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Hydrodynamic analogy approach for modelling reactive absorption

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HIGHLIGHTS

- Hydrodynamic analogy approach adequately describes reactive absorption processes.
- Different classes of reactions typical for absorption systems were studied.
- Both laminar and turbulent gas flow conditions were governed.
- Columns filled with different structured packings were successfully modelled.

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ABSTRACT

Design of separation units for reactive gas–liquid systems is usually based on conventional modelling methods employing the stage concept, either equilibrium or rate-based. The parameters of such models (e.g., mass transfer coefficients) are determined experimentally, and, most often, significant experimental effort is necessary when new processes are explored or new types of column internals are developed. In the context of a novel approach based on hydrodynamic analogies, rigorous partial differential transport equations are applied for modelling of non-reactive and reactive separation processes in columns filled with structured packings. The approach has already been verified for distillation and reactive desorption processes. In this work, its application to reactive absorption – also known as chemical absorption – is examined. Different types of reactions appearing in a wide range of absorption systems are considered. To account for absorption processes operated at high gas and liquid loads, an adjustment of the turbulent gas flow description is performed. Therefore, different test systems are used, namely physical absorption of ammonia into water, chemical absorption of sulphur dioxide and chemical absorption of carbon dioxide into sodium hydroxide solutions. The absorption of ammonia and sulphur dioxide took place under turbulent gas flow conditions, while in the absorption of carbon dioxide, the gas flow was laminar. Based on the carbon dioxide system, different types of corrugated sheet packings were compared. The hydrodynamic analogy model was successfully validated using available experimental data.

1. Introduction

Reactive absorption, also known as chemical absorption, is probably the most important example for reactive separation processes in industry. It is applied for production of acids and salts since the early 20th century [1]. In the field of gas purification, the use of reactive absorption has increasingly gained importance with growing restrictions on emission of harmful substances and potential greenhouse gases (see, e.g., [2,3]). An overview on important chemical absorption processes was recently given by Yildirim et al. [4].

Reactive absorption units may have very large dimensions, e.g., when exhaust gas purification of coal-fired power plants is considered. To keep equipment size and investment costs in an economic range, structured packings (Fig. 1) as column internals are often advantageous. They offer high separation efficiency, while their pressure drop is relatively low. However, the design and optimisation of structured packed absorption units requires adequate process model development [5,6].

A new modelling approach for the description of gas/vapour–liquid separation units with structured packings has been suggested in [7–9]. It is based on hydrodynamic analogies between real complex flows in structured packings and more simple (usually film-like) flow patterns. Unlike conventional process models,

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Nomenclature

a_P	specific packing surface, $m^2\ m^{-3}$
B	turbulence parameter, –
b_0	corrugation base length, m
C	concentration, dimensionless, see Eq. (25)
c	concentration, mol m^{-3}
c_{tot}	mean specific molar amount, mol/m^3
D	diffusivity, $m^2\ s^{-1}$
d_h	hydraulic diameter, m
F	F-factor, $F = u^G\sqrt{\rho^G}$, $Pa^{0.5}$
G	gas flow rate, mol s^{-1}
g	gravity, 9.81 m s^{-2}
H	height, m
h	corrugation height, m
I	ionic strength, mol/m^3
k_{eq}	gas-liquid equilibrium constant, –
k_R	reaction rate constant, $m^3\ mol^{-1}\ s^{-1}$
L	liquid flow rate, mol s^{-1}
N	absorption rate, mol $m^{-2}\ s^{-1}$
n_I	number of nodes in radial direction, –
n_J	number of nodes in axial direction, –
n_K	number of components, –
p	pressure, Pa
Re	Reynolds number, –
r	(radial) coordinate, m
r_S	interface reaction rate, mol $m^{-2}\ s^{-1}$
r_V	volumetric reaction rate, mol $m^{-3}\ s^{-1}$
R	gas constant, 8.3144 J $mol^{-1}\ K^{-1}$
Sc	Schmidt number, –
t	temperature, dimensionless, see Eq. (24)
T	temperature, K
u	velocity, m s^{-1}
u_τ	shear flow velocity, m s^{-1}
V	volume, m^3
w_L	liquid load, $m^3\ m^{-2}\ h^{-1}$
x	coordinate, m
x_i	liquid-phase mole fraction of component i, –
y	coordinate, m
y_i	gas-phase mole fraction of component i, –
z	coordinate, m
z^G	length of undisturbed gas flow, m
z^L	length of undisturbed liquid flow, m

Greek letters

α	sweep coefficient, see Eq. (31)
α_P	channel inclination angle
β	sweep coefficient, see Eq. (31)
γ	corrugation angle
δ	film thickness, m
η	(radial) coordinate, dimensionless, see Eq. (26)
φ	corrugation inclination angle
κ	von Kármán constant, 0.41
μ	viscosity, $kg/m^{-1}\ s^{-1}$
ν	stoichiometric factor, –
ρ	density, kg m^{-3}
ω	velocity, dimensionless, see Eq. (23)
ζ	(axial) coordinate, dimensionless, see Eq. (21)

Subscripts

av	average
eff	effective
i	radial node index
in	Inlet
j	axial node index
k	component index
lam	laminar
norm	normalised
out	outlet
P	packing
t	total
turb	turbulent

Superscripts

0	inlet conditions
G	gas-phase
L	liquid-phase
(m)	iteration index

in the hydrodynamic analogy approach, rigorous partial differential transport equations are applied and, therefore, expensive experimental determination of mass transfer coefficients is not required. The model was validated using experimental data of several distillation operations [9,10]. An extension was developed for the modelling of reactive stripping processes taking place in structured packings and in film-flow monoliths [11,12].

When the hydrodynamic analogy model is applied to processes with significant gas-phase turbulence, a relevant determination of the turbulence intensity is required. The latter depends on the specific packing geometry and can be evaluated by the so-called *virtual experiments*, in which the methods of computational fluid dynamics (CFD) are applied for the description of the gas flow in packing elements. In this way, mainly the dry pressure drop of structured packings could be predicted [13,14]. More recently, mean turbulent viscosity in the gas channel crossing section of a structured packing was directly determined [10]. However, the entire structured packing in a column unit can hardly be modelled because of computational limitations. For this reason, small representative elements (elementary units) are used. A good review on different methods for the selection and modelling of such representative elementary units is given by Said et al. [15] who also showed that the results obtained based on representative elementary units can agree very well with the results obtained from the modelling of larger packing domains.

In this work, the hydrodynamic analogy approach is used to model reactive absorption processes in structured packed columns. A focus is set on the description of different reaction mechanisms that are characteristic for a wide range of absorption systems. As absorption columns are often operated at high gas loads, an

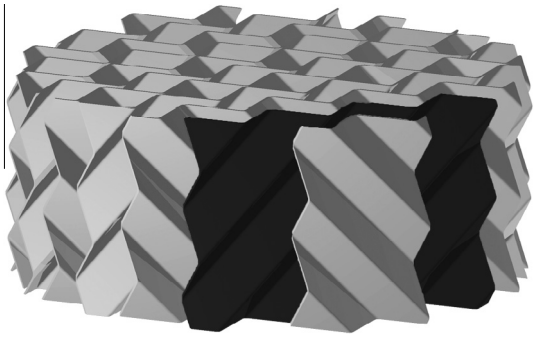

Fig. 1. Schematics of a corrugated sheet packing layer, a single corrugated sheet in dark colour.