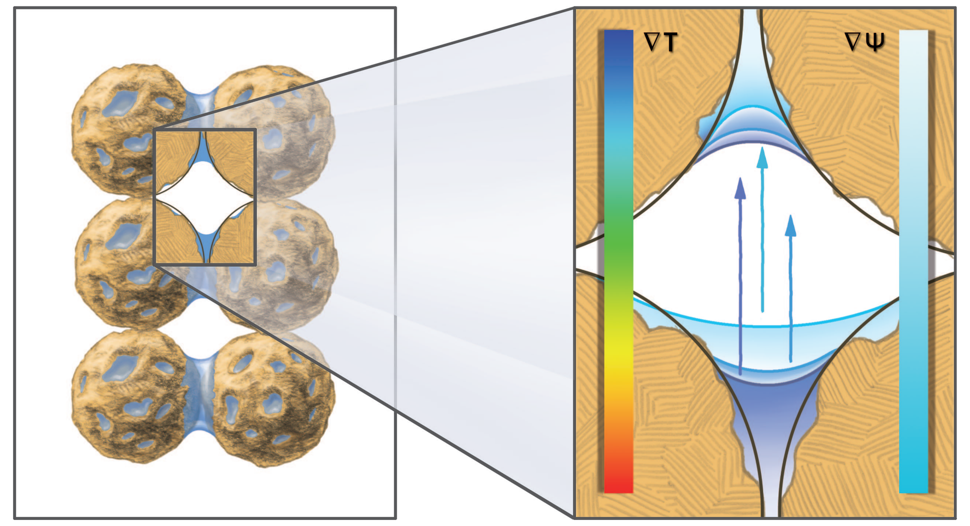

Figure 1: Schematic of a pore with two facing menisci in transition, pore scale saturation gradient results in a vapor flow between two menisci. Evaporation and condensation absorbs (releases) heat from (to) the interfaces which may cause a pore scale temperature gradient. Along with the pore scale gradients of temperature and vapor saturation, there might be macro scale gradients of vapor density and temperature which drives vapor flux between two interfaces.

Evaporation / Condensation Dynamics

- A 2D wedge shaped pore with known apex angle (α) is considered as the basic geometry of the problem (**Figure 2a**)
- Dynamics of the liquid - vapor interface profile composed of an adsorbed film and a capillary condensation meniscus can be modeled by the mean of two sets of PDEs expressing diffusion growth
- The building block can be extended to 3D as illustrated in **Figure 2c**. It could also be up scaled to represent an assemblage of rough grains in contact as **Figure 2b** and **d**

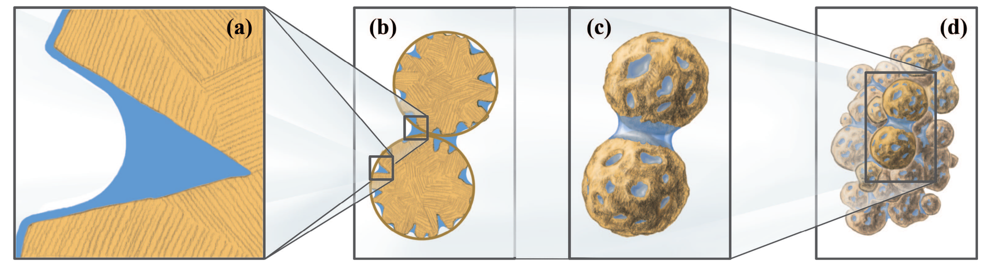

Figure 2: Different scales of modeling (a) a wedge shaped pore building block (b) 2D grains, water can deposit on and in-between the grains (c) extension to 3D grains (d) a population of spheres representing sand grains

