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Computational fluid dynamics simulations of direct contact heat and mass transfer of a multicomponent two-phase film flow in an inclined channel at sub-atmospheric pressure

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ABSTRACT

A method for simultaneous heat and multicomponent mass transfer incorporated with the volume of fluid surface tracking method was developed in a two-dimensional inclined channel. The process in the channel includes direct contact condensation of hydrocarbon mixtures with and without noncondensable gas, and distillation effect is also considered. Interfacial transport was performed by a multicomponent phase change model in kinetic forms considering the assumption of thermodynamic equilibrium at the vapor–liquid or vapor/gas–liquid interface using Peng–Robinson equations. The shear-stress transport k–ω turbulence model damped near the vapor–liquid or vapor/gas–liquid interface was used. The hydrocarbon mixtures in both phases were described by five pseudo-components, and Stefan–Maxwell equations were used to describe diffusional interactions in the multicomponent system. Parametric studies were performed to investigate further the model with various boundary conditions. Simulations for a binary system were also performed for a preliminary validation. For the liquid phase, similar trends of the Sherwood numbers were found between the results by simulations and predicted by the Penetration Theory. For the vapor phase, good agreement was observed between the results by empirical correlation and simulations.

1. Introduction

Direct contact heat and mass transfer in a vapor–liquid or vapor/gas–liquid two-phase film flow system occurs in various industrial applications such as gas absorption, ethylene quench, and distillation, among others. In particular, in the pump-around zone of a refinery vacuum tower, the oil vapor/gas mixtures are condensed partly in a limited space where structured packing is used commonly for the intensification of heat and mass transfer. Direct contact condensation (DCC) occurs in the pump-around zone, and a distillation effect is also included in most situations. In structured packing, a portion of the oil vapor/gas mixtures are condensed quickly by the supercooled oil liquid which flows counter-currently. Sensible heat and latent heat are transferred from the vapor/gas to the liquid phase with a temperature rise in the oil liquid. When the oil liquid is close to saturation or superheated locally, simultaneous condensation and evaporation of various components transpire at the vapor/gas–liquid interface, producing a distillation effect. Understanding this heat and mass transfer is important for the determination of the hydrodynamic and thermal characteristics in the structured packing of the pump-around zone.

Computational fluid dynamics (CFD) has been used widely for the research of flow pattern as well as heat and mass transfer in structured packing. Packing units such as representative elementary units (REUs) [1] are investigated commonly instead of the whole packing segment or column with complex geometry. For DCC in structured packing, the loads of vapor/gas and liquid vary evidently along with the height, which cannot be considered using REUs. However, structured packing can be simplified as a bundle of parallel inclined channels according to the hydrodynamic analogy approach reported by Shilkin and Kenig [2]. In this approach, two-phase countercurrent film flow is performed in a two-dimensional (2-D) axisymmetric inclined channel as a packing unit. The equations of momentum, energy, and mass transport are solved rigorously. Similarly, the hydrodynamic analogy approach can be combined with CFD for an in-depth description of the two-phase film flow system in the inclined channel such as the film wave caused by the interphase force (e.g., surface tension and drag force between the phases) and various surface textures at the wall.

