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A Modelling Approach of the Catalytic Oxidation of Volatile Organic Compounds in the SCR-DeNOx Monolithic Reactor

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Abstract: *Monolithic reactors play an important role in the integrated approach to environmental protection, especially in air pollution abatement. Mathematical modelling of catalytic reactors has become a key procedure in the design, development and optimisation of many industrial processes. The objective of this study was the modelling and simulation of the catalytic oxidation of volatile organic compounds by a commercial* V_2O_5-WO_3/TiO_2 *honeycomb catalyst, specific for the SCR-DeNOx process in high-dust flue gases from stationary incineration. The mathematical model is developed for the numerical simulation of a tubular plug flow reactor, using mass balance equation to predict results for benzene conversion under isothermal conditions.*

Keywords*: benzene catalytic oxidation,* V_2O_5-WO_3/TiO_2 *honeycomb catalyst, SCR-DeNOx*

1. Introduction

Monolithic catalysts play a key role for automotive exhaust control, selective catalytic reduction of NOx in flue gases and oxidative destruction of volatile organic compounds (VOCs) generated by industry or by incineration sources [1-5]. Selective catalytic reduction (SCR) is a widely used technology for the removal of NOx and VOCs from mobile and stationary emission sources [6-10].

Commercially employed catalysts in SCR-DeNOx technology are usually a homogeneous mixture of titanium dioxide (in the anatase form), vanadium pentoxide and tungsten trioxide or molybdenum trioxide [2, 4, 7, 11-13]. Monolithic catalysts offer a high specific geometric surface area and a low pressure drop, for use at high space velocities [4, 5, 13, 14]. Considerable effort has been made to develop the SCR-DeNOx process for simultaneous removal of NOx and dioxine [1, 7, 9, 15-17] as well as VOC pollutants in flue gases using commercial V_2O_5-WO_3/TiO_2 catalyst [6, 7, 18-23].

VOCs represent an important class of environmental pollutants. They as such and especially together with NOx participate in the degradation of the air quality and their secondary reaction products damage crops and vegetation. Even in trace amounts, these compounds and their reaction products may pose a potential risk for human health [24]. Heterogeneous catalytic oxidation is a technology for the abatement of VOCs in waste gas streams [8, 10, 18]. The catalysts may be applied in a monolithic form. Usually, the monolithic catalysts applied for this purpose have a honeycomb-like shape with parallel straight channels for the flow of the gas phase [4, 5, 12, 22].

The monolithic configuration is preferred with respect to the conventional packed bed because of the following advantages: (1) lower pressure drop especially under high gas throughputs; (2) reduction of external mass transfer and elimination of internal diffusion limitations when thin walls are used; (3) lower axial dispersion and back-mixing, and therefore high product selectivity; (4) larger specific geometric catalyst surface area; (5) uniform distribution of flow gas; (6) reduction of fouling and plugging, and thus extended catalyst lifetime; (7) easy scale-up [4, 5, 25-29].

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Mathematical modelling plays an important role in developing a new catalytic technology or for improving the design of existing reactors. The performance of a monolithic reactor is a complex function of design parameters, operating conditions, and properties of both the catalyst and reaction mixture [27, 30-33]. The approach to design and analyse catalytic SCR reactor customarily adopted in the early literature was based on pseudo-homogeneous models accounting for axial concentration gradients [4, 28, 29, 34]. Subsequently various mathematical models for monolithic reactor have been developed. These models are of different complexity, depending on the description of the reactant flow along the channels, the kinetic model of the chemical reaction, the heat and mass transfer in the gas and solid phase, etc. Depending on the objectives, applications and computational limitations, these models can be classified as one-dimensional (1-D), two-dimensional (2-D) and three-dimensional models (3-D), or as washcoat (catalyst layer), single channel, or multichannel (full reactor). [22, 27, 28, 31-35].

The presence of VOCs in flue gases from combustion sources led to investigations of their oxidative destruction in hybrid catalytic systems that simultaneously destroy VOCs and nitrogen oxide by V_2O_5-WO_3/TiO_2 catalysts. The aim of this study was to: (1) develop a mathematical model for the catalytic oxidation of VOCs on SCR-DeNOx monoliths; (2) predict the behaviour of the overall catalytic process and (3) validate the proposed model for the monolithic reactors. The proposed model is verified by comparing computer simulation data with experimental laboratory results using benzene as a model molecule for VOCs.

