



VOCs abatement in adiabatic monolithic reactors: Heat effects, transport limitations and design considerations



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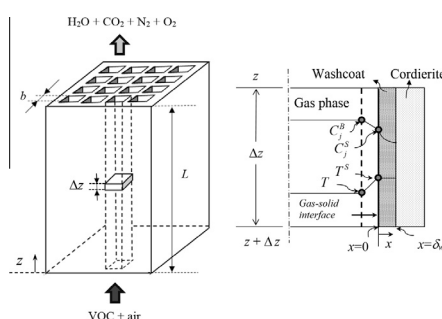
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HIGHLIGHTS

- The role of inlet temperature to control VOC emissions with low energy requirements is elucidated.
- Impact of internal mass transport limitations and external mass and heat transport limitations are analysed.
- Higher VOC concentrations increase heat effects and accelerate the reaction rates.
- Poor interfacial areas contribute to VOC abatement.
- Pseudohomogeneous models can significantly over – or underestimate the outlet VOC concentration.

GRAPHICAL ABSTRACT



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ABSTRACT

A simulation study of a monolithic reactor for the catalytic oxidation of Volatile Organic Compounds (VOC) over a Mn-Cu mixed oxide catalyst is presented. A heterogeneous 1D mathematical model is selected to describe the performance of the reactor under adiabatic and steady-state operation. Internal (washcoat) mass transport limitations and external (gas-solid) mass and heat transport limitations in the reactor are taken into account.

Proper quantification and analysis of both, internal and external resistances contribute to design and operate the reactor under conditions that favour VOC abatement.

The influence of the heat effects and different operating variables and design parameters on the reactor performance are analysed, aiming to meet environmental standards of VOC emissions with the lowest preheating energy requirements.

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1. Introduction

Emission control of hazardous air pollutants, including Volatile Organic Compounds (VOCs), is one of the priorities for environmental catalysis because of its many harmful effects on health and the environment [1].

VOCs are mostly generated by chemical and petrochemical industries. These emissions should be treated to reduce their concentration to the permitted levels currently established by global environmental standards. The European Commission sets an emission limit value (ELV) of 20 mg C/Nm³ in a stream discharged into the atmosphere [2].

Catalytic oxidation is a particularly suitable technology for treating large flows of low VOC concentrations [1,3].

Considerable efforts have been directed towards obtaining suitable catalysts for catalytic oxidation of VOCs [4–6]. It has been

