OPEN CELLULAR STRUCTURES FOR EXHAUST AFTERTREATMENT INTENSIFICATION

Tommaso Selleri, Matteo Ambrosetti, Mauro Bracconi, Gianpiero Groppi,
Isabella Nova, Enrico Tronconi*
Energy Department, Politecnico di Milano
Via La Masa 34, 20156, Milano (Italy)

Abstract

We present herein a numerical investigation of the potential of open cellular structures for intensification of the NH_3-SCR process, that is crucial for NOx control from lean burn engines. In the work, we develop a new modeling tool based on state of the art correlations for open cellular structures fundamental properties and use it as a basis for a preliminary computational assessment of the performances of these new catalytic supports and to select interesting configurations for dedicated experimental testing.

Keywords

NH_3-SCR, open-cell foams, POCS, process intensification, exhaust gas aftertreatment.

Introduction

NH_3-SCR is the leading technology for NOx abatement from lean burn and Diesel engines and is traditionally run in converters loaded with washcoated honeycomb monoliths. However, a paradigm shift is now required to tackle the progressively more stringent limits imposed by new emission regulations worldwide. Previous works in the literature have shown that open cellular structures are characterized by an enhanced fluid-solid mass and heat transport (Giani et al., 2005). These properties are of clear interest in aftertreatment applications since they might enable a faster dynamic response e.g. in rapid heat-up transients and an increased conversion. Moreover, it may be possible to reduce the weight of the aftertreatment unit, due to the structure high void fraction, and greatly increase the flexibility in design and flow configuration.

In this work, we provide a preliminary analysis of the potential of open random or regular cellular microstructures, like open-cell foams or periodic open cellular structures (POCS) as innovative catalyst supports to enhance the exhaust aftertreatment systems performances. In particular, a new modeling tool, based on state of the art correlations is developed and used to: i) gain insight in the general behavior of such innovative systems; ii) select interesting structures for experimental testing; iii) develop new ideas for system configuration.

Numerical tools

We have developed a transient 1D+1D heterogeneous model, embedded with a complete SCR kinetic scheme and with recently developed and already extensively validated correlations for heat and mass transfer as well as pressure drops (Bracconi et al., 2018). Open cellular structures geometry and morphological properties have been described with a state of the art analytical model (Ambrosetti, 2017). The resulting tool has been used to simulate both steady state and fast transient SCR operation of foam and POCS catalysts, as shown with some examples in the next section.

Results

Figure 1 compares a reference monolith substrate with 400 CPSI and a wall thickness of 5 mils to foams with 60 PPI and different void fractions (0.83-0.96) in steady-state Standard SCR tests. All samples are loaded with the same amount of catalyst and are tested at the same space velocity. Overall, it is evident how, on increasing the void fraction

* To whom all correspondence should be addressed

and adopting a sufficiently high PPI, foams can grant a relevant increase in the NO overall conversion at medium-high temperatures, due to a significant reduction in external mass transfer resistances. Unfortunately, this improvement in DeNOx performances corresponds to a notable increase in pressure drops, as also shown in Figure 1, which is related to the typical flow pattern inside these structures.

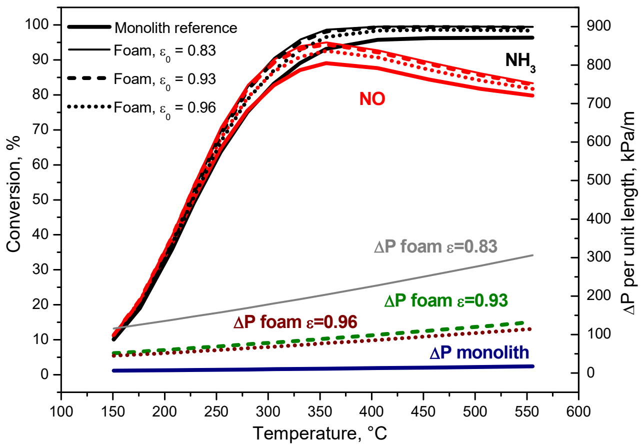

Figure 1. Std. SCR steady state simulation. Feed: $NO=NH_3=500$ ppm, $O_2 = H_2O = 10$ % v/v, GHSV = 175260 h^{-1}. ε effect @ 60 PPI