2. Materials and methods

The experimental tests for oxidative destruction of benzene were carried out on a commercial V_2O_5-WO_3/TiO_2 (anatase) catalyst. The catalyst had a low content of active component (0.53 %wt. V_2O_5), specific for the SCR-DeNOx process in high-dust system with low SO_2/SO_3 conversion. The main characteristics of the SCR-DeNOx commercial catalyst, according to the producers (CL-AS IHI-8070604/Japan), are presented in previous articles [20, 21]. The commercial catalyst was used in a monolithic form, with parallel straight channels by square section (Figure 1).

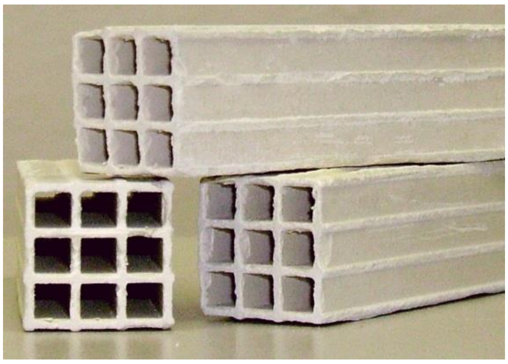

Figure 1. The commercial V_2O_5-WO_3/TiO_2 honeycomb catalyst

The experimental study concerning the catalytic oxidation of a benzene-containing flue gas was carried out with a laboratory scale set-up operated in a continuous and isothermal regime at atmospheric pressure. The model flue gas was obtained by mixing synthetic air with the appropriate amount of benzene.

The catalytic reactor consisted of two concentric quartz tubes (diameters of 40 x 1.5 mm and 32 x 1.5 mm, respectively). The monolith catalyst element was covered at both ends with quartz wool and placed into the reactor in such way to allow the gas to flow only through its channels. In order to monitor the process temperature on-line a Cr-Ni-Cr thermo-element was used. The catalytic reactor was placed into a temperature controlled electric oven.

VOC concentration analysis in the gas phases, at the inlet and outlet of the catalytic reactor, was carried-out by gas chromatography, using an Auto System XL gas chromatograph coupled with the Turbo Matrix ATD thermo desorber (PerkinElmer, USA). Gas samples were taken at a temperature of 322 K with a flow of 0.2 L/min, after a previous separation of water vapours in an adsorber packed with NaOH pellets (Merck/Germany). About 0.2 L/min of the water-free sample was fed to a Carbotrap 349 (Supelco/USA) adsorption tube, kept at 322 K in order to adsorb the hydrocarbons. The adsorbed hydrocarbons have been desorbed in the thermo desorber, gas chromatographically separated and quantified by a flame ionization detector (FID), and an electron capture detector (ECD). Calibration standards have been prepared by dissolving the hydrocarbons in 1-heptanol (from Merck/Germany) and injecting an appropriate μL volume into a Carbotrap tube and submitting these tubes to the thermo desorption gas chromatographic analytic procedure.

The qualitative and quantitative assessment of benzene oxidative destruction on the V_2O_5-WO_3/TiO_2 catalyst achieved through conversion is calculated with the following expression (in %):

$$X_{C_6H_6} = \frac{c^0_{C_6H_6} - c_{C_6H_6}}{c^0_{C_6H_6}} \cdot 100 \tag{1}$$

3. Results and discussions

A one-dimensional heterogeneous model was developed to describe the oxidation of VOCs in the SCR-DeNOx monolithic reactor. In according with literature [22, 27, 30, 35], the 1-D heterogeneous model was based on the assumption of negligible pore diffusion resistance within the thin catalytic wall of the honeycomb shaped monolith. The characteristics of 1-D monolithic reactor models are: (1) the simple form; neglecting the non-uniformity over the cross-section of the channel; (2) the results are often system specific due to lack of decoupling the physical processes from chemical kinetics; (3) fast computing and sufficient accuracy for certain system. The purpose of the application of 1-D monolith reactor models very often is: control, rapid design evaluations, kinetic studies, qualitative parametric studies. Basic assumption made during modelling include: isothermal conditions, laminar flow in the monolith channels, isobaric conditions, negligible axial diffusion, single-channel approach.

3.1. A 1-D mathematical model for the oxidation of VOCs by SCR-DeNOx honeycombs

Mathematical modelling of chemical processes and catalytic reactors are based on reasonable simplifying hypotheses so that by solving the models one obtains results close to reality. A commercial SCR-DeNOx (0.53 %wt. V_2O_5) catalyst in honeycomb form was used in the laboratory experiments, in order to establish the model. The model was based on the following simplifying assumptions: (1) the monolith element is a fixed bed micro-reactor with ideal mass flow; (2) the mass reaction volume (V_{MR}) is equal to the catalyst volume (V_{cat}) and the reactor volume (V_R), respectively; (3) the reactor is operated under isothermal conditions modelled by the mass balance equation (justified for small concentrations of VOC in the flue gases). For the establishment of the catalytic reactor model, a volume element was considered, for which a mass balance equation of the reactant subjected to transformation was written [27-29, 35, 36]. The schematics of the catalytic reactor employed for establishing the mathematic model is presented in Figure 2. In the same figure the notations and the characteristic equations used in the model are presented.

