Open cellular structures for NH_3-SCR intensification

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Introduction

NH_3-SCR is the leading technology for NOx abatement from lean burn and Diesel engines and is traditionally operated in catalytic converters made of 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 may significantly contribute to enhance the fluid-solid mass and heat transport [1] in catalytic processes.

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 substrates to improve the exhaust aftertreatment performances. 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 configurations.

Materials and Methods

A transient 1D+1D heterogeneous model of SCR converters, 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 [2], is herein developed. Open cellular structures geometry and morphological properties are described by a state-of-the-art analytical model [3]. The resulting tool is 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 and Discussion

Simulations in Figure 1A compare a reference monolith substrate with 400 CPSI and a 5 mils wall thickness to foams with 60 PPI and different void fractions (0.83-0.96) in steady-state Standard SCR runs. 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 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, which is related to the flow pattern inside these structures.
Figure 2 shows the beneficial effect on the heat-up dynamics of the SCR converter when an open-cell foam is used as catalyst support. 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 its lower thermal mass and enhanced volumetric heat transfer coefficient, the foam substrate can better follow the imposed heating ramp (dashed lines), leading to a faster onset of the SCR reactions, so important in cold-start transients but also during rapid changes of operating conditions, eventually achieving better performances in terms of overall deNOx efficiency.

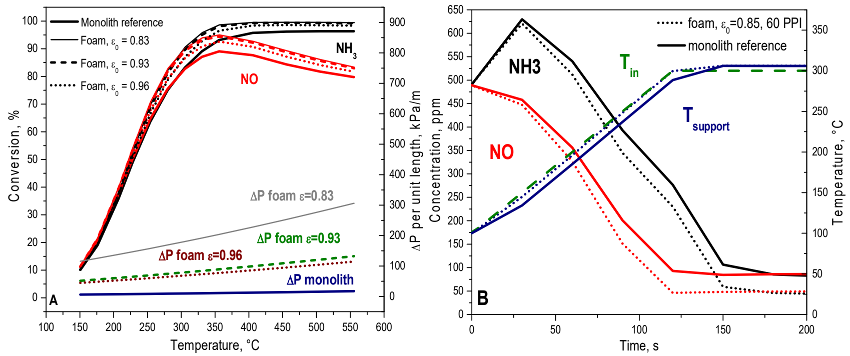

Figure 1. Std. SCR simulation. Feed: NO=NH_3=500 ppm, O_2 = H_2O = 10 % v/v, GHSV = 175000 h^{-1}. A) Steady-state conversion and pressure drops; B) Transient heat-up (100 °C/min)

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 synthetic gas rig.
Using the same approach, we are investigating both numerically and experimentally also regular cellular structures (POCS). Preliminary results show that the adoption of regular open-cell substrates (POCS), combined with different flow configurations impossible in conventional monoliths, 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.

Significance

We show that open-cellular structures are promising substrates for a new generation of SCR aftertreatment devices owing to their superior mass and heat transfer properties, as well as to their unique geometrical features. A new modeling tool based on state of the art correlations for the transport properties of open cellular structures has been developed and used for the preliminary computational assessment of the potential of these new catalytic supports and to select interesting configurations for dedicated experimental testing.

Acknowledgments

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