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Evaporation and transport of non-dilute, multi-component liquid mixtures in porous wicks: Simulation and experimental validation

Saman Beyhaghi[a], Krishna M. Pillai[a,*], Diab T. Qadah[b], Mark L. Dietz[b]

[a] Laboratory for Flow and Transport Studies in Porous Media, Department of Mechanical Engineering, University of Wisconsin-Milwaukee, 3200 N. Cramer Street, Milwaukee, WI 53211, USA

[b] Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, 3210 N. Cramer Street, Milwaukee, WI 53211, USA

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ABSTRACT

Modeling the transport and evaporation of multi-component liquids remains one of the most challenging problems in porous media studies. In this paper, slow isothermal evaporation of a *non-dilute* multi-component liquid mixture from a cylindrical porous wick made of sintered polymer beads is studied numerically and experimentally. Such wicks are used in several consumer products, such as air-fresheners and insect repellants, for dispensing volatile compounds into air. Since the evaporation rate is much smaller than the rate of capillary-pressure-driven liquid imbibition, the wick is considered fully-saturated while the evaporation from the wick top is modeled as a boundary effect. A volume-averaged model based on the work of Quintard and Whitaker is adapted to set the nonlinear species-transport equations inside the fully-saturated porous wick. Three numerical models with progressively increasing levels of complexity are employed to solve the governing equations in a one-dimensional domain representing the unidirectional, axial flow in a cylindrical wick. The Darcy velocity inside the wick is determined from evaporation rate at the wick-top, which in turn is a function of mole-fractions of all components at the liquid–air interface. Using the proposed numerical models, the evaporated liquid-mass and the composition of liquid mixture within the wick are predicted as functions of time. Results of the simulations are compared with experiments for a non-dilute mixture of decane, dodecane and hexadecane. Good agreement is observed for the three models, especially for the component concentration distributions along the wick, *without the use of any fitting parameters*. The evaporation rate is found to be a strong function of two model parameters: the porous-medium tortuosity and the air-film thickness at wick top.

1. Introduction

Understanding the flow and transport of multi-component liquid mixtures in cylindrical porous polymer wicks and the diffusive evaporation of such mixtures under isothermal condition from wick tops is an area of both fundamental and practical interest. From a fundamental perspective, modeling the transport and evaporation of multi-component liquids remains one of the most challenging problems in porous media studies. Of more immediate practical significance is that such wicks can be used for dispensing mixtures of fragrances (normally consisting of hydrocarbon compounds) into the ambient air. A variety of methods have previously been proposed to model the physics of transport and evaporation of liquids in porous media. This topic has a broad range of applications in science and industry, and has been the main subject of several studies in literature. Some of the applications include remediation of soil contaminated with chemicals [1–9]; heat pipe technology [10,11]; drying processes [12–19]; and the flow of gases in fuel-cell electrodes [20–22].

Gioia et al. [14] investigated theoretically the transient evaporation of a multi-component mixture of volatile organic compounds. The Stefan–Maxwell equation [23] has been used to find the molar flux of each component in the gas phase. Note that [14] dealt with the “tracer” form of the species equations (applicable to dilute mixtures) where the diffusivity matrix reduces to a scalar. Moreover, the composition of the mixture at the liquid–gas interface is considered to remain unchanged over time. Such assumptions give rise to an overly simplified, and perhaps inaccurate, model. (*Vide infra*, as will be evident from the theory used in the present paper, the full diffusivity matrix needs to be implemented and the transport equations of all mixture species need to be solved simultaneously due to the unsteady-state nature of the problem of transport in porous wicks as well as the non-dilute nature of the mixture.)

In other publications, the ecologically important problem of drying of the soil contaminated with hydrocarbon substances has been investigated [1–10]. Ho and Udell [2] introduced a theoretical

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* Corresponding author. Tel.: +1 414 229 6535; fax: +1 414 229 6958.
E-mail address: Krishna@uwm.edu (K.M. Pillai).

