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Rotary reverse flow reactor vs. adiabatic reactor with regenerative preheating - Design and comparison

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HIGHLIGHTS

- Two autothermal schemes for the treatment of VOCs are simulated and compared.
- Five different monolithic structures are considered for performance comparison.
- A design strategy is proposed considering a range of VOC content to be treated.
- The rotary reverse-flow reactor results more compact than the regenerator-reactor.
- The rotary reverse-flow reactor allows a more flexible operation.

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ABSTRACT

The autothermal catalytic-combustion systems are commonly used for the purification of waste air streams contaminated with low concentrations of volatile organic compounds (VOC). Within this type of devices, the reverse flow reactors (RFR) are known to be more efficient than systems employing recuperative (surface) heat exchangers to preheat the waste air stream with the lean air effluent from the catalytic incinerator. The advantage of the RFR is basically due to the regenerative heat-exchange mechanism, provided by the inert and catalytic solids inside the unit.

As an alternative, the regenerative mechanism of preheating can be achieved by an independent heat exchanger, which coupled to a catalytic reactor could be expected to produce similar performance as the RFR.

In this context, this contribution is devoted to analyse comparatively the performances of a rotary reverse flow reactor (RRFR) and a system comprising a rotary regenerative heat-exchanger and a catalytic reactor (RHE-SR system) for the treatment of a waste air stream contaminated with ethanol and ethyl acetate, by means of mathematical simulation. Both alternatives are assumed to be composed of monoliths with square channels. A strategy of design for both systems suitable for their comparison is proposed, attending to a range of VOC concentration in the waste stream. Both alternatives can be regarded as being suitable options to carry out the target. However, the resulting designs show clear advantages in favour to the RRFR, as this alternative requires a significantly more compact equipment than the RHE-SR does and, besides, it allows to be operated under a wider range of the rotational speed, which is the main control variable once the systems are operating.

1. Introduction

In the last decades, the environmental regulations have become more stringent in many countries. As a result, research and development of technologies for the control of air contamination has grown considerably. Volatile organic compounds (VOCs) are the most common air contaminants and catalytic oxidation is the most widespread option among destructive alternatives, when the levels of VOCs are low – i.e., ≤1% – (Kolaczkowski, 2005).

Depending on the nature of each VOC and the catalyst used, common temperatures for the catalytic combustion ranges between 200 and 400 °C. Additionally, the waste air streams are usually at near ambient temperature and the flow rates are quite high. Therefore, the need to efficiently recover part of the

