

Design of Catalytic Devices by Means of Genetic Algorithm: Comparison between Open-Cell Foam and Honeycomb Type Substrates

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ABSTRACT

Metallic foams or sponges are materials with a cell structure suitable for many industrial applications, such as reformers, heat catalytic converters, etc. The success of these materials is due to the combination of various characteristics such as mechanical strength, low density, high specific surface, good thermal exchange properties, low flow resistance and sound absorption. Different materials and manufacturing processes produce different type of structure and properties for various applications. In this work a genetic algorithm has been developed and applied to support the design of catalytic devices. In particular, two substrates were considered, namely the traditional honeycomb and an alternative open-cell foam type. CFD simulations of pressure losses and literature based correlations for the heat and mass transfer were used to support the genetic algorithm in finding the best compromise between flow resistance and pollutant abatement. The CFD analysis was conducted by means of numerical simulations carried out on a geometry sample obtained by the micro-tomography technique to investigate the flow regime type and to extract pressure drop information. The result of this analysis was used to set guideline for the design of foam type substrate and to provide a first estimation of cost effectiveness of new type of substrates.

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INTRODUCTION

The stochastic approach is nowadays one of the most applied technique for the study of a wide range of complex problems in different fields of application. In particular, the most common approach consists of the application of genetic algorithms (GA) to study the effect of the various parameters governing specific physical phenomena. Several authors successfully applied GA in many ICE fields for supporting the design and the optimization of components [1, 2, 3, 4].

In the present work a Genetic Algorithm (GA) was implemented in order to design a catalytic after-treatment device based on two different types of substrates, namely honeycomb monolith and open-cell foam. The first type represents the most widely adopted substrate for the manufacture of the catalyst. On the other hand, the second type has increasingly gained attention in the last years, since it seems to be a promising alternative for reducing the pressure drop and the loading noble metal compared to the traditional solutions, due to their properties of high porosity, high specific surface and tortuous structure which result in enhanced gaswall interactions [5, 6, 7]. However, in order to fully exploit the advantages of the open-cell foams, a proper design of the device should be found, in terms of both external dimensions (the ratio between length and diameter of

the converter) and geometrical micro-structural properties of the foam (pore density and porosity). The main focus of the analysis is to find guidelines for the design of a foam-based catalyst, highlighting the differences with respect to an optimum solution based on the traditional honeycomb substrate. Moreover, the performances of the two substrates are compared, showing the advantages related to the adoption of an open-cell foam substrate.

The present paper is structured as follow. In a first section, the development of the optimization model based on the genetic algorithm is reported. In particular, the input design parameters and the optimization target quantities are defined, along with the mathematical equations describing their relations. In a second section, micro-CT and CFD techniques are applied for the characterization of the geometrical and permeability properties of the open-cell foam substrate. This analysis was addressed in order to investigate the fluid-dynamic behavior of a foam substrate and to extract all the geometrical and permeability relations required for the application of the GA. Finally, in a third section, the application of the optimization model is described and the results obtained are discussed. In particular, the open-cell foam performances are compared to the ones of the honeycomb struts.

GENETIC ALGORITHM

Different types of genetic algorithms have been developed and applied for several purposes. In this work a multi-objective genetic algorithm named “Non-dominated Sorting Algorithm” (NSGA-II) [8, 9] was chosen due to its low computational cost and to the possibility of easy finding the Pareto optimal solutions. The NSGA-II performs the following three main stages:

- a non-dominated sorting of the population for ranking each element into a specific non-dominated front is performed;
- calculation of the “crowding distance”, i.e. the assessment of the crowding elements of the population;
- by means a further classification based on the crowded comparison operator, it is possible to address the algorithm towards the correct way in order to spread the Pareto optimal front out.

The whole process is repeated in a loop until complete convergence is reached. At every iteration half population is replaced using selection and crossover operators. It must be noted that the mutation operator is not activated because in this contest it is not necessary due to the nature of the implemented models.

From a literature survey, it appears that many authors have coupled directly GA to CFD analysis with proven effectiveness [10, 11, 12, 13]. However, computational cost is significant becoming a limiting factor, therefore stochastic approach is usually preferred. In this paper the authors applied the NSGA-II in order to find the best combination of the input parameters that allow the best trade-off of the output parameters. The input parameters are the intrinsic characteristics of the foams struts and the external geometric dimensions of the catalytic support. The output parameters are the pressure drop, the conversion efficiency and the cost effectiveness. For this purpose the equations available in the open literature were implemented in a proper version of the NSGA-II. These will be described in the following paragraphs for both the foam and the honeycomb substrates.

Foams

A steady state hot condition, with a constant temperature set to 400°C and pressure set to the atmospheric value, was considered. This hypothesis allows expressing all the variables, i.e. the density and the kinematic viscosity of the fluid, as well as the binary diffusion coefficients, as a function of the temperature. The fluid was set to air. The output parameters are the pressure drop, the conversion efficiency and the cost effectiveness. The GA focus was to find the minimum value for the following output parameters, which expressions are hereafter reported. In this work the analysis was restricted to consider only CO emissions, due to the lack of experimental correlations for foam catalytic substrates operating with more pollutant specie. However the approach hereafter described can be easily extended to take into account more pollutant specie and catalytic reactions.

