ABSTRACTS

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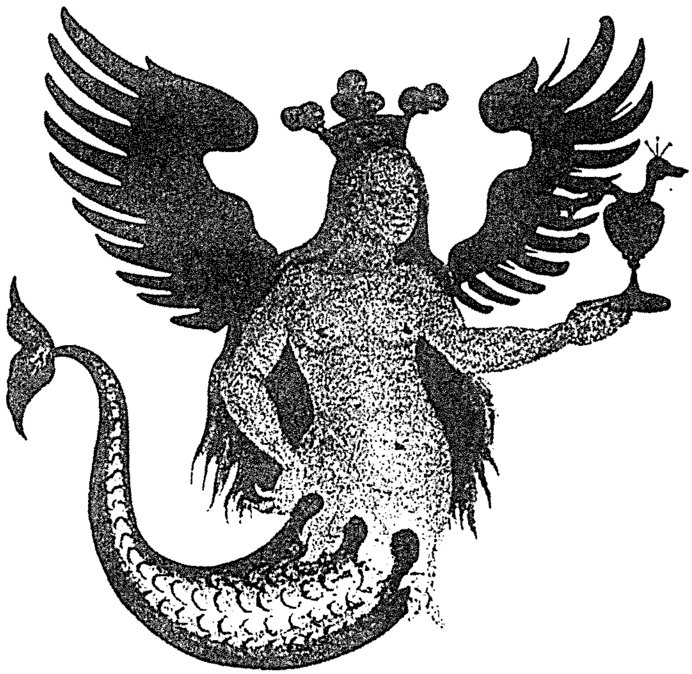

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PARAMETRIC ANALYSIS OF A MONOLITHIC CATALYTIC COMBUSTOR

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Introduction

Catalytic afterburners are nowadays a mature and available technology for pollution control and recently there is a renewed interest due to their energetic efficiency. The use of monolithic catalyst is particularly advantageous because they offer large geometric surfaces per unit volume and allow very low pressure drops. Therefore, the availability of simple and reliable models would be particularly useful for design purposes, and would contribute to the diffusion of this type of devices.

The aim of this work is the parametric analysis of the behaviour of a catalytic combustor for the abatement of low concentrations of organic pollutants in waste gases and particularly the investigation of the hysteresis phenomena. Previous works of other authors have shown that multiple steady states may occur, and hysteresis phenomena may be relevant and of practical interest in industrial or automotive applications [1].

Some preliminary results will be presented as the work is currently ongoing.

The model

A monodimensional model has been initially adopted for the combustor, with plug flow in the gas phase and heat transfer by conduction in the monolith. This representation is very simplified, but allows a sufficiently accurate prediction of the steady state behaviour of the system without making the parametric analysis too onerous. A bidimensional model will be developed as the next step, to obtain more accurate quantitative predictions [2] and to test the reliability of the monodimensional model.

The geometric characteristics of the monolith are reported in table 1. The system is the same investigated in previous modeling and experimental works [3, 4]. A superficial reaction has been assumed and the benzene oxidation reaction [5] adopted in this first stage, in order to make a comparison between experimental and predicted results possible. Other more general kinetic expressions will be considered in the proceeding of the work in order to have a wider parameter range.

Heat and mass transfer between the gas bulk and the catalyst surface has been modeled using the transfer coefficients proposed by Votruba *et al.* [6].

The differential equations have been numerically solved by a finite difference method, employing the second order centered difference formula.

In order to plot the conversion vs inlet gas temperature graphs, a continuation algorithm with automatic step control was implemented. This method uses each found solution as an approximation for the next one. Its most peculiar characteristic is the possibility to choose automatically at each iteration the variable that has to be incremented. This is particularly useful in our case because it is not possible to use exclusively the inlet temperature as the integration variable; in fact, in correspondence of the point where the conversion curves show a vertical tangent, the solution would be lost. An exhaustive description of the method is given by Seydel [7].

Results

The main variable considered is the inlet temperature of the gas in the combustor, that operatively is also the variable that in the system can be easily manipulated acting on the preheater. The influence of the inlet gas velocity and of the hydrocarbon concentration has been investigated, too.

Figures 1-3 show the steady state response of the reactor at different gas velocities and benzene concentrations. The outlet conversion (z) as a function of inlet gas temperature is plotted.

As expected higher conversions are obtained at lower gas velocities (higher residence times) and lower concentrations: this is a consequence of the zeroth-order oxidation kinetics, because in the range of temperature tested the reaction is not completely mass-transfer controlled.

Significant hysteresis effects can be observed, especially at low gas velocity and relatively high concentration.

Conclusions

Preliminary results on the parametric investigation of the behaviour of a monolithic catalytic combustor are presented. Significant hysteresis effects have been predicted; these results may be interesting for the design of afterburners operating at very low feed temperatures.

