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Simplified Pressure Drop and Flow Distribution Modelling in Radial Catalytic Converters

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A simplified model of a radial hydrocarbon reforming catalytic converter is presented. It focuses on fluid flow, distribution along the annular catalytic packed bed, and overall pressure drop. As for the chemistry aspect of the problem or possible issues due to pore blockages, these are not considered in the paper.
The model is based on a set of several well-known equations such as the continuity equation, Euler's equation for inviscid flow, equation of state, etc. and is built with utilization in geometry optimization algorithms in mind. An optimization software implementing the discussed model and a comparison of results and experimental data related to a series of existing catalytic converters are presented as well.

1. Introduction

Radial catalytic converters are typically employed in petroleum refineries to convert low-octane intermediates into higher-quality products, such as high-octane gasoline, with hydrogen being a by-product (Rahimpour et al., 2013). This process is highly endothermic (Zagoruiko et al., 2014) and therefore the entire catalytic conversion unit usually consists of several converters connected in series each of which is preceded by a fired heater where the feed is re-heated.
Pressure drops in packed beds of catalytic converters tend to be quite significant which, combined with pressure drops in fired heaters, induces considerable pumping costs. Converters must therefore be designed in such a way that the resulting pressure drops are as low as possible. Moreover, flow distribution along the catalytic packed bed should be as uniform as possible – especially if regeneration of the catalyst (Bartholomew, 2000) is not performed. This helps to achieve uniform aging of the catalyst and consequently longer service life of the catalytic bed.
Neither the chemistry aspect of the problem (except for an estimated temperature gradient in the packed bed) nor pore blockages (Jiménez-García et al., 2013) are considered in this paper. What is of interest to us is pressure change modelling as pressure gradients also largely influence flow distribution. Earlier, pressure drop of a packed bed had usually been estimated en bloc using for instance the Ergun equation as discussed in (Green and Perry, 2008); however, this did not enable incorporation of incremental changes in temperature, viscosity, etc. into the models or reasonable prediction of flow distribution. Current modelling approaches therefore favor direct numerical simulation, often via customized finite-element or finite-volume methods as described for instance by Palle and Aliabadi (2013) in case of regular packing or by Mousazadeh et al. (2013) for random particle distribution. Some of the models even consider effective transport properties of packed layers as discussed by Bertei et al. (2013). Computational fluid dynamics (CFD) is very popular as well (see e.g. Zhou et al., 2013), especially in case of automotive industry applications (Kumar and Mazumder, 2010). Other models such as those based on artificial neural networks can also be encountered (Zamaniyan et al., 2013). Nonetheless, for optimization purposes one needs a simple-enough model if reasonable optimization times are to be expected. Hence, although one-dimensional simplified models of packed beds exist for chemical phenomena (Srinivasan and Depcik, 2013a), heat and mass transport (Srinivasan and Depcik, 2013b), or both (Saouli et al., 2011), these are still quite complex and their implementation in geometry optimization algorithms would lead to optimization times that are prohibitively long if used in engineering practice. What is more, the implementation itself

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would certainly not be easy. A simple yet accurate enough pressure drop and flow distribution model allowing fast and effortless geometry optimization is therefore presented in this paper.

2. Description of the catalytic converter unit

Figure 1 shows a typical radial catalytic converter. Desulfurized naphtha feedstock enters the converter at the top through the inlet duct. Then it flows into the inlet dome through the inlet distributor and continues into the channels along the perimeter of the annular catalytic packed bed. Converted feed then leaves the unit through the central outlet duct.
Both cylindrical surfaces of the packed bed consist of two layers. Rigid outer layer made of a perforated steel sheet prevents deformations of the bed. Inner layer – a wire mesh screen – keeps the packing from falling through the holes in the outer perforated sheet.