The mass balance equation of benzene corresponding to its transformation in the catalyst volume element (dV_{cat}) is:

$$\left(n_{C_6H_6}\right)_x = \left(n_{C_6H_6}\right)_{x+dx} + \left(dn_{C_6H_6}\right)_{transformed} \tag{2}$$

or:

$$V_g \cdot c_{C_6H_6} = V_g\left(c_{C_6H_6} + dc_{C_6H_6}\right) + \left(-r_{C_6H_6}\right)_{ef} \cdot dV_{cat} \qquad (3)$$

Using the notations corresponding to the volume element (Figure 2), relation (3) becomes:

$$A_T \cdot u_g \cdot dc_{C_6H_6} = -\left(-r_{C_6H_6}\right)_{ef} \cdot A_T \cdot dx \qquad (4)$$

After replacing the benzene concentration as a function of time, the mass balance differential equation for the model reactor results in the form:

$$c^0_{C_6H_6} \cdot \frac{dX_{C_6H_6}}{d\tau_c} = \left(-r_{C_6H_6}\right)_{ef} \qquad (5)$$

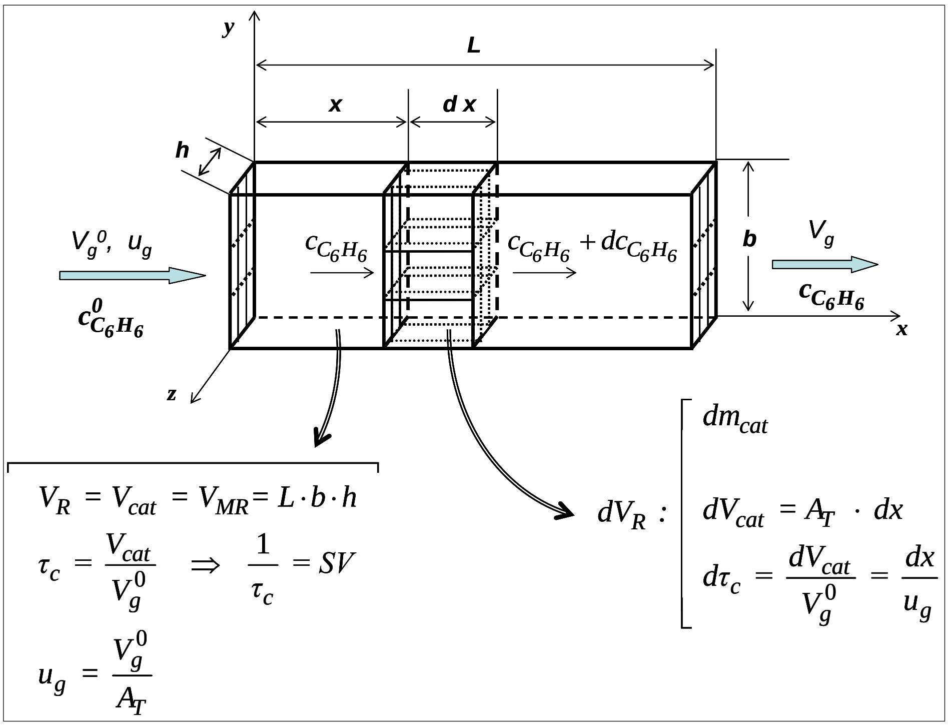

Figure 2. Schematic of the 1-D catalytic reactor model:
V_R – monolith reactor volume; V_{cat} – monolith catalyst volume; V_{MR} – the volume of the reaction mass; m_{cat} – mass of monolithic catalyst; dV_R – volume element; dx – the size of the volume element at distance x; A_T – cross-sectional area of the monolith catalyst; L, b, h – geometric dimensions of the monolith; V_g^0, V_g – initial flow gas and final flow gas, respectively; u_g – linear velocity; SV – space velocity; τ_c – contact time

3.2. Prediction of the overall catalytic process

The experimental studies of the catalytic oxidation of benzene by the V_2O_5-WO_3/TiO_2 monolithic catalyst have shown that: (1) for low concentrations in the influent gas (< 150 ppm C_6H_6), the relative conversion of benzene is not influenced by concentration, (2) but increases with temperature and (3) is influenced by the presence of water vapour.

