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A multifluid-PBE model for simulation of mass transfer limited processes operated in bubble columns

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ABSTRACT

Modeling of reactive dispersed flows with interfacial mass transfer limitations require an accurate description of the interfacial area, mass transfer coefficient and the driving force. The driving force is given by the difference in species composition between the continuous and dispersed phases and thus depends on bubble size. This paper shows the extension of the multifluid-PBE model to reactive and non-isothermal flows with novel transport equations for species mass and temperature which are continuous functions of bubble size. The model is demonstrated by simulating the Fischer-Tropsch synthesis operated in a slurry bubble column at industrial conditions. The simulation results show different composition and velocity for the smallest and largest bubbles. The temperature profile was independent of bubble size due to efficient heat exchange. The proposed model is particularly useful in investigating the effects of bubble size on strongly mass transfer limited processes operated in the heterogeneous flow regime.

1. Introduction

1.1. Interfacial mass transfer limited processes

For interfacial mass transfer limited processes the interfacial mass transport phenomena are limiting the overall reaction rate and thus the efficiency of the process. A typical example is bubble columns where gas is injected into the reactor and forms gas bubbles. The gaseous reactants must be transported out of the gas bubbles and into the bulk liquid phase in order to be converted to products.

For interfacial mass transfer limited processes the mass transfer through the liquid film surrounding the bubble is generally the limiting step, as the diffusion coefficient in a liquid is much smaller than in a gas. The mass transfer of species s from the bubble to the bulk liquid can then be modeled as (e.g. Jakobsen, 2014):

$$\Gamma_s = a_L k_{L,s} \rho_L (\omega^*_{L,s} - \omega_{L,s}) \tag{1}$$

where a_L is the gas–liquid interfacial area, $k_{L,s}$ the mass transfer coefficient, $\omega^*_{L,s}$ the weight fraction of species s at the interface and $\omega_{L,s}$ the concentration of s in the bulk liquid. A proper description of mass transfer thus relies on:

- An accurate description of the gas–liquid interfacial area a_L,
- an accurate description of the driving force for mass transfer (here: $\omega^*_{L,s} - \omega_{L,s}$))
- and an accurate parameterization of the mass transfer coefficient $k_{L,s}$.

The driving force for the interfacial mass transfer flux is generally related to the difference in composition in the two phases. In this work the gas composition is considered a function of bubble size. This means that the driving force for mass transfer is a function of bubble size – whether considering the overall mass transfer resistance or simplifying using only the liquid resistance as in Eq. (1).

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Nomenclature

Latin letters

A	bubble surface area [m^2]
a_L	interface area for gas–liquid interface [$m^2\ m^{-3}$]
b	breakage frequency [s^{-1}]
c	coalescence rate [s^{-1}]
$\boldsymbol{c}$	microscopical velocity in spatial space [$m\ s^{-1}$]
$\boldsymbol{C}$	peculiar velocity; $\boldsymbol{C} = \boldsymbol{c} - \boldsymbol{v_r}$ [$m\ s^{-1}$]
C_{BP}	bubble pressure proportionality constant [–]
$C_{D,G}$	drag coefficient [–]
C_L	lift force coefficient [–]
C_p	heat capacity [$J\ K^{-1}\ kg^{-1}$]
C_{VM}	virtual mass force coefficient [–]
$\boldsymbol{C}_s$	peculiar velocity for a molecule of species s [$m\ s^{-1}$]
C_ξ	peculiar velocity in property space; $C_\xi = \Xi - v_\xi$ [$m\ s^{-1}$]
$D_{G,z,\text{eff}}$	effective axial dispersion coefficient [$m^2\ s^{-1}$]
$\boldsymbol{e}$	unit vector [–]
f	number density function [$\#\ m^{-1}\ m^{-3}$]
f_d	mass density function [$kg\ m^{-1}\ m^{-3}$]
$\boldsymbol{f}_{\text{drag}}$	drag force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{f}_{\text{lift}}$	lift force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{f_g}$	gravity force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{f_p}$	external pressure force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{f}_{TD}$	turbulent dispersion force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{f}_{vm}$	virtual mass force [$kg\ m\ s^{-2}\ m^{-1}$]
$\boldsymbol{F}_r$	force in physical space [$kg\ m\ s^{-2}$]
$F_{G,z}$	cross-sectionally averaged force term [$kg\ m\ s^{-2}$]
F_ξ	force in property space [$kg\ m\ s^{-2}$]
$\boldsymbol{f}_{\text{drag}}$	drag force [$kg\ m\ s^{-2}\ m^{-1}$]
h	mass averaged enthalpy [$J\ kg^{-1}$]
$H(\alpha)$	dimensionless function in model for bubble pressure [–]
h'	fluctuating enthalpy [$J\ kg^{-1}$]
h_{G-L}	gas–liquid heat transfer coefficient [$W\ m^{-2}\ K$]
h_p	particle enthalpy [$J\ kg^{-1}$]
h_v	specific heat of vaporization [$J\ kg^{-1}$]
$h_{p,s}$	particle specific heat for component s [$J\ kg^{-1}$]
$\boldsymbol{I}$	unit tensor [–]
k	thermal conductivity [$W\ m^{-1}\ K^{-1}$]
$k_{L,s}$	liquid side mass transfer coefficient for species s [$m\ s^{-1}$]
K_s	weight based vapor–liquid equilibrium constant [–]
m	average mass [kg]
m_p	mass of particle p [kg]
$\bar{M}_w$	average molar mass [$kg\ kmol^{-1}$]
p	microscopical number density function [$m^{-3}\ m^{-1}\ s\ m^{-1}\ s\ m^{-1}\ K^{-1}\ kg^{-1}$]
p	pressure [Pa]
P	normalized number density function [$s\ m^{-1}\ s\ m^{-1}\ K^{-1}$]
$\boldsymbol{P}$	pressure tensor [$kg\ m^{-1}\ s^{-2}$]
$\boldsymbol{P}_b$	bubble pressure tensor [$kg\ m^{-1}\ s^{-2}$]
$\boldsymbol{P}_r$	viscous stress tensor in spatial space [$kg\ m^{-1}\ s^{-2}$]
Pr	Prandtl number [–]
$\boldsymbol{p}_\xi$	viscous stress vector in inner coordinate (bubble diameter) space [$kg\ m^{-1}\ s^{-2}$]
$Q_{cd,p}$	heat exchange for a single particle due to convection and conduction [$J\ s^{-1}$]
$Q_{r,p}$	heat exchange for a single particle due to radiation [$J\ s^{-1}$]
$\boldsymbol{q_r}$	heat flux [$W\ m^{-2}$]
$q_{G,z}$	cross-sectionally averaged heat transfer term [$m^2\ s^{-2}$]
q_ξ	space-property heat flux [$W\ m^{-2}$]
$\boldsymbol{r}$	spatial position [m]
S	source term not due to collisions [$p^{-1}s^{-1}$]
S_m	source term due to coalescence and breakage in the equation of change for mass [$kg\ m^{-1}\ m^{-3}\ s^{-1}$]
$S_{\omega_{s,p}}$	source term due to coalescence and breakage in the equation of change for species mass [$kg\ m^{-1}\ m^{-3}\ s^{-1}$]
$S_{\boldsymbol{c}}$	source term due to coalescence and breakage in the equation of change for momentum [$kg\ m^{-3}\ s^{-2}$]
S_{h_p}	source term due to coalescence and breakage in the equation of change for enthalpy or temperature [$J\ m^{-3}\ m^{-1}$]
t	time [s]