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Mass transfer performance of CO_2 capture in rotating packed bed: Dimensionless modeling and intelligent prediction

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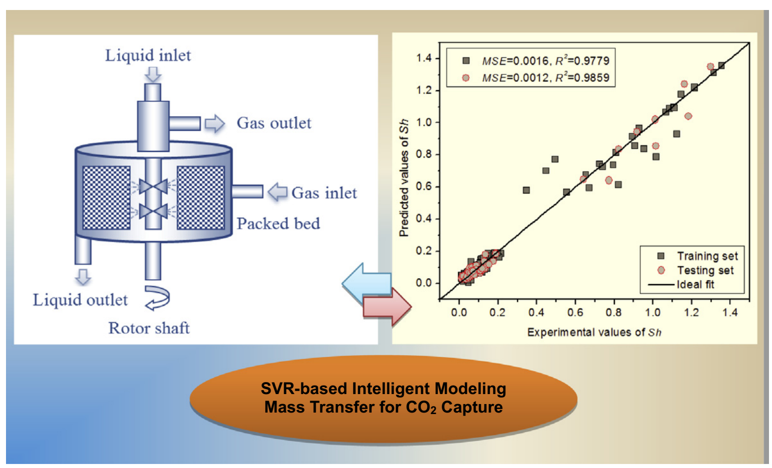
HIGHLIGHTS

- Intelligent modeling for mass transfer of CO_2 capture in rotating packed beds.
- Dimensional analysis was used to obtain the independent and dependent variables.
- Support vector regression (SVR)-based approach is developed for prediction.
- SVR is superior to multiple nonlinear regression and artificial neural network.

GRAPHICAL ABSTRACT



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ABSTRACT

Rotating packed beds have been demonstrated to be able to intensify the physicochemical process of multiphase transportation and reaction in the fields of energy and environment, and successfully applied in the field of CO_2 emission control. However, modeling and prediction of gas–liquid mass transfer especially for mass transfer with chemical reaction are rare due to the complexity of multiphase fluid flow and transportation. In view of the inaccuracy of semi-empirical models and the complexity of computational fluid dynamics models, an intelligent correlation model was developed in this work to predict the mass transfer coefficient more accurately for CO_2 capture with NaOH solution in different type rotating packed beds. This model used dimensional analysis to determine the independent variables affecting the mass transfer coefficients, and then used least squares support vector regression (LSSVR) for prediction. An optimized radial basis function was obtained as kernel function based on grid search coupled with simulated annealing (SA) and 10-fold cross-validation (CV) algorithms. The proposed model had the mean square error of 0.0016 for training set and 0.0012 for testing set. Compared with the models based on multiple nonlinear regression (MNR) and artificial neural network (ANN), the present model decreased mean squared error by 91.06% and 38.46% for training set and 94.57% and 53.85% for testing set respectively, suggesting it had superior performance on prediction accuracy and generalization ability.