The kinetic studies of the catalytic oxidation of benzene (experimental conditions: 75 ppm C_6H_6 in initial gas phase, 5 %vol. H_2O, gas area velocity between 5 and 24 m/h) have shown that the conversion of benzene increases with increasing contact time between the gas phase and the catalyst. The effects of inter- and intra-phase mass transfer limitations were lumped into an effective pseudo first-order rate constant, k_{ef} in equation (6), which is specific for each catalyst:

$$c^{0}_{C_6H_6}\frac{dX_{C_6H_6}}{d\tau_c}=k_{ef}\cdot c^{0}_{C_6H_6}\left(1-X_{C_6H_6}\right) \qquad (6)$$

The kinetic equations have been obtained previously and are presented in early papers [37, 38]. Based on the formal kinetics it was shown that the benzene oxidation reaction on the V_2O_5-WO_3/TiO_2 monolithic catalyst in a humid gas stream at a space velocity equal to 6388 h^{-1} is a first order reaction expressed by relations:

$$\begin{cases}\left(-r_{C_6H_6}\right)_{ef}=-\dfrac{dn_{C_6H_6}}{V_R\cdot d\tau}=k_{ef}\cdot c^{0}_{C_6H_6}\cdot e^{\left(-k_{ef}\cdot\tau_c\right)},\ \text{mol/m}^3\cdot\text{s}\\ \left(\text{k}_{ef}\right)_{exp}=5.577\cdot10^{2}\cdot e^{\left(-3399.09\cdot T^{-1}\right)},\ \text{s}^{-1}\end{cases} \qquad (7)$$

3.3. Validation of the proposed model for the monolithic reactor

The equation of the reactor (eq. 5) and the process rate (eq. 6) were used for calculating of the kinetic curve. Considering the ideal flow of the reaction mass characterized by a smooth profile of the rate, temperature and concentration in every cross section of the reactor and neglecting the volume variation, the mathematic model for the experimental reactor is described by four equations (Table 1).

Table 1. Mathematic model for the catalytic reactor

No.	Mathematic equation
I.	Mass balance differential equation $c^{0}_{C_6H_6}\dfrac{dX_{C_6H_6}}{dx}=\left(-r_{C_6H_6}\right)_{ef}=F\left(X_{C_6H_6},\ T\right)$
II.	Catalytic process equation rate $\left(-r_{C_6H_6}\right)_{ef}=\left(k_{ef}\right)_{exp}\cdot c^{0}_{C_6H_6}\left(1-X_{C_6H_6}\right)$, kmol /m^3·s
II.	Effective rate constant, experimentally established $\left(k_{ef}\right)_{exp}=5.578\cdot10^{2}\cdot e^{\left(-33.99\cdot10^{2}\cdot T^{-1}\right)}$, s^{-1}
IV.	Mass balance equation for benzene $c_{C_6H_6}=c^{0}_{C_6H_6}\left(1-X_{C_6H_6}\right)$

The mathematical model of the catalytic reactor was solved by the fourth order Runge-Kutta method, [36, 39, 40] with a constant step of the grating, and the experimental conditions (250 ^{0}C and an influent gas system containing: 75 ppm = 0.003345 mol/Nm^3 C_6H_6 and 5 %vol. H_2O in air). Calculations have been done using the Excel and Math Lab program. The resulting *conversion – contact time* kinetic curve is presented in Figure 3.

A good correlation between the experimental kinetic curve and the one calculated on the basis of the proposed model was obtained. The rate of the benzene oxidation on the SCR-DeNOx (0.53 %wt. V_2O_5) catalyst was correctly chosen (for ensuring the process occurrence in concordance with the transfer through pores- transformation combined model, while kinetic parameters were correctly determined).

Extrapolation of the reaction rate of the catalytic process to the temperature range of 150 – 400 ^{0}C leads to the data given in Figure 4. From the kinetic curves it can be concluded that in order to achieve benzene conversions higher than 90 % for process temperature in the range 300 – 350 ^{0}C a contact time of 1 – 2 seconds should be ensured. When the temperature is decreasing, a given benzene conversion involves a higher contact time. At a given gas flow rate, achieving a high contact time implies the need for an increased catalyst volume.