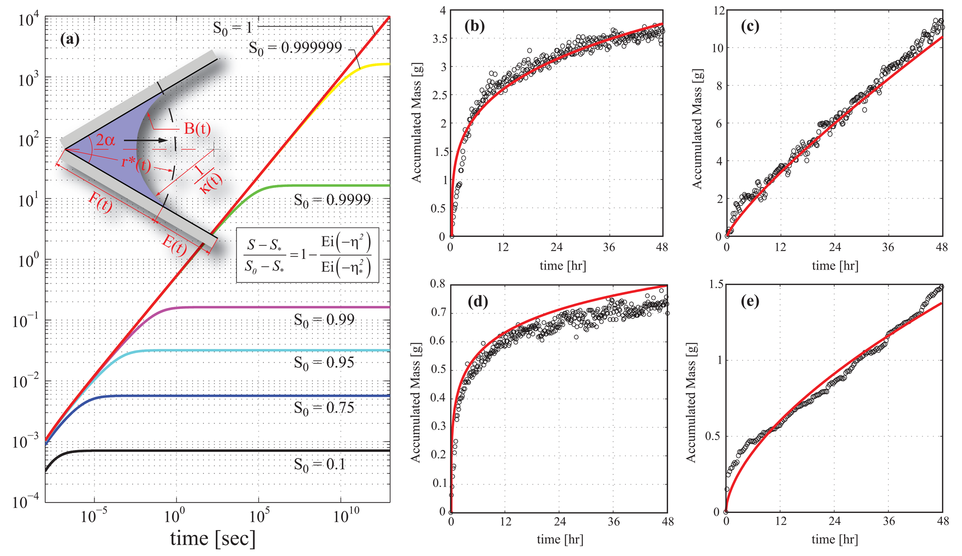

Figure 3: (a) Model predictions and measurements of capillary condensation kinetics into a wedge shaped pore for different ambient vapor saturations (b-e) water deposition due to condensation in different ambient conditions and sample grain sizes from direct measurement (markers) and numerical simulations (lines) (b) 100g of fine sand in low RH, (c) 200g of coarse sand in low RH, (d) 100g of fine sand in high RH, and (e) 200g of coarse sand in high RH

Pore Scale Interfacial Evolution

- In a recent study, Shahraeeni and Or [Langmuir, 2010] evaluated the model at the **macro** scale using experimental data of condensation dynamics in sand samples. Mass deposition dynamics confirms model validity in this scale.
- To validate the result of modeling at pore scale, dynamics of interfacial evolution have been measured in a series of experiments conducted in the controlled ambient condition in **micro** scales in the synchrotron X-ray facility at Swiss Light Source (SLS) / Paul Scherrer Institute (PSI).

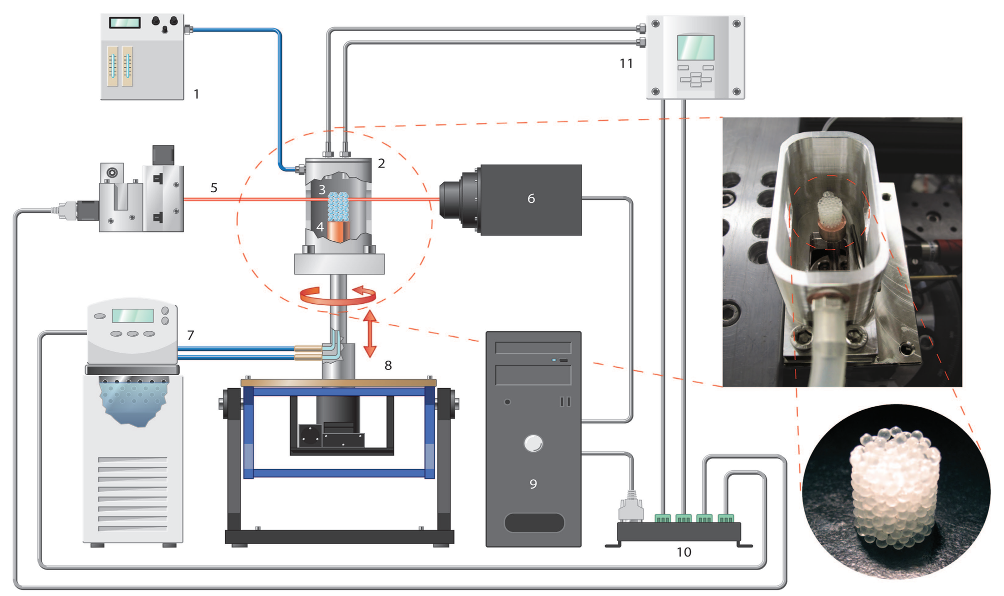

Figure 4: Experimental setup consists of (1) dew point generator (2) climate-controlled chamber (3) sintered glass bead sample (ϕ5mm, h10mm) (4) temperature controlled copper table (5) X-ray synchrotron beam line (6) TOMCAT camera (7) temperature-controlled water bath, (8) TOMCAT rotating-moving table (9) computer for data acquisition and control (10) measurement and control data logger and (11) high-precision temperature and relative humidity sensor measuring ambient conditions in the chamber

