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Incorporation of Eulerian–Eulerian CFD framework in mathematical modeling of chemical absorption of acid gases into methyl diethanol amine on sieve trays

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ABSTRACT

A two-dimensional mathematical model for removal of acid gases (H_2S and CO_2) by methyl diethanol amine in a commercial sieve tray column has been developed. The velocity profile in the liquid both in radial and axial directions of each plate has been calculated by Eulerian–Eulerian computational fluid dynamics framework. In order to establish the temperature and concentration profiles in radial and axial directions of plates, mass and energy balance equations have been developed and solved numerically. A non-equilibrium rate based method combined with the two-film theory has been considered to obtain concentration profile. In this model most of the important parameters in the gas absorption process have been included, therefore one can expect that the model will be able to predict the performance of the columns at wide ranges of operating conditions. The results obtained by the model using operational data of a commercial plant indicate that there exists appreciable distribution of velocity, concentration and temperature in radial and axial directions. More interesting finding is that the extent of these distributions decline from bottom to top of the column as is expected. In fact, good agreement was noticed when the results of model were compared with operating conditions of an industrial column.

1. Introduction

Natural gas is considered sour if it contains H_2S and CO_2. Before the gas can be used, these acid gases should be removed by sweetening process. In this processes usually N.G. is sweetened by separation of H_2S and CO_2 in a sieve plate or packed type columns. In these columns, usually the gas and amine get in contact by a counter-current flow pattern in order to transfer these gases into the amine.

The gas absorption is a well-known technique and it is one of the most common method for separation of acid gases in gas refineries. Although this method is energy intensive, nevertheless it is the first choice among different separation techniques. Alkanolamines are widely used for purposes of separation of acid gases from natural gas. These amines have high ability to absorb the acid gases because the chemical reactions between the alkanolamines and these gases create a good driving force, which is necessary for absorption process. Since these chemical reactions are reversible, therefore, the alkanolamines can be recovered easily.

The occurrence of ionic reactions in one hand and lack of information about the tray hydraulics in the other hand raise a challenging design task. There are enough evidence that in the commercial size trays there exist velocity, concentration and temperature gradients in the radial direction. These non-uniform distributions not only reduce efficiency but also inaccurate prediction of column performance will be obtained once they are ignored. In order to account for these mal-distributions in the model one should incorporate the fundamental concepts of fluid mechanics. In fact, in the most of previous studies the fluid mechanics have been ignored altogether [1–3]. One reason for the reluctance to approach the modeling in a more fundamental way is the difficulty of solving the large and complex equations of two- or three-dimensional multi-phase systems.

For a given set of operating conditions (gas and liquid flows), tray geometry (column diameter, weir height, weir length, diameter of holes, fractional hole area, active bubbling area, downcomer area) and system properties, it is required to predict the fluid flow on the tray, residence time distributions and the mass transfer rates in each fluid phase.

One of the major assumptions made in modeling of distillation and gas absorption processes is considering each tray as an equilibrium stage (liquid and vapor streams leaving the tray are at equilibrium) and usually hydrodynamics of the tray is neglected. Neglecting this phenomenon shadows the predicted parameters in the large scale tray based on efficiency of a small scale tray. The inadequacy in the models to some extent was corrected by using the concept of (a) tray Murphree efficiency or (b) by non-equilibrium concepts [4]. Currently the most common assumption in distillation and absorption models is the concept of the fully mixed