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Nomenclature

a	gas–liquid interfacial area (m^{-1})
a_c	centrifugal acceleration ($m^2\ s^{-1}$)
a_p	surface area per unit volume of the bead (m^{-1})
a_t	surface area of the packing per unit volume of the bed (m^{-1})
b	bias term
c_L	concentration of NaOH solution (mol L^{-1})
c_G	concentration of CO_2 in inlet gas (mol L^{-1})
D_G	diffusion coefficient in the gas phase ($m^2\ s^{-1}$)
D_L	diffusion coefficient in the liquid phase ($m^2\ s^{-1}$)
d	degree of the polynomial function
d_e	hydraulic diameter (m)
d_p	spherical equivalent diameter of the packing (m)
E^2	mean squared error
e_i	slack variable
G	gas mass flux (kg $m^{-2}\ s^{-1}$)
g	acceleration due to gravity (m s^{-2})
H	Henry's law constant ((mol/mol)/(mol/mol))
H'	solubility coefficient (kmol $Pa^{-1}\ m^{-3}$)
h	axial height of the rotor (m)
$\mathbf{I}$	an identity matrix
K	kernel function
K_Ga	overall volumetric gas-side mass transfer coefficient (s^{-1})
K_La	overall volumetric liquid-side mass transfer coefficient (s^{-1})
k	the number of sub-samples for cross-validation
k_G	local gas-side mass transfer coefficient (kmol $m^{-3}\ s^{-1}$ - Pa^{-1})
k_Ga	local volumetric gas-side mass transfer coefficient (s^{-1})
k_L	local liquid-side mass transfer coefficient (m/s)
k_La	local volumetric liquid-side mass transfer coefficient (s^{-1})
k_s	a constant obtained from experimental results (mol^2 - s $m^{-8}\ Pa^{-2}$)
L	liquid mass flux (kg $m^{-2}\ s^{-1}$)
l	characteristic length (m)
N	number of samples
N_H	neuron number in hidden layer
N_P	the number of input variables
P	operating pressure (Pa)
ΔP	pressure drop (Pa)
Q_G	gas flow rate ($m^3\ s^{-1}$)
Q_L	liquid flow rate ($m^3\ s^{-1}$)
$\mathbf{R}$	space of the output features y_i
$\mathbf{R}^d$	space of the input features x_i
R^2	coefficient of determination (COD)
r_h	hydraulic radius of the packings, ε/a_t, (m)
r_i	inner radius of the packed bed (m)
r_o	outer radius of the packed bed (m)
r_{avg}	average radius of packings, $(r_h + r_o)/2$ (m)
T	operating temperature (K)
t	a constant in polynomial kernel function
u_G	actual gas velocity (m s^{-1})
u_{Gf}	superficial gas velocity (m s^{-1})
u_L	actual liquid velocity (m s^{-1})
u_{Lf}	superficial liquid velocity (m s^{-1})
V	volume of 1mol gas
V_i	volume inside the inner radius of the bed (m^3)
V_o	volume between the outer radius of the bed and the stationary housing (m^3)
V_t	total volume of the RPB (m^3)
$\boldsymbol{w}$	weigh vector
X	surface renewal parameter (m)
$\boldsymbol{x}$	input variable
x_i	ith input variable
x_{Ni}	scaled value of the observed variable
x_{min}	minimum observation value of the dataset
x_{max}	maximum observation value of the dataset
Δx	spacing between plate corrugations (m)
$\boldsymbol{y}$	output variable
y_i	target output corresponding to the ith input
$\hat{y}$	predicted value of y
$\bar{y}$	mean value of y
z	axial height of packing (m)

Greek letters

α_i	ith Lagrangian multiplier
γ	regularization parameter
ε	porosity of the packing or voidage (m^3/m^3)
μ_G	dynamic viscosity of gas (Pa s)
μ_L	dynamic viscosity of liquid (Pa s)
ν_G	kinematic viscosity of gas ($m^2\ s^{-1}$)
ν_L	kinematic viscosity of liquid ($m^2\ s^{-1}$)
ρ_G	density of gas (kg m^{-3})
ρ_L	density of liquid (kg m^{-3})
σ	surface tension (kg s^{-2})
σ_c	critical surface tension of packing (kg s^{-2})
σ_w	surface tension of water (kg s^{-2})
σ^2	squared bandwidth of RBF kernel
φ	mapping function
ψ	sphericity of packing
$\boldsymbol{\Omega}_{i,j}$	scalar product between a pair of input points
ω	rotational speed (rad s^{-1})
η	CO_2 capture efficiency (%)

Dimensionless groups

Gr_G	Grashof number of the gas phase ($l^3 a_c/\nu_G^2$)
Gr_L	Grashof number of the liquid phase ($l^3 a_c/\nu_L^2$)
Mr	liquid–gas molar ratio ($(Q_L c_L)/(Q_G c_G)$)
Re_G	Reynolds number of the gas phase ($d_e u_G/\nu_G$ or $G/a_t \nu_G$)
Re_L	Reynolds number of the liquid phase ($d_e u_L/\nu_L$ or $L/a_t \nu_L$)
Re_ω	rotational Reynolds number ($\omega r_{avg}^2/\nu_G$)
Sc_G	Schmidt number of the gas phase (ν_G/D_G)
Sc_L	Schmidt number of the liquid phase (ν_L/D_L)
Sh	Sherwood number ($K_G a/(D_G a_t^2)$)
We_L	Weber number of the liquid phase ($L^2/\rho_L a_t \sigma$)

1. Introduction

It has been demonstrated that carbon dioxide (CO_2) as a greenhouse gas from human activity especially from combustion of fossil fuel is responsible for the global warming and the greenhouse effect [1,2]. Anthropogenic CO_2 emissions control and reduction have become an important scientific, environmental and even international economic and political issue.

Currently, post-combustion CO_2 capture can be roughly categorized as chemical absorption, physicochemical adsorption, membrane, cryogenics, chemical looping combustion (CLC) and biological sequestration according to their scientific principles [3,4]. Among these approaches, chemical absorption is comprehensively considered as a good choice for its advantages of high efficiency, low cost and mature technology [3]. Over last decades, conventional gas–liquid contactors such as packed tower, spray

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