

## Heat losses in monolithic reactors for VOC abatement

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### Highlights

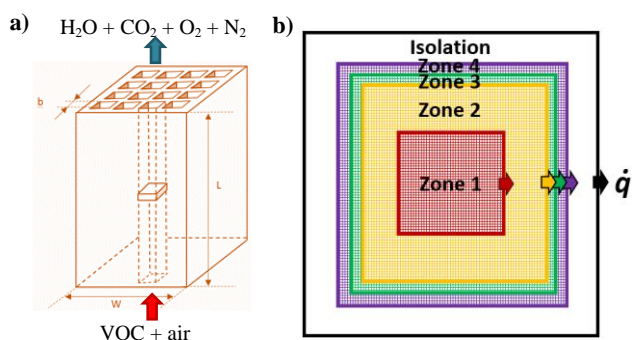
- Thermal effects associated to heat losses in monoliths are discussed.
- Higher energetic requirements to reach the minimum inlet temperatures are necessary.
- Heat losses lead to incomplete VOC abatement despite an appropriate insulation is provided.
- Higher conversion differences between zones for small scale reactors are registered.

### 1. Introduction

The success of monoliths as converters of engine emissions has encouraged researchers to carry out other gas phase reactions using monolithic reactors [1]. Catalytic oxidation in monoliths for VOC (Volatile Organic Compounds) abatement is an example. A typical end-pipe VOC emission is characterized by a very low concentration of organic species (in the range of 50–2000 ppm) and large gas flow-rates (1700–17000 m<sup>3</sup>/h) [2]. In the case of high feed concentrations of VOC, the heat released by the combustion reaction favors VOC abatement. If feed concentrations are low, then auxiliary fuel requirements for preheating may be substantial, increasing the operating costs. In addition, heat losses contribute to decrease reactor efficiency and extra feed preheating is needed. In this contribution a theoretical study of the thermal effects due to heat losses in monolithic reactors of different scales for the catalytic combustion of VOC is performed. The influence of heat losses on the efficiency of the process is analyzed.

### 2. Methods

A *Multiple Channel Model* is used to describe the reactor performance under steady-state conditions. As shown in Figure 1, the monolith is represented as concentric square-rings zones, every zone containing a set of squared channels. For each reactor zone, a heterogeneous, 1D, non-isothermal model is proposed. Internal and external mass-transfer limitations and external (gas-solid) limitations to heat transfer are taken into account. Heat transfer by conduction through the solid (cordierite) is considered along the radial coordinate of the monolith, i.e., from the central zones to peripheral zones at lower temperatures, due to heat dissipation to the environment. The reactor feed consists in a stream of ethanol diluted in air.



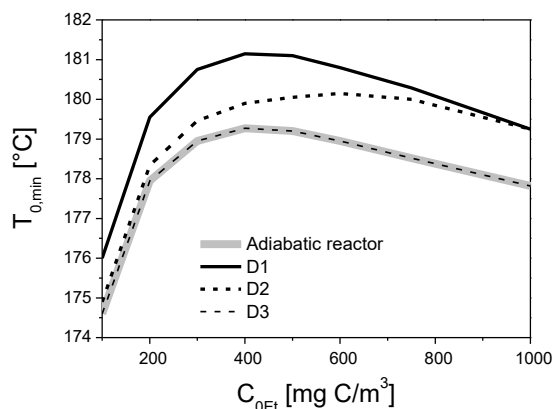
**Figure 1.** a) Schematic representation of the monolithic reactor. b) View of the cross-section of the concentric discretization of the reactor covered with an insulation.

Channels of square section are impregnated with a Mn-Cu mixed oxide catalyst. The assumed reaction system includes the partial oxidation of ethanol to acetaldehyde (reaction 1) and the total oxidation of acetaldehyde (reaction 2) [3].

Three different reactor scales are considered, which are determined by the total number of channels ( $NC$ ). The following designs were selected:  $NC = 2500$  ( $D1$ ), 13924 ( $D2$ ) and 102400 ( $D3$ ) channels. The total cross-sectional area for each reactor design yields:  $A_{D1} = 48 \text{ cm}^2$  (6.9 cm x 6.9 cm),  $A_{D2} = 262 \text{ cm}^2$  (16.2 cm x 16.2 cm) and  $A_{D3} = 1936 \text{ cm}^2$  (44 cm x 44 cm), respectively. For the three scales analyzed

the four zones in which the cross-section of the monolith is subdivided contain the following percentages of the total number of channels: zone 1 = 40%, zone 2 = 40%, zone 3 = 10% and zone 4 = 10% (see Fig. 1.b).