- Data from synchrotron X-ray tomography for the evolution of liquid - vapor interface due to the capillary condensation resulted from a series of controlled changes in the ambient conditions (T_0, RH_0) accurately instrumented as the interaction between dew point generator, sample and chamber temperatures (T_{DPG}, T_{smple} and $T_{chamber}$)
- Data are in reasonable agreement with the corresponding simulation result in pore scale, although owing to nonuniformity in the chamber vapor distribution, equilibrium condition would not be uniform over the sample (**Figure 5b**)
- An extensive experimental data set at the nano scale was reported by Kohonen et al [1999] which was used for the model verification during early stages of the condensation (**Figure 5d**)

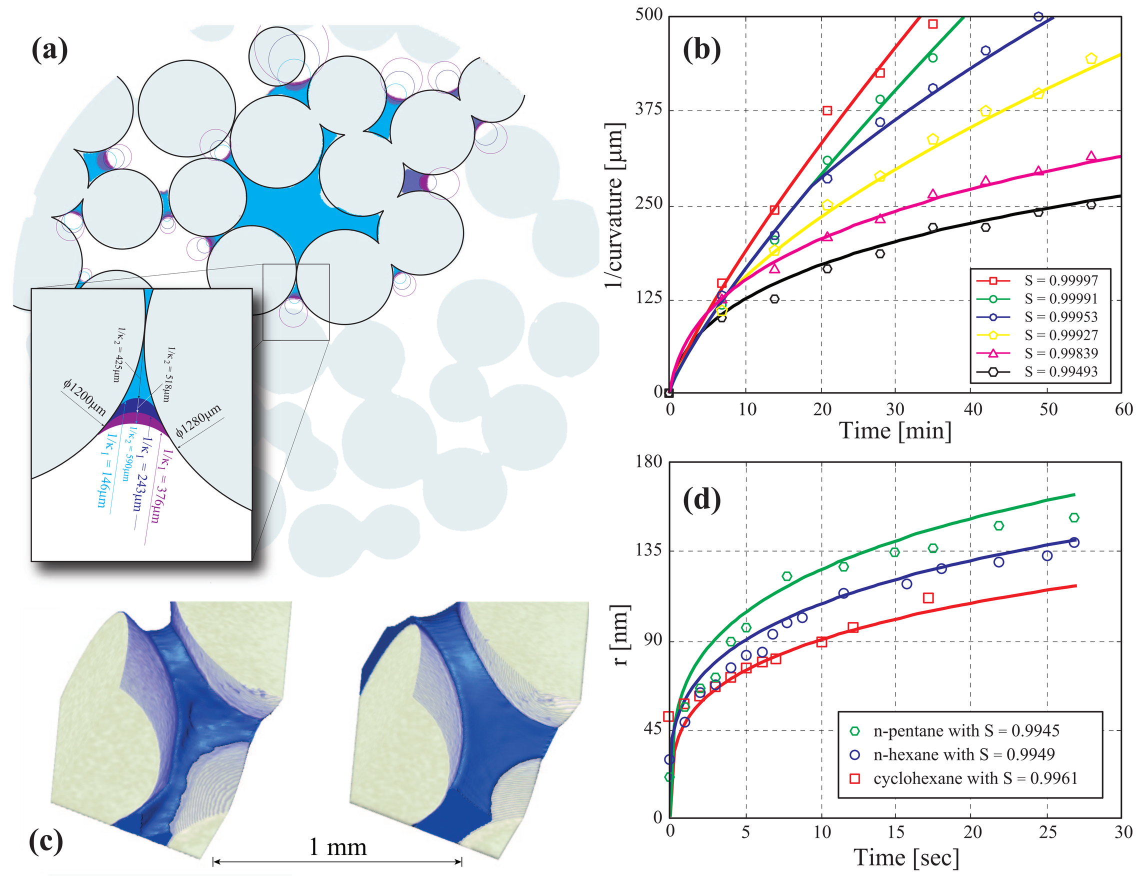

Figure 5: (a) Evolution of the interface due to the condensation in 2D cross section, nonuniform saturation distribution in-between the beads results in different rates for different interfaces as illustrated in (b), (c) 3D structure of the menisci in-between the grains, it illustrates how the interfaces evolve and collide (d) comparison of numerical simulation of interfaces dynamics with the experimental data from Kohonen et al [1999] for early stages of condensation in nano scale.

