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Comparison of geometrical, momentum and mass transfer characteristics of real foams to Kelvin cell lattices for catalyst applications

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ABSTRACT

Open cell foams are considered promising catalytic substrates providing high surface area and a tortuous structure resulting in enhanced mass transfer characteristics. CFD analysis, recently, has focused in pointing structures with favourable reactivity-flow resistance characteristics. In order to reduce the geometrical complexity and computational efforts, foams have been modelled as regular (polyhedric) open cell structures. In this study a comprehensive comparison of real foams with equivalent Kelvin cell lattices is performed in CFD. Therefore 4 typical foams (two ceramic and two metallic) have been chosen. Geometric properties have been accessed with Micro-Tomography scans. Randomised Kelvin cell lattices have been generated matching porosity and specific surface area of the scanned real foams. Geometric, momentum and mass transfer characteristics of real foams and Kelvin cell lattices are analysed with CFD. Kelvin cell lattices showed similar behaviour in respect to their real foam equivalents, had though clearly better reactivity-pressure drop trade-offs. Based on the results presented best performances as a catalyst can be expected by 3D printed, additive manufactured, high porosity polyhedric structures.

1. Introduction

Catalyst technologies for exhaust aftertreatment for internal combustion engine applications have succeeded in reducing emissions dramatically. Cold start and low temperature emissions are though still a major concern. Catalytic acceleration of chemical reactions in the exhaust gases occurs on finely dispersed noble metal particles (Pt, Pd and Rh), which constitute a significant cost factor. The most common substrates for modern automotive catalysts are honeycomb structures. The exhaust flow in the channels is laminar with low heat and mass transfer characteristics. For compensation, modern catalysts have far too large dimensions.

Compared to conventional honeycombs, open cell structures (foams) reach the same conversion rate but with reactors 2.5–3 times smaller [1]. Tortuous flow paths through porous structures achieve a higher chemical activity per unit of volume [2,3]. In addition open cell structures result in higher flow uniformity which is a key factor for the pollutant conversion efficiency and for the catalyst durability [4–8]. The higher porosity and lower thermal inertia of foams are beneficial during light off [9], helping to reduce cold start emissions of vehicles. Open cell foam structures allow also more flexibility in the geometrical configuration of the reactor, since they do not restrict the lateral flow [10].

The increased mass and momentum transfer properties of foams compared to standard honeycombs result in higher conversion efficiencies but also in a higher pressure drop per unit of length [11,12], which, especially in the automotive field, is a crucial aspect, since it affects the global engine efficiency. Thus, to properly evaluate the reactor performance, pollutant conversion needs to be weighted by the pressure drop [2]. Experimental analysis by Giani et al. [2] and Patcas et al. [13] reported that the conversion to pressure drop trade off is higher on honeycombs compared to foams. Similar conclusion can be reached by comparing pressure drop correlations present in literature [14]. However CFD analysis by Lucci et al. [15,16] suggested that the trade off is on favour of foams when their porosity is high enough.

Computational analysis has been proved useful to study flow resistance and heat transfer in open cell structures [17–26]. Despite these efforts to characterize foam transfer properties, there

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Nomenclature

η	conversion efficiency $\eta = \frac{C_{in}-C_{out}}{C_{in}}$ [−]
v	kinematic viscosity [m^2/s]
σ_x	standard deviation of quantity x
d_p^{KC}	pore diameter of Kelvin Cell structures before randomization [m]
D_h	hydraulic diameter [mm]
D_p	external pore or cell diameter $D_P = d_p + d_s$ [mm]
d_p	internal pore/cell diameter of randomized KC structures or of foam [mm]
d_w	window diameter of foam or randomized KC structures [mm]
D_{air}	air diffusivity [m^2/s]
Hg	Hagen number $Hg = \frac{\Delta P}{\Delta x} \cdot \frac{D_h^3}{\rho v^2}$ [−]
K	mass transfer coefficient $K = -\frac{ln(1-\eta)}{S_v L_R/U}$ [m/s]
KC	Kelvin cell
L_R	reactor length [mm]
$L_{x,y,z}$	domain dimensions [mm]
PPI	Pores Per Inch
Re	Reynolds number $Re = \frac{D_h u}{\varepsilon v}$ [−]
Sh	Sherwood number $Sh = KD_P/D_{air}$ [−]
U	inflow velocity [m/s]
Y_i	mass fraction of specie i [−]
ε	porosity [−]
S_v	specific surface area [m^2/m^3]
CT	X-ray computer tomography

is no agreement for correlations that reliably predict foam performance [27], in agreement with experimental data. Edouard et al. [27] reported that no pressure drop correlation resulted consistently in good results and that standard deviations of experimental values can be as high as 100%. More recently, Dietrich [28] proposed a pressure drop correlation in non dimensional form predicting most of data reported in literature within an error range of ±40%. A similar uncertainty is shown in a number of studies dealing with heat and mass transfer [29–32]. Main reasons for the ambiguities in characterizing foams are their wide range of pore sizes, different connectivities and strongly varying ligament lengths.