Figure 2 shows a simulation where the beneficial effect on the heat-up dynamics of the SCR converter when an open-cell foam is used as catalyst support is evident. In this example, the catalyst is firstly exposed to 500 ppm of NO and NH_3 at 100 °C (not shown) and then the temperature is rapidly increased from 100 °C to 300 °C (100 °C/min) in NO and NH_3 flow. Due to the lower overall thermal mass and the enhanced volumetric heat transfer coefficient of the support, the foam substrate can better follow the imposed heating ramp (dashed lines in figure), leading to a faster onset of the SCR reactions, so important in cold-start transient but also in rapid changes of operating conditions, and to achieve better performances in terms of conversions.

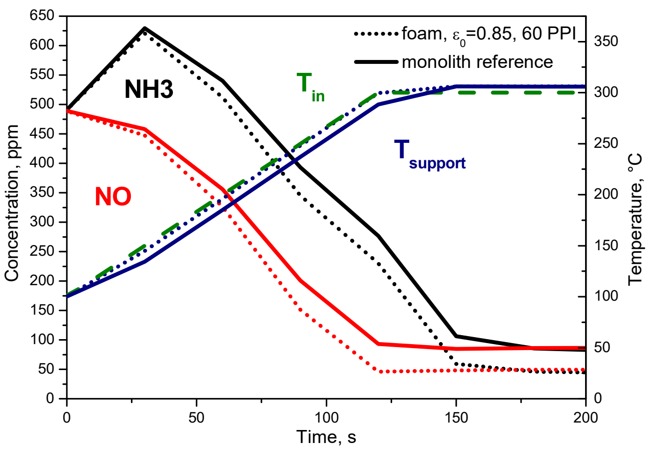

Figure 2. Transient Std. SCR simulation. Feed: $NO=NH_3=500$ ppm, $O_2 = H_2O = 10$ % v/v, GHSV = 175260 h^{-1}.

Based on these simulations, cordierite foams with different ranges of ε (0.8-0.9) and PPI (20-60), are currently under testing in a dedicated gas rig. Using the same approach, it is possible to study also regular structures (POCS) which are indeed under investigation both numerically and experimentally. In general, both simulations and experiments emphasize the trade-off between improvement in NOx conversion, due to increased mass/heat transfer, and higher pressure drops across the converter. In addition, volume constraints are relevant in mobile aftertreatment applications. Thus, to better exploit the improved mass transfer of cellular substrates without significant penalties on pressure drops, a radial flow configuration, impossible for conventional honeycombs, has been also investigated. In this new scheme, the flow enters from a central hole and is forced to go through the catalyst substrate in radial direction and is collected at the external surface of the catalyst, or vice versa. In principle, this approach can enable an increased overall flow area, minimizing at the same time the gas path length through the foam structure. This leads to an improvement in the overall conversion with a significant reduction of pressure drops (to values in line or even lower with respect to honeycombs).

Notably, preliminary results show that the adoption of regular open-cell substrates (POCS), combined with different flow configurations (e.g. radial flow), can provide additional degrees of freedom, to be exploited for EAT system design and optimization, and might result in more flexible, compact and lightweight converters.

Conclusions

In this preliminary work, we show that open-cellular structures are promising substrates for a new generation of aftertreatment devices owing to their superior mass and heat transfer properties as well as their unique geometrical features. We develop a numerical tool to investigate system geometry and optimal conversion and pressure drops performances in NH_3-SCR converters. Simulation results suggest that the possibility of adopting highly void supports with reduced thermal mass, as well as the flexibility in flow configurations, are unique features of cellular substrates, which could provide significant benefits over the traditional honeycomb technology and help lean burn engines aftertreatment devices to overcome the emission regulation challenges.

Acknowledgments

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References

Giani, L., Groppi, G., Tronconi, E. (2005). *Ind. Eng. Chem. Res.*, *44*, 4993.

Bracconi, M., Ambrosetti, M., Maestri, M., Groppi, G., Tronconi, E. (2018). *Chem. Eng. J.*, *352*, 558.

Ambrosetti, M., Bracconi, M., Groppi, G., Tronconi, E. (2017). *Chem. Ing. Tech.*, *89*, 7.