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Mathematical modeling of electrothermal regeneration of modified carbonaceous adsorbent bed in inductively heated column



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ABSTRACT

A novel, two-dimensional, non-isothermal, non-adiabatic and non-equilibrium mathematical model of desorption step (regeneration) in electrothermal temperature swing adsorption (ETSA) process in cylindrical coordinates was proposed. Regeneration concerns desorption of the carbonaceous adsorbent (modified Sorbonorit 3 adsorbent bed) loaded with *n*-butanol. The unique mathematical model has been developed for the internal volumetric heat source capacity, generated in adsorbent bed by induction heating. The internal volumetric heat source capacity depends on temperature, concentration of desorbed compound in solid phase, volumetric fraction in bed of granular iron, electric current intensity, and radial coordinate.

Mathematical model of ETSA process was solved by numerical method of lines in non-dimensional, cylindrical coordinate system.

The fairly good agreement of computed and experimental results with respect to process characteristics was obtained.

1. Introduction

Volatile organic compounds (VOCs) are a significant group responsible for the about 45–50% of the total emissions to atmosphere. Various industrial chemical processes, bonding, coating, painting, lacquering, drying and cleaning with use of organic solvents, pharmaceuticals, dyes and lacquers production, extraction, impregnation and lamination of wood-like and plastics as well as engine fuels distribution are the main emission sources [1].

Waste gases are characterized by large volumetric fluxes in which VOCs concentration practically does not exceed 50 g/m³ [2]. Adsorption methods of air purification enable removal and recovery of various VOCs such as hydrocarbons, chlorohydrocarbons, perfluorocarbons etc. with efficiency above 95% at relatively low investment costs [3–7]. The costs of adsorbent regeneration are crucial when concerning the adsorption process to be used to purify gases from VOCs. A life time of carbonaceous adsorbents is about 1000 adsorption-desorption cycles. In practice, typical adsorbent regeneration methods used to restore the adsorbent capacity make use of hot inert gas or superheated water vapor flowing through the adsorbent bed [7–9]. However, these methods are expensive, energy consuming and do not guarantee effective recovery of adsorbed components.

The novel electrothermal heating methods of the adsorbent bed

include ohmic (resistive), induction or microwave treatment. As a result of electric or magnetic field energy conversion, the heat is generated directly in the adsorbent bed volume.

The cyclic ETSA process is a novel method used to remove volatile organic compounds (VOCs) from gaseous streams, especially from polluted waste gases emitted mainly by chemical and petrochemical industries.

Most commonly, the resistance [10–16] and microwave heating [17] are used. In the resistance heating the Joule's heat is generated during passing an electric current through the bed of granular adsorbent. In microwave heating intermolecular friction of dipoles (dipolar rotation phenomenon) or ions (ionic conduction phenomenon) takes place due to changing direction of electric field.

Induction heating is based on well-known physical phenomena: electromagnetic induction and then the Joule effect [18–22]. It can be applied to regeneration of carbonaceous adsorbent fixed bed in a column after the adsorption step of the ETSA process, when activated carbon is loaded with the volatile organic compounds (VOCs) [22,23] adsorbed from an air stream. Induction heating has several advantages: high capacity of internal volumetric heat source, no contact between adsorbent and heating medium, simplicity of heating system control, etc.