3. Mathematical model

Let us first consider flow through a simple channel. Figure 2 shows a segment of a straight channel with the control volume being delimited by a dotted line. Pressure, density, and flow velocity at the inlet are denoted as p_1, ρ_1, and v_1, respectively. Channel area at the inlet into the control volume is A_1. Quantities at the outlet from the control volume are denoted analogously with the subscript "2". Since the segment delimited by the control volume is of a very short length dl, we can approximate the outlet cross-sectional area by $A_2 = A_1 + (\partial A / \partial l)\, \mathrm{d}l$ and proceed similarly for the remaining quantities.
We must also consider friction, $\mathrm{d}F_F$, standard gravity, g, the rate at which fluid leaves the control volume through the wall of the channel, $\delta \mathrm{d}l$, and the angle of inclination of the segment from the direction of g, φ. Please note that δ is positive for outflow and negative for inflow.
The first equation that we will need is the continuity equation, that is

$$\rho v A = \text{const.} \tag{1}$$

After writing Eq (1) for the segment in Figure 2, expanding it, and removing higher-order terms

$$\frac{1}{\rho}\frac{\partial \rho}{\partial l} + \frac{1}{v}\frac{\partial v}{\partial l} + \frac{1}{A}\frac{\partial A}{\partial l} + \frac{\delta}{\rho v A} = 0. \tag{2}$$

Next, by performing a balance of forces acting on the fluid delimited by the control volume

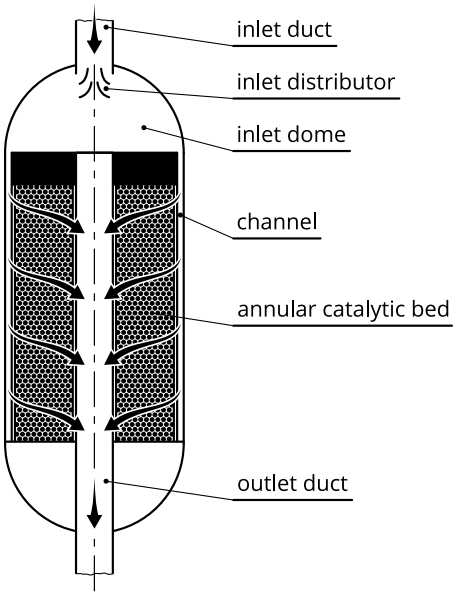

Figure 1: Cross-section of a typical radial catalytic converter

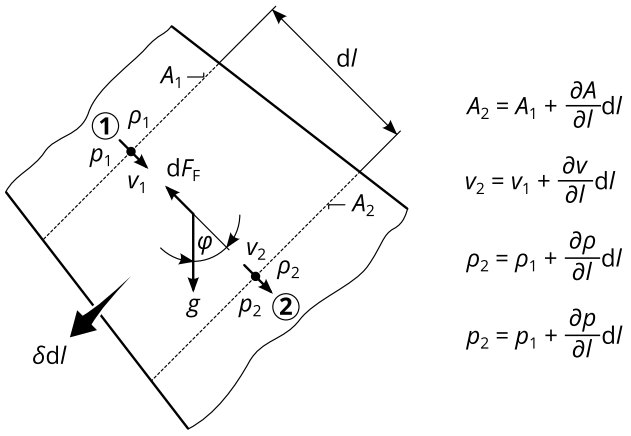

Figure 2: Short segment of an inclined channel with variable cross-section and porous wall

$$v\frac{\partial v}{\partial l}+\frac{1}{\rho}\frac{\partial p}{\partial l}-g\cos\varphi+\frac{1}{\rho A}\frac{\mathrm{d}F_{\mathrm{F}}}{\mathrm{d}l}=0 \tag{3}$$

which, in fact, is the Euler's equation for steady one-dimensional compressible inviscid flow. The last term in this equation can be replaced for convenience – per the Darcy-Weisbach equation (Brown, 2002) – by specific energy loss,

$$\frac{1}{\rho A}\frac{\mathrm{d}F_{\mathrm{F}}}{\mathrm{d}l}=\frac{\mathrm{d}E}{\mathrm{d}l}=\lambda\frac{\mathrm{d}l}{D_{\mathrm{h}}}\frac{v^2}{2}. \tag{4}$$

Here, λ denotes Darcy friction factor and D_{h} hydraulic diameter of the channel. The modified equation thus is

$$v\frac{\partial v}{\partial l}+\frac{1}{\rho}\frac{\partial p}{\partial l}-g\cos\varphi+\lambda\frac{\mathrm{d}l}{D_{\mathrm{h}}}\frac{v^2}{2}=0. \tag{5}$$

Finally and most importantly, it is needed to find the equation governing pressure change in the segment. To do so, we will utilize two other equations, namely the equation of state,

$$p=\rho RT, \tag{6}$$

and the first law of thermodynamics for an adiabatic process,

$$\frac{\partial q}{\partial l}=c_{\mathrm{v}}\frac{\partial T}{\partial l}-\frac{p}{\rho^2}\frac{\partial \rho}{\partial l}. \tag{7}$$