Pressure Drop

The pressure drop was obtained from the general expression that considers both the viscous and the inertial contributions [14, 15]:

$$\Delta p = \left(\frac{\mu}{K} u + \rho C u^2 \right) L \quad (1)$$

where K and C are respectively the permeability and the form coefficient. These two terms are both function of the geometric properties of the foam only, which are the porosity ϵ and the characteristic diameter d_p , computed as the average dimension of the pore. The CFD characterization of the foam allows the determination of the permeability and the form coefficient by means respectively the dimensionless parameters A and B :

$$K = \frac{d_p^2}{A} \quad (2)$$

$$C = \frac{B}{d_p} \quad (3)$$

In the next section, the procedure adopted for evaluating the parameters A and B will be described: these depend only on the porosity and the morphology of the foam [16]. Minimizing the Equation (1) leads to the minimum of the pressure drop.

Conversion Efficiency

The conversion efficiency was evaluated modeling the mass transfer of the pollutants from the highest concentration to the washcoat surface during the crossing time of the catalyst. Giani et al. [17] proposed a relation for evaluating the mass transfer coefficient starting from the conversion efficiency in CO (η) measured in the experimental tests:

$$k_m = -\frac{\ln(1-\eta)}{S_V V_0 / Q} \quad (4)$$

where V_0 is the catalytic volume and Q the volumetric flow rate. The specific surface S_V was also expressed by the cubic cell model of the foam structure:

$$S_V = \frac{2}{d_p} \sqrt{3\pi(1-\epsilon)} \quad (5)$$

This model is very simple but rather inaccurate: the specific surface evaluated by the Equation (5) overestimates the real one computed for the actual samples. Hence the specific surface expression was changed in the present work as follows:

$$S_V = \gamma \frac{2}{d_p} \sqrt{3\pi(1-\epsilon)} \quad (6)$$

where the coefficient γ and morphology of the foams are related.

Moreover, a dimensionless expression of the mass transfer coefficient k_m is given by the Sherwood number:

$$Sh = \frac{k_m d_p}{D_{1,2}} \quad (7)$$

Experimental results [18] showed the correlation between the Sherwood number Sh , the Schmidt number Sc and the Reynolds number Re for the range of porosity of interest (84% - 95%):

$$Sh = 0.91 Re_{s_{max}}^{0.43} Sc^{\frac{1}{3}} \quad (8)$$

It should be noted that $Re_{s_{max}}$ is the Reynolds number computed considering the superficial velocity u and the average structure diameter d_s as characteristic length:

$$u_{max} = u \frac{d_p^2}{(d_p - d_s)^2} = \frac{u}{\left(1 - \frac{2}{\sqrt{3\pi}} \sqrt{1 - \epsilon}\right)^2} \quad (9)$$

$$Re_s = Re_p \frac{2}{\sqrt{3\pi}} \sqrt{1 - \epsilon} \quad (10)$$

where u_{max} is the interstitial velocity expressed as the maximum mean velocity in the smallest area among the struts of the cubic cell model up to now considered.

Finally, combining the expressions above presented and considering that the GA tries to find the absolute minimum value of a certain function, the final expression for the inefficiency of the CO conversion was evaluated as follows:

$$\ln(1 - \eta) = -k_m S_V \frac{L}{u} = -\frac{Sh D_{1,2}}{d_p} S_V \frac{L}{u} \quad (11)$$

Cost Effectiveness

In order to determine eventual advantages of the foams as a catalytic support in comparison to the honeycomb the Geometric Surface Area (GSA) could be a key parameter. In fact, a better mass transfer of the foams allows to lower the catalyst loading on the surface, reducing the amount of precious metals needed. This leads to a reduction of the cost of the device. Thus, the GSA can be assumed as the third parameter than should be minimized:

$$GSA = S_V V_0 \quad (12)$$

Honeycomb

The same approach was adopted for the honeycomb struts, thus the expressions of the pressure drop, the conversion efficiency and the geometric surface area were re-written as a function of the external diameter and the length of the catalytic monolith. The case of the honeycomb substrate was treated as the open-cell foam one, but in this case the porosity and the pore density (ppi) were replaced by the Open Frontal Area (OFA) (that is equal to honeycomb porosity) and the cell density (cpsi) respectively.

Pressure Drop

The expression proposed by Patcas et al. [19] for the pressure drop in the honeycomb monolith has been adopted:

$$\Delta p = \frac{32\mu}{d_h^2 \epsilon} u L \quad (13)$$

where d_h indicates the hydraulic diameter. This equation is directly derived from the Hagen-Poiseuille formulation and shows a linear dependency of the Darcy velocity to the pressure drop. The results coming from this expression showed to properly match the experimental trend up to a velocity value of about 10 m/s. Over this value the concentrated pressure losses at inlet and outlet boundaries become relevant: these hydraulic resistances vary following the quadratic law of the velocity [20].

Conversion Efficiency

The conversion inefficiency was estimated by the Equation (11) where the Sherwood number was expressed as [7, 19]:

$$Sh = 2.976 \left(1 + 0.078 Re_c Sc \frac{d_c}{L}\right)^{0.45} \quad (14)$$

instead of Equation 8. For the specific surface the following relation was used [17]:

$$S_V = \frac{4\epsilon}{d_c} \quad (15)$$

Cost Effectiveness

The Equation (12) has been applied for honeycombs as well.

CFD CHARACTERIZATION OF THE FOAM SAMPLES

As previously described, the optimization algorithm needs a set of relations describing the geometrical and fluid-dynamic properties of the catalytic substrates. In this section, the properties of the open-cell foams hereafter considered will be characterized by means of a combination of micro-CT and CFD techniques.