Pore Scale Enhanced Vapor Transport

- We combine evaporation - condensation dynamics with pore scale geometry to study capillary assisted vapor transport between menisci within prototype pore ('unit cell')
- We consider magnitude of EVT for various pore scale thermal and capillary gradients relative to inert gas diffusion

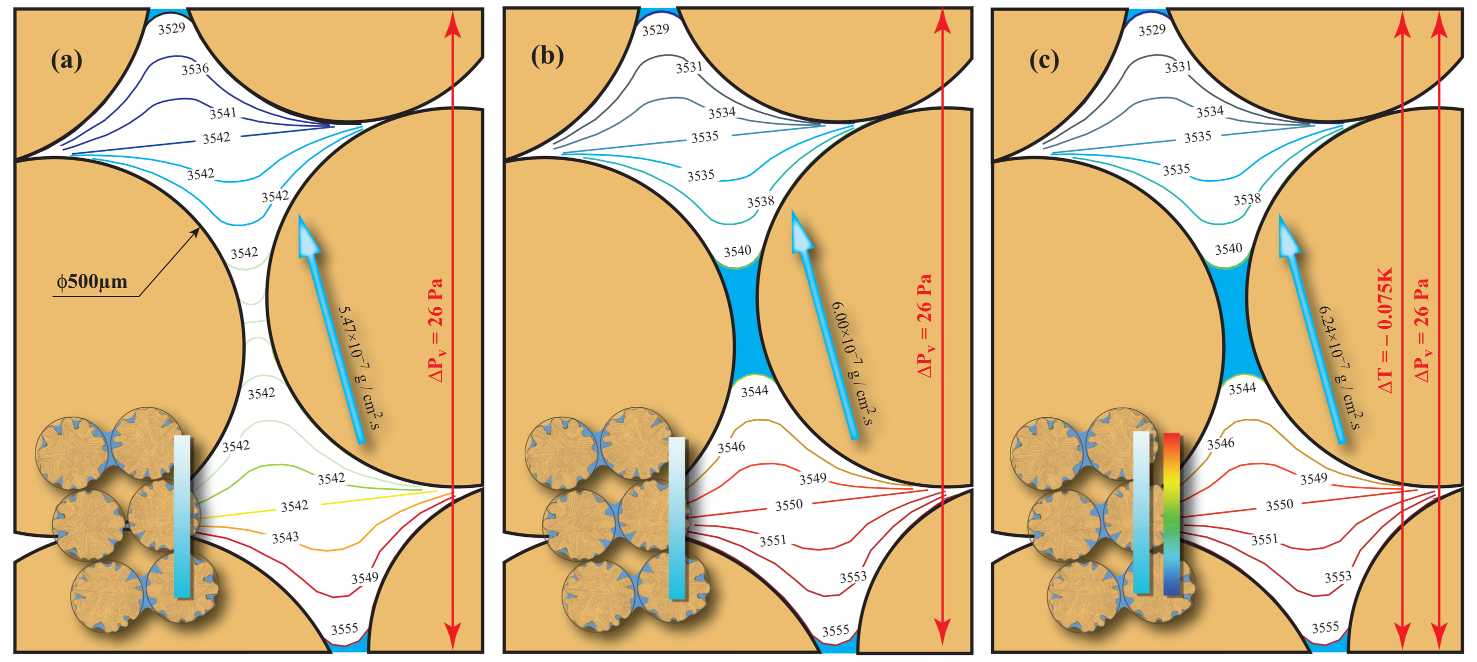

Figure 6: Scalar field of vapor density distribution for different scenarios (a) pure isothermal vapor diffusion (b) capillary driven isothermal vapor diffusion through a liquid island (c) same as (b) in the presence of local thermal gradient. Different cases illustrate pore scale enhancement as tabulated below in terms of 'η'