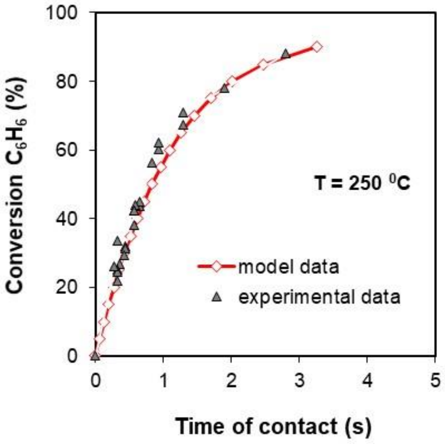

Figure 3. Validation of the benzene oxidation rate in humid air (75 ppm C_6H_6, 5 %vol. H_2O) on a SCR-DeNOx (0.53 %wt. V_2O_5) catalyst at T = 250 ^{0}C

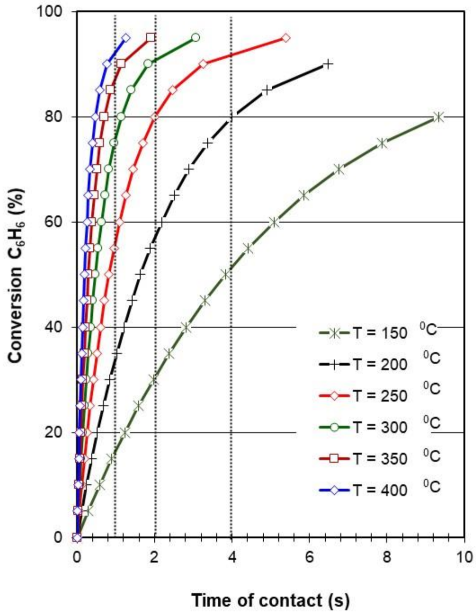

Figure 4. Kinetic curves for temperatures between 150 – 400 ^{0}C calculated using the catalytic reactor model for the benzene oxidation process in a humid air stream (5 %vol. H_2O)

Expressing the rate equation and using the Runge-Kutta method allows the plotting of a diagram describing the dependence between the catalyst volume, contact time and benzene conversion as a function of the gas flow volume (Figure 5).

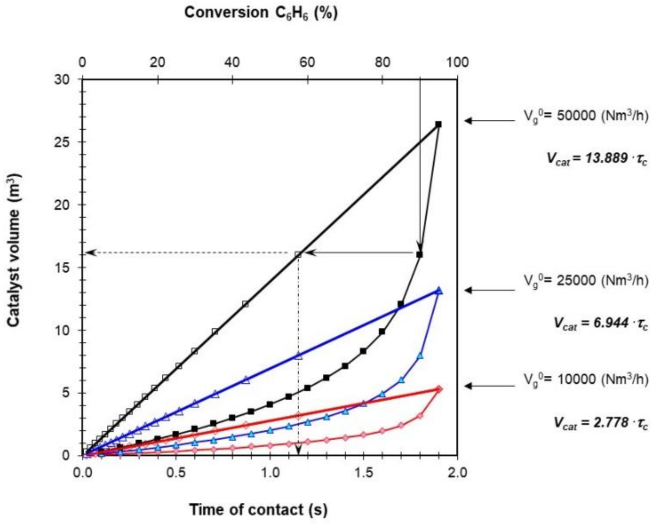

Figure 5. Prediction of the volume of a SCR-DeNOx (0.53 %wt. V_2O_5) catalyst needed for benzene oxidation in humid air stream (5 %vol. and 350 °C)

This diagram of Figure 5 may be used for assessing at a given temperature the catalyst volume necessary for achieving a desired conversion of VOCs in a given flue gas flow rate. Considering that initial benzene concentration up to 150 ppm showed no influence on the conversion [20, 21, 37], the diagram may be used for benzene concentration in influent gas in the range 0 – 150 ppm C_6H_6.

4. Conclusions

Monolithic catalysts are widely used in mobile and stationary emission control reactors for the selective catalytic reduction of nitrogen oxides and the removal of volatile organic pollutants.

This paper reports the results of experimental and modelling investigations of the oxidation of the VOC benzene by commercial V_2O_5-WO_3/TiO_2 (0.53 % V_2O_5) honeycomb catalysts, as used for SCR-DeNOx processes in high-dust flue gases from stationary incineration processes. A 1-D heterogeneous model of the monolith reactor was developed to predict the axial concentration profiles in the monolithic channels of the reactor. The 1-D model can be used for the evaluation of experimental kinetic parameter studies and for the qualification of the effects of some design variables on the performance of the reactor. The mathematic model of the catalytic reactor involves the use of mass balance differential equation under isothermal conditions.

The good agreement between experimental results and 1-D model predictions indicates that the proposed model could be used for more detailed considerations of physical-chemical processes in the monolithic reactor.

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