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Notation

a_v	gas-solid interfacial area, m^2/m^3	$\text{C}_2\text{H}_5\text{OH}$	ethanol
A_l	lateral area, m^2 , calculated as $A_l = 4(b - 2\delta_w)CNL$	$\text{C}_2\text{H}_4\text{O}$	acetaldehyde
A_o	open frontal area, m^2 , calculated as $A_o = (b - 2\delta_w)^2 CN$	CO_2	carbon dioxide
A_r	transversal area, m^2 , calculated as $A_r = b^2 CN$	H_2O	water
b	channel width = height, mm	LHHW	Langmuir-Hinshelwood
C_j	concentration of j component, mol_j/m^3 or $\text{mg C}/\text{m}^3$	O_2	oxygen
$C_{s,j}$	concentration of j component in the solid phase, mol_j/m^3 or $\text{mg C}/\text{m}^3$		
$C_{s,j}^s$	concentration of j component at surface of the solid phase, mol_j/m^3 or $\text{mg C}/\text{m}^3$	<i>Greek letters</i>	
$C_{\text{VOC}}^{\text{VOC}}$	emission limit value of VOC, $\text{mg C}/\text{m}^3$	δ_w	washcoat thickness, μm
CN	channels number, dimensionless	ΔH_{ri}^o	heat of i reaction at standard conditions, J/mol
Cp_j	specific heat of j component, $\text{kJ}/(\text{kmol K})$	ΔH_{ri}	heat of i reaction, J/mol
$D_{e,j}$	effective diffusion coefficient for j component, m^2/s	ΔT	total temperature gradient (inlet-outlet) in the gas phase, $^\circ\text{C}$
E_i	activation energy of i reaction, J/mol	ΔT_{s-g}	interfacial temperature gradient, $^\circ\text{C}$
<i>GHSV</i>	gas-hourly space velocity, $1/\text{h}$	$\Delta T_{s-g,max}$	maximum interfacial temperature gradient, $^\circ\text{C}$
h_c	convective heat transfer coefficient, $\text{J}/(\text{s m}^2 \text{K})$	$\eta_{i,ext}$	external effectiveness factor of i reaction, dimensionless
$k_{g,j}$	convective mass transfer coefficient from gas to solid interface, $\text{m}^3/(\text{m}^2 \text{s})$	$\eta_{i,int}$	internal effectiveness factor of i reaction, dimensionless
$k_{ref,1}$	kinetic constant of reaction 1, $1/\text{s}$	$\bar{\eta}_{i,ext}$	axially averaged external effectiveness factor of i reaction, dimensionless
$k_{ref,2}$	kinetic constant of reaction 2, $\text{mol}/(\text{m}^3 \text{s})$	$\bar{\eta}_{i,int}$	axially averaged internal effectiveness factor of i reaction, dimensionless
KC_j	adsorption constant of j component, m^3/mol	ρ_w	washcoat density, kg/m^3
L	channel length, m	<i>Subscripts</i>	
m_w	catalyst mass, g	<i>Ac</i>	acetaldehyde
P	pressure, atm	<i>Et</i>	ethanol
q_{gen}	heat generation rate, $\text{J}/(\text{m}^3 \text{h})$, calculated as $q_{gen} = \eta_{1,int} r_1^s (-\Delta H_{r1}) + \eta_{2,int} r_2^s (-\Delta H_{r2})$	<i>ext</i>	external
Q_0	volumetric feed flow rate, $\text{N m}^3/\text{h}$	<i>i</i>	i reaction
r_i	reaction rate of i reaction, $i = 1, 2$, $\text{mol}/(\text{m}_w^3 \text{s})$	<i>int</i>	internal
r_i^B	reaction rate of i reaction at gas phase, $i = 1, 2$, $\text{mol}/(\text{m}_w^3 \text{s})$	<i>j</i>	j component
r_i^{eff}	effective reaction rate of i reaction, $i = 1, 2$, $\text{mol}/(\text{m}_w^3 \text{s})$	<i>max</i>	maximum
r_i^S	reaction rate of i reaction at gas-solid interface, $i = 1, 2$, $\text{mol}/(\text{m}_w^3 \text{s})$	<i>min</i>	minimum
R	universal gas constant, $\text{J}/(\text{mol K})$	<i>ref</i>	reference
T	gas phase temperature, $^\circ\text{C}$	<i>s-g</i>	solid-gas interface
T^S	solid phase temperature, $^\circ\text{C}$	<i>VOC</i>	volatile organic compound
$T_{0,min}$	minimum inlet temperature, $^\circ\text{C}$	<i>w</i>	washcoat
u_s	average gas velocity, m/s	<i>0</i>	at the axial coordinate $z = 0$
V_g	gas volume, m^3	<i>Superscripts</i>	
V_w	washcoat volume, m^3	<i>B</i>	at bulk gas phase
x	transversal coordinate, m	<i>eff</i>	effective
y_j	molar fraction of j component, dimensionless	<i>S</i>	at solid surface
z	axial coordinate, m	<i>*</i>	reference condition
C	carbon		

demonstrated that Mn–Cu mixed oxide catalysts are highly active at moderate temperatures for the catalytic oxidation of a wide variety of VOCs [7]. Catalysts have a finite life in terms of activity, and exposure to high temperature over time reduces the catalytic activity [4,8]. Additionally, for large flow rates, the preheating of the gaseous stream to achieve the required temperature levels that guarantee full VOCs conversion, produces a significant operative cost [9]. Recuperative catalytic conversion is a promising choice to preheat the gaseous stream, in which the thermal energy in the effluent gas is exchanged with the influent [10] but is not always suitable when the stream presents temporal emissions patterns.

An accurate determination and setting of the minimal inlet temperature of the gaseous stream according to its flow rate and VOC inlet concentration as an anticipative control strategy, would

contribute to reaching the ELV of VOCs emissions with minimum economic loss.

In the last three decades, the success of monoliths as converters of engine emissions has encouraged researchers to improve other gas phase reactions by using monolithic catalysts and reactors [11]. The major advantages of this design are low pressure drops under high fluid throughputs leading to an energy-efficient operation, short diffusion path in the catalyst and high external surface area, among others [11,12]. All these advantages become monoliths particularly appropriate for catalytic combustion [12,13].

Detailed modelling and simulation play a very important role in the designs of these systems [14–17]. Since catalytic combustion reactions are extremely fast, both inter-phase and intra-phase transport limitations are likely to be significant and have to be properly considered to analyse a reactor performance. Numerous

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