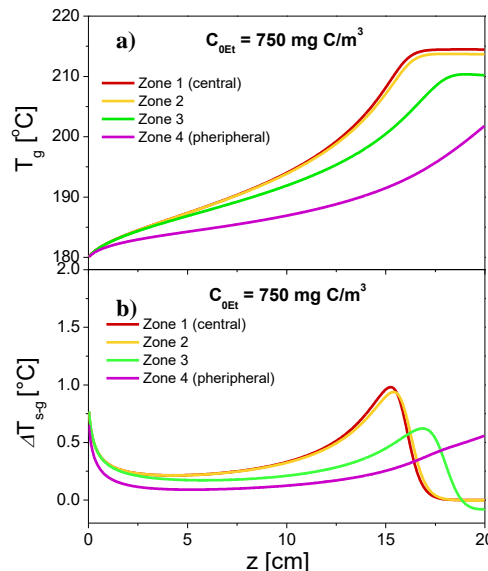
### 3. Results and discussion



**Figure 2.**  $T_{0,min}$  for different  $C_{0Et}$  for a perfect adiabatic reactor and three designs ( $D1$ ,  $D2$  and  $D3$ ) of non-adiabatic reactors.

Figure 2 shows the minimum inlet temperatures which are required to ensure the environmental specifications ( $20 \text{ mg C/m}^3$ ) for different inlet ethanol concentrations and the same space velocity ( $GHSV = 2.42 \times 10^5 \text{ h}^{-1}$ ) and design parameters ( $b = 1.115 \text{ mm}$  (width),  $\delta_w = 20 \text{ }\mu\text{m}$  (washcoat thickness),  $L = 20 \text{ cm}$ ) [4]. Four different designs are considered: a perfectly isolated reactor and three non-adiabatic monoliths ( $D1$ ,  $D2$  and  $D3$ ). To make the insulation conditions comparable, an insulation thickness for each design was chosen so that the same average tube skin temperature ( $T_{TS,av} = 31 \text{ }^\circ\text{C}$ ) was obtained. The external area/volume ratios are: ( $A_{ext}/V_R$ ) =  $133.76 \text{ m}^2/\text{m}^3$  ( $D1$ ),  $41.39 \text{ m}^2/\text{m}^3$  ( $D2$ ) and  $13.66 \text{ m}^2/\text{m}^3$  ( $D3$ ). As the reactor scale is diminished, it the feed temperatures have to be raised above those of the adiabatic case, to satisfy the

emission limit value. This fact is a direct consequence of the heat losses, leading to an increase in the preheating costs. Figure 3.a shows axial temperature profiles in each of the four transverse discretization zones of the monolith (see Fig.1b), for design  $D2$ . Although thermal insulation is efficient, the peripheral channels operate several degrees colder than the channels in the central zones. The heat loss to the environment has a greater impact for the smaller reactors, where the external area / volume ratio of the reactor is higher. Figure 3.b shows the corresponding temperature differences between the solid and gaseous phase,  $\Delta T_{s-g}$ . The maximum in the curves of  $\Delta T_{s-g}$  correspond to axial positions where the rate of heat generation is maximum (associated with the strong consumption of acetaldehyde, results not shown). As the peripheral zones are colder due to heat dissipation, the effective reaction rates decrease, and thus the heat generation and the interfacial temperature differences. The lower values of  $\Delta T_{s-g}$  further contribute to the reaction extinction in the peripheral zone, as the temperature of the solid phase decreases. In addition, in zones 3 and 4 the axial position of the maximum temperature drop in the external film is shifted towards the reactor outlet.



**Figure 3.a)** Axial temperature profiles, and **b)** temperature drop over the external film in each zone for  $D2$ ,  $C_{0Et} = 750 \text{ mg C/m}^3$ ,  $T_0 = 180 \text{ }^\circ\text{C}$ ,  $GHSV = 2.42 \times 10^5 \text{ h}^{-1}$ , with design parameters  $b = 1.115 \text{ mm}$ ,  $\delta_w = 20 \text{ }\mu\text{m}$  and  $L = 20 \text{ cm}$ .

### 4. Conclusions

As the reactor scale decreases and the external area/volume ratio increases, the effect of heat losses on VOC emissions is magnified and the monolith exhibits non-uniform behavior between channels, leading to an incomplete VOC abatement, mostly at the outlet of peripherals channels. The inlet temperature set point should be high enough to prevent high VOC emissions due to lower inlet VOC concentration in a heat loss scenario. This undoubtedly results in higher energetic requirements to ensure VOC complete conversion.

### References

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### Keywords

VOC catalytic combustion; monolith; multiple channel model; thermal effects