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Nomenclature

a	catalytic activity
a_0	catalytic activity of the fresh catalyst
a_{crit}	critical value of a for reactor extinction
a_v	specific interfacial area (m^2/m^3)
c_p	specific heat ($J\ kg^{-1}\ K^{-1}$)
C_j	molar concentration of the jth component in the gas phase (mol/m^3)
C_T	total molar concentration in the gas phase (mol/m^3)
D	diameter of the RRFR (m)
D_{RHE}	diameter of the regenerator (m)
D_R	diameter of the reactor (m)
d_h	hydraulic diameter of the channels (m) ($4\varepsilon_L/a_v$)
E_i	activation energy of the ith reaction ($J\ mol^{-1}\ K^{-1}$)
f_C	cleaning fraction
f_{cold}	fraction of the total cross-section of the regenerator used for the cooling step of the solid (m)
f_I	ratio of the length of the inert zone to the total length of the unit
G	superficial mass velocity ($kg\ m^{-2}\ s^{-1}$)
G_{mC}	cleaning mass flow rate ($kg\ s^{-1}$)
G_{mT}	total mass flow rate to be treated ($kg\ s^{-1}$)
h	heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
h^*	modified heat transfer coefficient (Eq. (9)) ($W\ m^{-2}\ K^{-1}$)
k_i	specific rate constant of the ith reaction (s^{-1})
$k_{i,ref}$	specific rate constant of the ith reaction, evaluated at T_{ref} (s^{-1})
K_j	adsorption constant of the jth component ($m^3\ mol^{-1}$)
$k_{m,j}$	mass transfer coefficient for the jth component ($m\ s^{-1}$)
ℓ	equivalent washcoat thickness (m) ($\delta_{cat}[1+\delta_{cat}/(L_{cell}-\delta_T)]$)
L	length of the RRFR (m)
L_{cell}	side of the unit cell of the monolith (m) ($N_{cell}^{-1/2}$)
L_{RHE}	length of the regenerator (m)
L_R	length of the reactor (m)
M_{air}	molecular weight of air
n	current half-cycle to be simulated
N_{cell}	number of cells per unit of cross-sectional area (m^{-2})
Nu	Nusselt number
r_i	ith reaction rate ($mol\ m^{-3}\ s^{-1}$)
$\mathbf{r}_j^{ef}$	effective rate of consumption of the jth component ($mol\ m^{-3}\ s^{-1}$)
R	ideal gas constant. ($J\ mol^{-1}\ K^{-1}$)
Re	Reynolds number (evaluated at feed conditions)
S	total cross-section of RRFR (m^2)
S_{RHE}	total cross-section of the regenerator (m^2)
S_R	total cross-section of the catalytic reactor (m^2)
Sh	Sherwood number
$\langle T_G\rangle^{RS}$	average temperature of the air stream at the output of the reaction step (K)
$\langle T_G\rangle^{cool}$	average temperature of the air stream at the output of the cooling step (K)
$\langle T_G\rangle^{C}$	average temperature of the air stream at the output of the cleaning step (K)
t	time (s)
$t_{\alpha 0}$	time at which a channel in the position α_0 at initial time (in the reaction step), reaches the cleaning step for the first time ($[(\pi-\varphi)-\alpha_0]t_{cycle}/(2\pi)$)
t_{cycle}	cycle period (s)
$t_{cycle}^{\min}$	minimum cycle period (s)
$t_{cycle,crit}$	critical cycle period (s)
$t_{cycle,low}$	minimum **operating** cycle time for the nominal operation (s)
t_{CS}	duration of a cleaning step (s)
t_{cool}	duration of a cooling step of the solid (s)
t_{reg}	duration of a heat regeneration step of the solid (RHE-SR) (s)
t_{RS}	duration of a reaction step (RRFR) (s)
T	temperature (K)
$T_G^{0,R}$	temperature of the air stream at the reactor inlet (K)
$T_G^{L_R,R}$	temperature of the air stream at the reactor outlet (K)
T_{ref}	reference temperature for the calculation of the kinetic coefficients (K)
$T_{S,\max}$	maximum temperature reached in the solid phase (K)
$T_{S,\max}^{adm}$	maximum allowable temperature in the solid phase used in the design (K)
V	total volume of the RRFR (m^3)
V_{RHE}	total volume of the regenerator (m^3)
V_R	total volume of the reactor (m^3)
W_{act}	total mass of the active material (kg)
W_I	total mass of the inert material (kg)
$X^{(n)}$	any of the variables T_S, T_G or $y_{j,G}$ for the nth half-cycle
$X_{ini}^{(n)}$	any of the variables T_S, T_G or $y_{j,G}$ at the beginning of the nth half-cycle
$X_{end}^{(n)}$	any of the variables T_S, T_G or $y_{j,G}$ at the end of the nth half-cycle
$\langle y_{j,G}\rangle^{RS}$	average mole fraction of the jth component in the gas phase at the output of the reaction step
$\langle y_{j,G}\rangle^{cool}$	average mole fraction of the jth component in the gas phase at the output of the cooling step
$\langle y_{j,G}\rangle^{C}$	average mole fraction of the jth component in the gas phase at the output of the cleaning step
$\langle y_{VOCs}\rangle$	average mole fraction of VOCs at the output
$y_{j,G}^{0,\min}$	minimum VOC concentration
$y_{j,G}^{0,nom}$	nominal VOC concentration
$y_{j,G}^{L_R,R}$	mole fraction of the jth component in the air stream at the output of the reactor
$\langle y_{VOCs}^{adm}\rangle$	allowable mole fraction of VOCs at the output
y_j	mole fraction of the jth component
z	axial position in the channel (m)

Greek letters

α_0	angular location of the channels at the operation start time
δ_{cat}	catalytic coating thickness (m)
δ_T	wall thickness (m)
ΔH_j	enthalpy of combustion of the jth component ($J\ mol^{-1}$)
$\lvert\Delta P\rvert$	pressure drop in a cycle (mbar)
$\lvert\Delta P\rvert^{adm}$	allowable pressure drop (absolute value) (mbar)
Δt_{oper}	difference between $t_{cycle,crit}$ and $t_{cycle,low}$ (s)
ΔT_{ad}	maximum adiabatic temperature rise (K)
ΔT^R	temperature rise in the reactor (K)
ε	void fraction of the bed
ε_T	tolerance for the maximum temperature (1 K)
ε_a	tolerance for the determination of the relative critical catalyst activity ($5\cdot10^{-4}$)
λ_S	thermal conductivity of the solid on the axial direction ($W\ m^{-1}\ K^{-1}$)
ρ	density ($kg\ m^{-3}$)
τ	time at which the channel just reaches the cleaning step
φ	angle span by the compartments discharging or collecting the cleaning stream

Subscripts

cat	catalyst-associated property
C	cleaning step