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Nomenclature

a_c	accommodation coefficient
A	interfacial area density (m^2/m^3)
$D_{i,m}$	diffusivity of species i in mixture (m^2/s)
D_{ij}	the Fick's law binary diffusion coefficient (m^2/s)
$D_{ij,M}$	the Stefan–Maxwell binary diffusion coefficient (m^2/s)
$D^{o}_{ij,M}$	binary i–j infinite dilution diffusion coefficient (m^2/s)
$[D]$	matrix based on Fick's law binary diffusion coefficient $D_{i,j}$
D_ω	cross-diffusion term, ω equation ($kg/m^3\ s^2$)
E	energy (J/kg)
$\boldsymbol{F}$	source term, momentum equation (N/m^3)
$\boldsymbol{g}$	acceleration due to gravity (m/s^2)
G_k	production of turbulence kinetic energy ($kg/m\ s^3$)
G_ω	production of specific dissipation rate ($kg/m^3\ s^2$)
h	sensible enthalpy (J/kg)
H_{fg}	latent heat of vaporization (J/kg)
J	species mass diffusion flux, ($kg/m^2\ s$);
J_i	mass flux for species i, ($kg/m^3\ s$);
J'	net mass flux over the vapor–liquid interface ($kg/m^2\ s$)
J_{eva}	mass flux of evaporation ($kg/m^3\ s$)
J_{cond}	mass flux of condensation ($kg/m^3\ s$)
k	thermal conductivity (W/m K); turbulence kinetic energy (m^2/s^2)
K	relaxation parameter
M	molecular weight (kg/kmol)
n	number of species
P	pressure (Pa)
P_c	critical pressure (Pa)
P_{sat}	saturation pressure (Pa)
Q	total latent heat transfer in the channel (W)
R	universal gas constant (J/mol K)
S_{α_q}	source term, VOF equation (kg/m^3)
S_E	source term, energy equation (W/m^3)
S_k	source term, k equation (W/m^3)
S_ω	source term, ω equation (W/m^3)
t	time (s)
T	interfacial temperature (K)
T_b	bubble point temperature (K)
T_{sat}	saturation temperature (K)
T_c	critical temperature (K)
T_d	dew point temperature (K)
T_l	temperature of the liquid phase (K)
T_v	temperature of the vapor phase (K)
$\boldsymbol{u}$, u	velocity (m/s)
X	liquid phase mass fraction
Y_k	dissipation of turbulence kinetic energy ($kg/m\ s^3$)
Y_ω	dissipation of specific dissipation rate ($kg/m^3\ s^2$)
Y	vapor or vapor/gas phase mass fraction

Greek symbols

α	volume fraction
β_1, β_2	mass transfer time relaxation parameter (1/s)
Γ_k	effective diffusivity of k (kg/m s)
Γ_ω	effective diffusivity of ω (kg/m s)
δ	liquid film thickness (mm)
μ	viscosity, (kg/m s)
ρ	density, (kg/m^3)
ω	specific dissipation rate, (1/s); acentric factor

Subscripts

c	critical
cond	condensation
e	equilibrium
eff	effective
eva	evaporation
min	minimum value
max	maximum value
q	the qth fluid
s	species

The gas–liquid film flow in a 2-D channel has been examined extensively using the CFD method [3–6], whereas the volume-of-fluid (VOF) [7] method is used for the interface tracking of film flow on various walls among numerous other numerical methods. Considering the heat and mass transfer at the gas–liquid interface in an inclined channel, Banerjee [8,9] investigated the evaporation of methanol and ethanol/isooctane mixtures. The evaporation rate was determined by the diffusion flux of gas species at the gas–liquid interface in the form of Fick's Law, and turbulence was treated using the renormalization group k–ε turbulence model. Banerjee and Issac [10] studied the evaporation of gasoline, which mainly considered the diffusion effect in gas mixtures. The gasoline mixtures were described by the continuous thermodynamics approach. Haroun et al. [11] performed direct numerical simulation (DNS) of reactive absorption in a gas–liquid two-phase flow on structured packing based on the VOF method. The mass transfer at the gas–liquid interface was described by a continuum mechanical modeling of two phases flow and Henry's law with constant coefficient. Haelssig et al. [12] studied the simultaneous interfacial heat and mass transfer of an ethanol–water system by DNS within the framework of the VOF method. Both diffusion and convection flux were considered. The interfacial area as well as the gradients of species and temperature near the vapor–liquid interface was calculated based on the piecewise linear interface calculation method. In these investigations [8–12], mixtures with binary or ternary components were studied, and the gradients of mass fraction and temperature at the interface were obtained to determine the interfacial jump conditions (the discontinuity of species concentration and energy at the vapor/gas–liquid interface). Evaporation, absorption, or distillation was investigated. However, the condition of DCC was not considered.

In the present study, DCC with and without noncondensable gas were performed in an inclined channel, and a distillation effect was also considered. The interfacial jump conditions were described in kinetic forms without calculating the gradients of mass fraction and temperature at the vapor–liquid or vapor/gas–liquid interface. The convection flux at the interface was included because it was not negligible relative to the diffusion flux under DCC [13]. The hydrocarbon mixtures in both phases were described by five pseudo-components. Stefan–Maxwell equations were used for multi-component system considering diffusional interactions. The shear-stress transport (SST) k–ω model with turbulence damping [14] was used in both phases considering that the k–ε or the k–ω turbulence model without turbulence damping usually generates a too high turbulence near the interface. Parametric studies were presented for a further investigation of the model with various boundary conditions. Simulations for a binary system were performed for a preliminary validation of this model.