Full adsorption cycle of the electrothermal temperature swing

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Nomenclature		r_e	Mean pore radius of adsorbent (m)
		R	Bed radius (m)
$a_{s_{AC}}$	Specific area of activated carbon particle (m^2/m^3)	R_g	Universal gas constant (J/(molK))
b_0	Toth multitemperature isotherm constant (Pa ⁿ)	R_{PAC}	AC particle radius (m)
bei	Imaginary part of the Bessel-Kelvin function of the first	$R_{p_{Fe}}$	Fe particle radius (m)
	type, zero order (–)	t	Time (s)
bei'	Imaginary part of the Bessel-Kelvin function of the first	t _{ads}	Total duration time of adsorption step (s)
	type, first order (–)	t _{des}	Total duration time of desorption step (s)
ber	Real part of the Bessel-Kelvin function of the first type,	Т	Temperature (K)
	zero order (-)	T_{des_0}	Inlet inert gas temperature in desorption step (K)
ber'	Real part of the Bessel-Kelvin function of the first type,	T_{con}	Desorbed component condensation temperature (K)
	first order (–)	T_{reg}	Regulation temperature in adsorbent bed (K)
В	Vector of magnetic induction (T)	T_{wall}	Internal wall temperature of adsorption column (K)
$c_{b_{AC}}$	Specific heat capacity of dry activated carbon bed (J/kg K)	V	Volume (m ³)
c_{bFe}	Specific heat capacity of dry granular iron bed (J/kg K)	Y	Mole ratio of component in gas phase (mol/mol inert)
$c_{s_{eff}}$	Specific heat capacity of unloaded bed of AC and granular	Y_{adsin}	n-Butanol concentration in gas phase at column inlet
	Fe mixture (J/kg K)		during desorption step (mol/mol inert)
C_{l_A}	Molar specific heat of adsorbed component (liquid) (J/	Y_{adsout}	n-Butanol concentration in gas phase at column outlet
	mol K)		during desorption step (mol/mol inert)
$C_{p_{g_A}}$	Molar specific heat of adsorbed component in gas phase (J/mol K)	Z	Axial coordinate (m)
C_{n}	Molar specific heat of gas phase $(J/mol K)$	Greek sy	rmbols
C_{p_g}	Molar specific heat of inert gas (J/mol K)	5	
$D^{p_{inert}}$	Diffusion coefficient (m^2/s)	δ	Penetration depth of magnetic field in cylindrical ad-
D	Vector of electric induction (C/m^2)		sorbent bed (m)
D_{ic}	Inductor coil diameter (m)	δ_n	Penetration depth of magnetic field in particle of ad-
D_{κ}	Knudsen diffusion coefficient (m^2/s)	F	sorbent bed (m)
D_I	Axial mass dispersion coefficient (m^2/s)	ΔH	Isosteric heat of adsorption (J/mol)
D_M	Molecular diffusion coefficient (m^2/s)	ε	Absolute permittivity of dielectric (F/m)
D_R	Radial mass dispersion coefficient (m^2/s)	ε_{b}	Bed voidage (activated carbon or iron) $(-)$
D_{s}	Surface diffusion coefficient (m^2/s)	ε_{eff}	Effective bed voidage (additive fraction of activated
<i>d</i> _n	Effective diameter of AC and Fe mixture (m)	-55	carbon and iron voids – Eq. (56), $(-)$
d_{n}	Equivalent iron particle diameter (m)	ε_{n}	Particle porosity (m^3/m^3)
$d_{p_{e}}$	Equivalent AC particle diameter (m)	ϕ	Volumetric fraction of granular iron in the adsorbent bed
\boldsymbol{E}^{PAC}	Vector of electric field intensity (V/m)		(-)
$E_{\rm m}$	Amplitude of electric field intensity (V/m)	γ	Electrical conductivity ($\Omega^{-1} m^{-1}$)
f	Current frequency (Hz)	YAC	AC particle electrical conductivity ($\Omega^{-1} m^{-1}$)
G _{inert}	Molar flux density of inert gas $(mol/m^2 s)$	γ_{Fe}	Fe particle electrical conductivity ($\Omega^{-1} m^{-1}$)
G_{air}	Molar flux density of air (carrying gas) $(mol/m^2 s)$	η_{σ}	Gas phase viscosity (Pa s)
H	Magnetic field intensity (A/m)	η_{rmv}	Efficiency coefficient of adsorbed component removal
H_m	Amplitude of magnetic field intensity (A/m)	•	from adsorbent bed (%)
H_{m0}	Magnetic field intensity (A/m)	η_{rcv}	Efficiency coefficient of adsorbed component recovery (%)
Iic	Current intensity of the inductor coil (A)	nend	Efficiency coefficient of adsorbed component condensa-
Ĵ	Vector of magnetic field strength (A/m)		tion (%)
Kic	Nagaoka coefficient of the inductor coil $(-)$	λ	Effective thermal conductivity (W/(mK))
L	Adsorbent bed height (m)	λ_{bAC}	Thermal conductivity of bulk activated carbon bed (W/
Lic	Inductor coil length (m)		(mK))
m	Toth multitemperature isotherm constant (mol/kg)	$\lambda_{b_{Fe}}$	Thermal conductivity of bulk iron bed (W/(mK))
m _{ads}	Mass of the adsorbed component (kg)	λ_{inert}	Inert gas thermal conductivity (W/(mK))
m _{cnd}	Mass of the condensed component (kg)	$\lambda_{L,R_{eff}}$	Effective heat dispersion coefficient in axial or radial di-
m_{rmv}	Mass of the removed component from adsorbent bed (kg)	-50	rection (averaged value for activated carbon and iron – Eq.
M_A	Molar mass of adsorbed component (kg/mol)		(55) (W/(mK))
n	Toth multitemperature isotherm constant $(-)$	μ	Magnetic permeability (H/m)
N _{ic}	Number of turns of the inductor coil $(-)$	μ_{AC}	AC particle magnetic permeability (H/m)
N	Number of particles $(-)$	μ_{Fe}	Fe particle magnetic permeability (H/m)
Р	Pressure (Pa)	ν_{g}	Gas phase kinematic viscosity (m^2/s)
q	Concentration of component in solid phase (mol/kg)	ρ _b	Adsorbent bed bulk density (kg/m ³)
\dot{q}_0	$=q_{ads}$, initial concentration of component in solid phase in	$\rho_{h,\sigma}$	Adsorbent bed mixture (activated carbon and iron) bulk
**	desorption step (mol/kg)	, _{Dejj}	density (kg/m ³)
<i>q</i> _{ads}	Final concentration of component in solid phase in ad-	ρ _м	Gas molar density (mol/m^3)
	sorption step (mol/kg)	$\rho_{M_{0}}$	Gas molar density at column inlet (mol/m ³)
Q_V	Internal volumetric heat source capacity (W/m ³)	ρ_p	Adsorbent particle density (kg/m ³)
Q_{V_n}	Internal volumetric heat source capacity generated in a	ρ _g	Gas phase density (kg/m ³)
P	particle (W/m ³)	$(\Sigma v)_A$	Sum of atomic diffusion volumes of component molecule
r	Radial coordinate (m)		(cm ³)

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