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Nomenclature

a	interfacial area (m^{-1})
A	tray area (m^2)
A_1	dimensionless concentration of CO_2 in the liquid film
A_2	dimensionless concentration of H_2S in the liquid film
B_2	dimensionless concentration of MDEA in the liquid film
A_h	hole area (m^2)
C	concentration (kg/m^3), (mol/m^3)
C_D	drag coefficient
C_p	specific heat (J/mol K)
d_G	diameter of bubble (m)
D	diffusivity (m^2/s)
De	Eddy diffusivity (m^2/s)
E	enhancement factor
E_2	dimensionless concentration of $HCO_3{}^-$ in the liquid film
E_3	dimensionless concentration of HS^- in the liquid film
F_2	dimensionless concentration of $MDEAH^+$ in the liquid film
G	dimensionless group defined in Table 2
$\mathbf{g}$	vector of gravity acceleration (m/s^2)
H	specific enthalpy (J/mol)
h	molar enthalpy (J/mol)
h_{cl}	clear liquid height (m)
h_f	froth height (m)
h_w	weir height (m)
k_l°	mass transfer coefficient (m/s)
L	molar flow rate of liquid phase (mol/s)
l_{mix}	Prandtl mixing length (m)
L_w	weir length (m)
$\mathbf{M}_{L.G}$	interphase momentum transfer ($kg/m^2\,s^2$)
P	pressure (Pa)
p_i	dimensionless concentration of species defined in Table 2
Q	volumetric flow rate (m^3/s)
R_{MDEA}	dimensionless reaction rate of CO_2 and MDEA defined in Table 2
$r_{p,k}$	interface momentum transfer caused by mass transfer ($kg/m^2\,s^2$)
Sc	Schmidt number
pi	dimensionless diffusivity of species defined in Table 2
T	temperature (K)
u	x-component of velocity (m/s)
U	superficial velocity (m/s)
v	velocity vector (m/s)
v_{slip}	sleep velocity (m/s)
v	y-component of velocity (m/s)
V	molar flow rate of gas phase (mol/s)
w	z-component of velocity (m/s)
x	Cartesian coordinate, mole fraction of liquid phase
y	Cartesian coordinate, mole fraction of gas phase
z	Cartesian coordinate, only is defined for liquid film geometry (m)

Greek symbols

α	molecular temperature conductivity (m^2/s)
δ	film thickness (m)
φ	volume fraction of each phase
Γ	interphase mass transfer ($kg/m^2\,s$)
μ	dynamic viscosity (kg/m s)
ν	kinematic viscosity (m^2/s)
ρ	density (kg/m^3)
τ	shear stress (Pa)
τ'	Reynolds stress (Pa)
ξ	dimensionless distance from liquid interface

Superscripts

abs	absorption
liq	referring to liquid phase
vap	referring to gas phase
tr	transpose

Subscripts

avg	average
blk	bulk
G	referring to gas phase
k	phase number
L	referring to gas phase
ref	reference
t	turbulence
wall	tray wall

ideal tray—i.e. spatial variations in concentration, temperature and velocity are ignored.

In recent years, advancements have been made by applying CFD for simulating the liquid flow on a tray by means of various theoretical models, such as the stream function model [5], the k–ε turbulence model [6] and the two-fluid turbulence model [7].

Several investigators have attempted to include the hydrodynamics of plate in the model by using CFD [8–12]. Although the previous models are able to give satisfactory results for the velocity profile at different liquid rates, but they have overlooked effect of chemical reactions in the liquid. The vapor–liquid flow on a tray is also characterized by cross flow of the two phases. In this theory, the liquid phase is usually considered as continuous phase and the upward vapor flow is supposed to be dispersed phase [9].

Mehta et al. [8] have analyzed the liquid phase flow patterns on a sieve tray by solving the time-averaged equations of transport only for the liquid. Interactions with the vapor phase are taken into account using of interphase momentum transfer coefficients determined from empirical correlations. Yu et al. [12] attempted to model the two-phase flow behavior using a two-dimensional model, focusing on the description of the hydrodynamics along the liquid flow path, ignoring the velocity profile of gas along the height of the plate. Fischer and Quarini [10] have attempted to describe the three-dimensional transient gas–liquid hydrodynamics. An important key assumption made in the simulations of Fischer and Quarini concerns the interphase momentum exchange (drag) coefficient; these authors assumed a constant drag coefficient of 0.44, which is appropriate for uniform bubbly flow. This drag coefficient is not appropriate for description of the hydrodynamics of trays operating in either the froth or spray regimes.

van Baten and Krishna [11] developed a three-dimensional transient CFD model, within the two-phase Eulerian framework, to describe the hydrodynamics of a sieve tray. The required exchange coefficient of interphase momentum transfer is estimated based on the correlation of Bennett et al. [13] for the liquid hold-up. Krishna has carried out his simulations with varying superficial gas velocity, liquid weir loads, and weir heights.

There are yet other excellent surveys of the literature in this area [14]. Literature contains correlations for tray hydrodynamics which