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References

[1] Barresi A., Mazzarino I. and Ruggeri B., 1989, Incenerimento catalitico di effluenti gassosi. *Chim. Ind. (Milan)* 71, 64-75.

[2] Finlayson B.A. and Young L.C., 1979, Mathematical models of the monolithic catalytic converter - Part III. Hysteresis in carbon monoxide reactor. *A.I.Ch.E. J.* **25**, 192-196.

[3] Barresi A.A., Mazzarino I., Vanni M. and Baldi G., 1993, Catalytic afterburners with not fully developed flow: modeling and experimental performances. *Chem. Eng. J.*, in press.

[4] Barresi A., 1990, Ossidazione catalitica di composti organici volatili presenti nelle emissioni gassose. Ph.D. Dissertation, Politecnico di Torino.

[5] Barresi A.A. and Baldi G., 1992, Deep catalytic oxidation kinetics of benzene-ethenylbenzene mixtures. *Chem. Eng. Sci.* **47**, 1943-1953.

[6] Votruba J., Mikuš O., Nguen K., Hlaváček V. and Skřivánek J., 1975, Heat and mass transfer in honeycomb catalysts - II. *Chem. Eng. Sci.* **30**, 201-206.

[7] Seydel R., 1988, *From equilibrium to chaos*. Elsevier, New York.

Table 1. Catalyst features

Monolith diameter	22 mm
Monolith length	12.4 mm
Monolith mass	2.42 g
Cell geometry	square
Cell size	1.5 mm
Wall thickness	0.3 mm
Open area	69%
Geometric surface/volume	1850 m^2/m^3

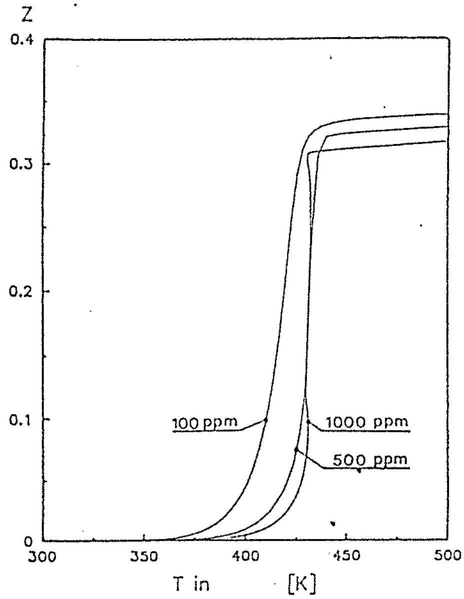

Figure 1. Outlet conversion vs inlet gas temperature. Hot flow inlet gas velocity=1 m/s.

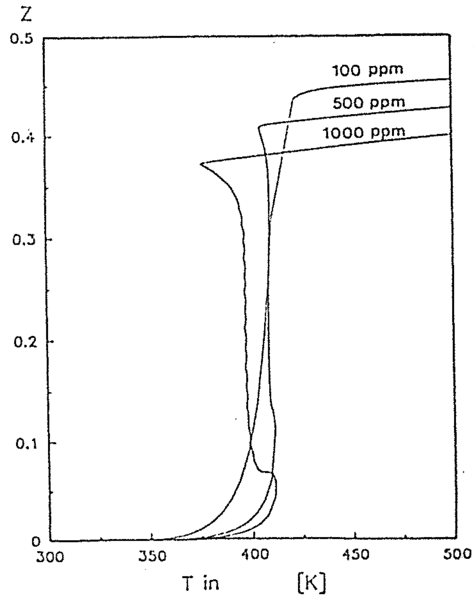

Figure 2. Outlet conversion vs inlet gas temperature. Hot flow inlet gas velocity=0.5 m/s.

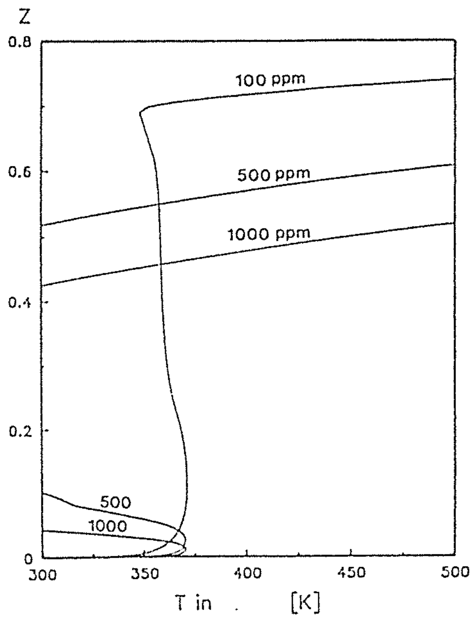

Figure 3. Outlet conversion vs inlet gas temperature. Hot flow inlet gas velocity=0.1 m/s.