In literature, foams are frequently modelled as regular cell structures. These models are used for theoretical analysis [33–35], or to derive properties which are difficult to extract experimentally, like the specific surface area (S_v) [2,36,37].

Current computing capabilities allow performing computational analysis of real CT foam scans [38,23,25,39]. Alternatively, foams can also be accurately reconstructed with elaborate algorithms based on Voronoi tessellations [40,41]. However, regularly structured geometries are easier to handle [17,42,43,21,44,45,26]. Automatic procedures can be implemented to quickly generate regular structures with prescribed properties. Moreover the geometrical scalability and the reduced complexity of regular structures allow more systematic analysis. In fact, while real foam structures are typically characterized by three parameters (porosity, pore diameter and specific surface), only two parameters are necessary for the regular structures since the specific surface can be obtained by precise correlations from the cell dimension and the porosity. Frequently used geometries for cell modelling are cubic cells [33,46,30,34,35] and tetrakaidecahedrons, also called Kelvin cells (KC) [36,43,37,21,47,16]. The Kelvin cell structure model can be further improved by the Weaire–Phelan structure which uses multiplication of two kinds of cells (pyritohedron and dodecahedron) instead of one (tetrakaidecahedron) as in the case of Kelvin cell structure. The Weaire–Phelan foam model is recognised to be more accurate in terms of foam representation, since it reduces the surface energy of 0.3% compared to the Kelvin cell model and it has a wider variability in windows and pore distributions. However, it has been demonstrated by [48] that differences on pressure drop are small, especially for high porosities.

A flow resistance comparison between Kevin Cell and foams was performed by Habisreuther et al. [43]. The authors calculated the pressure drop from a scan of an 45 PPI allumina foam with a porosity of 0.79. In their case a randomized Kelvin Cell structure with the same properties underestimated the pressure drop compared to the foam scan. Then they show that by closing about 40% of the pores in the Kelvin cell structure similar pressures drops were achieved, they also show that by closing the structure pores they achieve similar tortuosity between the two structures. Iasiello et al. [49] also contains comparisons between real and Kelvin Cell foams in terms of convective heat transfer and pressure drop, but the matching parameter were the pore size and the porosity, leading to pressure drop in the Kelvin structure up to 100% higher than the real foams.

Moreover, recent developments in additive manufacturing techniques have opened the possibility to manufacture real regular structures [50,51] and potentially elevating these structures from being a model to be an actual catalytic support for commercial use. Thus, recently regular structures have also been investigated experimentally [52,44].

In the present work open cell foams are reconstructed with randomised Kelvin cell structures and both flow resistance and mass transfer properties are analysed. At first, the micro-structure of 4 different foam samples is reconstructed by means of micro-CT scans in order to have a reliable characterization of all the geometrical properties, even those (e.g. specific surface, pore diameter) which are usually difficult to assess experimentally. Then, randomized KC structures are modelled by matching the porosity and the specific surface of the foam samples considered. Geometrical properties of the reconstructed KC structures are compared to the original micro-CT foam scans, to evaluate the deviations between the two 3D models. Finally, CFD investigations are performed to compare the momentum and mass transfer performances of the two kind of structures.

2. Method

2.1. Micro-CT foam reconstruction

Micro Computed Tomography has been applied for the reconstruction of the actual geometry of the samples. In a micro-CT scanner a X-ray cone beam passes through the sample and is collected by a detector; the sample is rotated providing a series of 2D projection images at different angles. A 3D voxel dataset is then reconstructed from the stack of 2D images using inverse methods. In the current case a Nikon Metrology Benchtop 160 micro-CT system was used; this uses an electron gun operating at up to 160 keV and a metal target to generate a cone of X-rays through bremsstrahlung; both the electron gun voltage and target metal can be altered to provide a range of spectra and penetration suitable for imaging a range of material compositions from soft biological samples to metal composites, including the foams used here. The sample is mounted in the beam between the target and a flat panel detector, and rotated to provide the 2D projection images. The exact resolution depends on the ratio between the target-sample