Table 1: The enhancement factor (η) for different pore scale vapor transport scenarios in the pore geometry of Figure 6 due to the vapor and temperature gradients in the presence and absence of the liquid phase

		Temperature Gradient		
		Isothermal $\nabla T = 0$	Assisting $\nabla T = -1.1$K/cm	Opposing $\nabla T =$ 1.1K/cm
Liquid Phase Presence	Pure Diffusion, $L_{liquid} = 0$	1	1.035	0.965
	Capillary Diffusion, $L_{liquid} = 200\mu m$	1.097	1.141	1.053

Sample Scale Enhanced Vapor Transport

Sample scale vapor transport is estimated by representing a partially saturated porous medium as a bundle of tortuous pathways consisting of unit cells similar to those studied for pore scale vapor transport (**Figure 6** above) arranged in series.

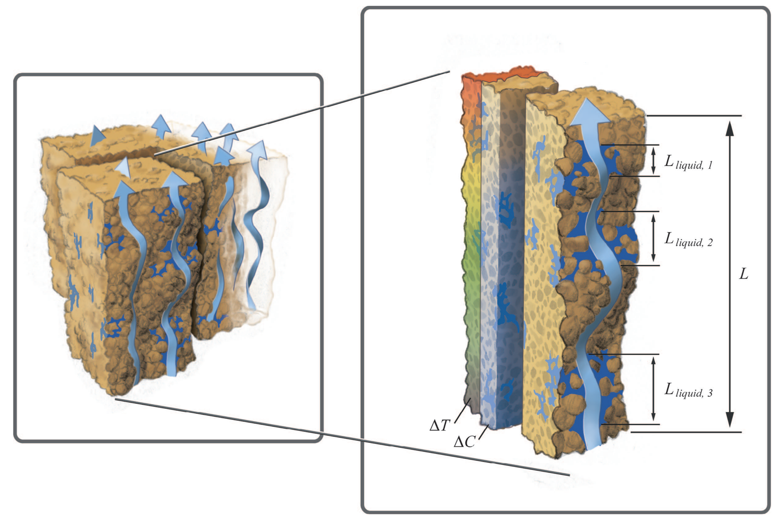

Figure 7: Simulation of a 3D sample as a bundle of tortuous pathways, distribution of the liquid islands along the pathways satisfies the macroscopic saturation according to the equation:

$$\tau \frac{\sum_{j=1}^{m} L_{liquid,j}}{\sum_{i=1}^{n} L_i} = \frac{\theta_w}{\varphi}$$

There are macroscopic temperature and vapor gradients which drive flow. Some of the pathways have no liquid phase obstruction ($\Sigma_i L_{liquid,i} = 0$) letting pure diffusion while the others partly filled with water resulting capillary assisted diffusion

The resulting simulations of vapor transport enhancement as function of water content and temperature gradients are depicted in **Figure 8**.