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Nomenclature

A_{cs}	cross-sectional area of the wick (m^2)
A_{ls}	liquid–solid interface area (m^2)
$\mathbf{b}$	closure variable (m)
C_g	total molar concentration in the gas phase (Kmol/m^3)
$c_{A,l}$	molar concentration of any component A in the liquid phase (Kmol/m^3)
c_l	total molar concentration in the liquid phase (Kmol/m^3)
D	effective diffusivity of species in the mixture, when treated as a constant
D_{AB}	binary diffusion coefficient for any two species A and B (m^2/s)
$D_{A,g}$	diffusivity of component A in gas phase (air) (m^2/s)
D_{Am}	effective diffusivity of component A in the liquid mixture (m^2/s)
$[\langle \mathrm{D} \rangle^l]$	volume-averaged form of the diffusivity matrix (m^2/s)
$[\mathbf{D}_{eff}]$	effective diffusivity tensor as defined in (11-c) (m^2/s)
$[\mathbf{D}_h]$	hydrodynamic dispersion tensor as defined in (11-d) (m^2/s)
H	total height of the wick (m)
$\mathbf{I}$	unity tensor
$\mathbf{J}_{A,l}$	diffusive flux of component A (Kmol/m^{2}s)
M_A	molar mass of component A (20) (kg/Kmol)
m	mass (kg)
$\dot{m}_A$	rate of evaporation of component A from the wick-top (kg/s)
$\dot{m}_{evap}$	rate of evaporation of liquid mixture from the wick-top (kg/s)
m_R	mass of the liquid mixture in the supplying reservoir (kg)
N	number of species components in the mixture
N''_A	molar evaporation flux of component A (Kmol/m^{2}s)
n_A	pressure ratio of species A (defined as P_A^{sat}/P^{tot})
$\mathbf{n}_{ls}$	unit vector normal to the liquid–solid interface (directed away from the liquid phase toward the solid phase)
P	pressure (kPa)
[P]	nodal matrix used for diagonalization of matrices, used in (11-c) and (11-d)
R	universal gas constant (kJ/Kmol K)
[R]	an intermediate matrix introduced for obtaining the diffusivity matrix
T	absolute temperature (K)
t	time (s)
$\mathbf{u}_{A,l}$	velocity of any species A in the liquid mixture (m/s)
$\mathbf{u}_l$	liquid mixture velocity (m/s)
u_l	component of the liquid mixture velocity along the wick axis (m/s)
$\tilde{\mathbf{u}}_l$	spatial deviation of the liquid mixture velocity from its volume-averaged value (9) (m/s)
V_l	volume of the liquid (or pore) region within the REV (m^3)
V_R	volume of the liquid mixture in the supplying reservoir (m^3)
$x_{A,l}$	mole-fraction of any component A in the liquid mixture
$\tilde{x}_{A,l}$	Spatial deviation in the mole-fraction of component A from its volume-averaged value, (8)
y_A	mole-fraction of component A in the gas phase
z	vertical coordinate

Greek symbols

δ	thickness of the diffusive layer introduced for evaporation flux (16) (m)
ε	V_l/V, porosity
ρ	density (kg/m^3)
$\rho_{A,l}$	density of any species A in the liquid mixture (kg/m^3)
ρ_l	density of the liquid mixture (kg/m^3)
τ	scalar tortuosity
$\boldsymbol{\tau}$	tortuosity tensor
υ	dummy variable showing time-step in (34)

Subscripts

0	initial time
A	corresponding to any component A of the liquid mixture ($A = 1, 2, \ldots, N$)
g	gas phase
int	liquid–air interface
l	liquid phase
R	liquid reservoir
s	solid phase
δ	corresponding to the distance of δ above the liquid–air interface

Superscripts

n	corresponding to time-step n in the computational domain
Sat	saturation
tot	total

model to predict the composition of the liquid mixture at different underground depths, to track the position of the evaporation front (liquid–air interface) over time, and to estimate the mixture composition in both the dry and wet regions. Due to the slow motion of fluids during drying, there is no need to incorporate the liquid-mixture velocity through the advection term in the species transport equations. Again, the assumption of a constant interface composition as well as the use of a scalar diffusion coefficient has enabled the authors to assume fixed-value boundary conditions for species concentrations at the liquid–air interface and solve the decoupled set of governing equations analytically.

The problem of mass transport in porous media has been extensively investigated by Quintard and Whitaker in several publications where the method of volume averaging has been used to propose a more accurate representation of the governing equations for mass-transport applications in porous media [5,24–28]. This body of work remains the most definitive and seminal contribution in this area. In order to compare the level of rigor of the volume-averaging based method with the other available methods, remarks regarding the species transport equations from recent publications are presented in Table 1. As seen in the table, even though the main structure of the species equation as a convection–diffusion equation is retained in the majority of the included models, several assumptions including the dilute condition (i.e., the diffusion of one component remains uninfluenced by the diffusion of the others), binary mixture, scalar diffusion coefficient (i.e., ignoring the tensor nature of the diffusivity and dispersion tensors), and simplified tortuosity models (i.e., inadequate representation of the role of the porous medium microstructure) are made in order to facilitate the development of analytical or numerical solutions. However, the volume-averaging method not only predicts the transport of non-dilute multicomponent mixtures accurately, but also provides a rigorous mathematical procedure for estimating parameters such as tortuosity, the effective diffusivity, and