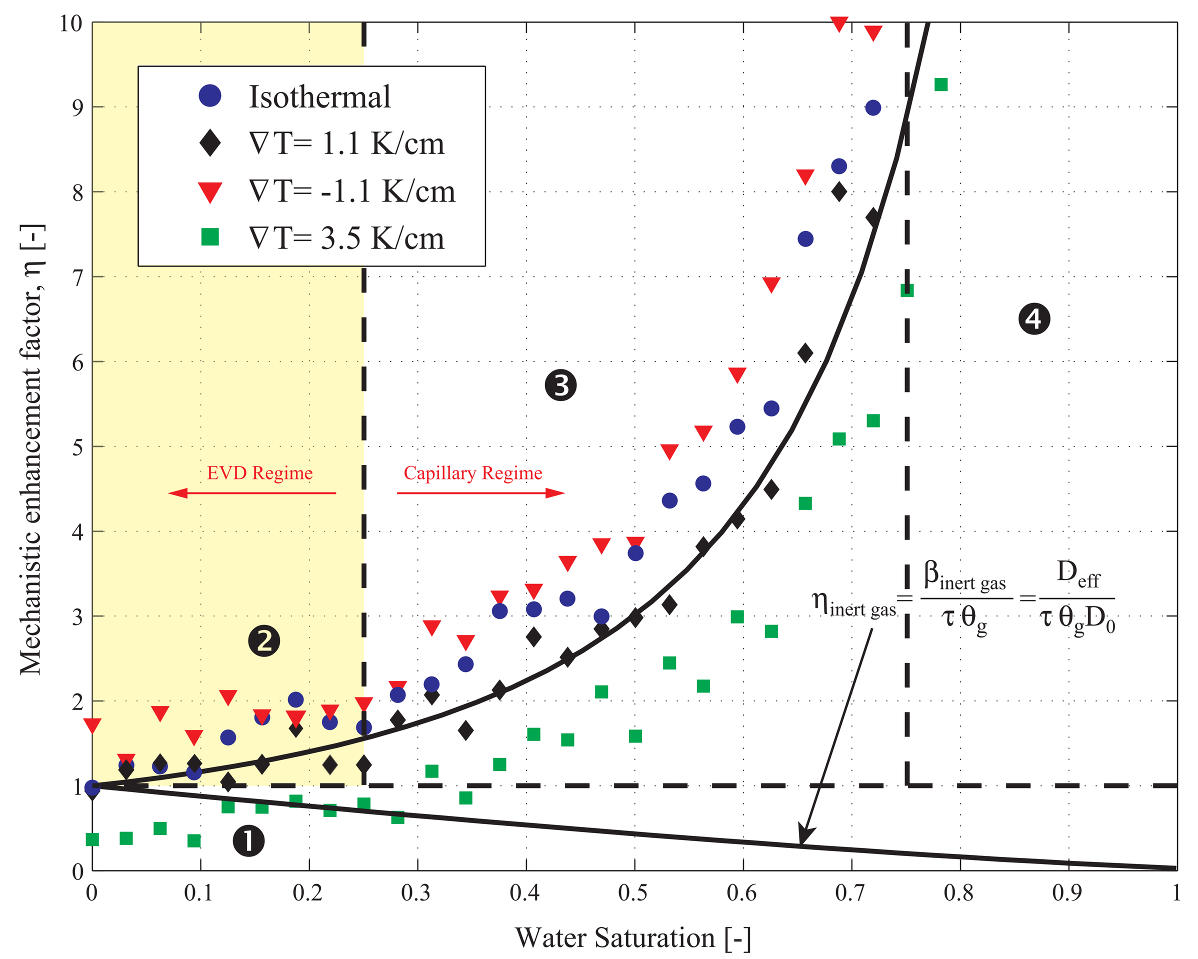

Figure 8: Simulated vapor transport enhancement at the macroscale (considering unit pores in series), curves show while diffusive flux of an inert gas in porous media monotonically reduced to zero by the increase of saturation level, in the case of vapor diffusion it can enhanced over several order of magnitude. The plane is divided to four zones. In zone (1) vapor diffusion is retarded mainly due to the opposing temperature gradient; in zone (2) thermally induced enhancement results higher vapor flux than the inert gas; for zone (3), characterized between percolation threshold and when the mean pore size would be invaded by liquid phase, capillary assisted diffusion leads to the vapor flux rates higher than the inert gas values; and finally in zone (4), majority of the pathways convey mass in capillary mode and transport phenomena would not be vapor flow anymore

Summary

- To reconcile discrepancies between predicted and observed vapor fluxes in porous media, two pore scale enhancement mechanisms were proposed by the pioneering work of Philip and de Vries [1957]. These mechanisms however, were seldom studied at the pore scale.
- We conducted pore scale experiments using synchrotron X-ray tomography to measure and verify a mechanistic model of evaporation – condensation dynamics as a building block for the modeling of vapor diffusion dynamics through porous media.
- Simulations of vapor diffusion in the presence of liquid phase reveal that the so-called enhanced vapor diffusion under isothermal condition is in fact a result of reduced diffusion length. Thermal gradient may augment or hinder this effect depending on the direction of thermal gradients.
- We have identified various transport regimes where the true pore scale enhancement as postulated by Philip and de Vries [1957] takes place at low water contents and could result in doubling of the vapor flux relative to diffusion of an inert gas. Once the liquid content exceeds the percolation threshold, the transport becomes dominated by capillary flow.

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