Therefore, by combining Eq(5) through (7)

$$\frac{1}{\rho}\frac{\partial \rho}{\partial l}-\frac{1}{\rho v^2}\frac{\partial p}{\partial l}+\frac{g\cos\varphi}{v^2}-\frac{\lambda}{2D_{\mathrm{h}}}+\frac{1}{A}\frac{\partial A}{\partial l}+\frac{\delta}{\rho vA}=0. \tag{8}$$

Since in this simplified case heat is generated solely due to friction, it can re-written the above equation as

$$\frac{\partial p}{\partial l}\left(\frac{1}{\kappa p}-\frac{1}{\rho v^2}\right)=\frac{\lambda}{2D_{\mathrm{h}}}\left(1+\frac{\kappa-1}{\kappa}\frac{\rho v^2}{p}\right)-\frac{g\cos\varphi}{v^2}-\frac{1}{A}\frac{\partial A}{\partial l}-\frac{\delta}{\rho vA} \tag{9}$$

in which $\kappa = c_{\mathrm{p}} / c_{\mathrm{v}}$ denotes heat capacity ratio. From here, it immediately follows that

$$\frac{\partial p}{\partial l}=\frac{\frac{\lambda}{2D_{\mathrm{h}}}\left(1+\frac{\kappa-1}{\kappa}\frac{\rho v^2}{p}\right)-\frac{g\cos\varphi}{v^2}-\frac{1}{A}\frac{\partial A}{\partial l}-\frac{\delta}{\rho vA}}{\frac{1}{\kappa p}-\frac{1}{\rho v^2}}. \tag{10}$$

At this point it is easy to obtain equation for pressure change in a segment of the length Δl in the discretized representation of the geometry. Other quantities are calculated accordingly with difference versions of the equations above.

Considering minor losses (flow through the perforated steel sheets, wire meshes, etc.), these can be calculated via the standard equation

$$\Delta p=\zeta\frac{\rho v^2}{2} \tag{11}$$

with coefficients of hydraulic resistance, ζ, computed according to the formulas available in (Idelchik, 2001).

It is assumed that the bed is packed regularly (Afandizadeh and Foumeny, 2001). Pressure changes therein are calculated in the same manner as in Eq(11) since the usual equations for en bloc estimation of pressure drop (especially Ergun equation) are not suitable for prediction of pressure drop in case of turbulent flow regime (Allen et al., 2013). Temperature changes caused by energy dissipation due to induced turbulence are then estimated similarly as in Eq(4), i.e., via specific energy loss. Such an approach allows us to incorporate gradual changes in temperature, pressure, viscosity, and other quantities.

4. Software implementation of the model

The model has been implemented in a geometry optimization tool (see Figure 3) developed in Java (Oracle, 2014). The entire geometry is discretized automatically and a quasi-1D mesh is produced based on the provided input data. Equations are then solved sequentially in an upwind-like (Patankar, 1980, Section 5.2-2) iterative manner until convergence is reached. Considering physical properties of the fluid (density, dynamic viscosity, etc.), these are always calculated ad hoc with respect to actual temperature and pressure.

The tool is primarily intended for catalytic bed geometry optimization with the domain being given by ranges of characteristic dimensions (inner and outer diameters and length of the catalytic bed). Even though extensive evaluation of all possible geometries in the domain would certainly yield an optimum, the process would be rather time-consuming. An appropriate optimization method is therefore selected according to the actual dimension of the domain. The Golden Section Method (Ravindran et al., 2006, pp. 51–53) is employed for a one-dimensional domain. Two-dimensional domains are explored using the Hooke and Jeeves method (Ravindran et al., 2006, pp. 92–97) enhanced with intelligent selection of initial estimate and with an algorithm for adaptive pattern step length. A 3D extension of this enhanced Hooke and Jeeves method is used for three-dimensional optimization domains. Additionally, the application can take full advantage of contemporary multi-core processors – it splits the optimization domain into several smaller domains so that all available processor cores are utilized and that optimization times are shortened even further.

Based on our tests, both objective functions, that is, pressure drop and relative standard deviation from uniform flow distributions, are smooth and unimodal for any reasonable set of input data. It is therefore safe to use the above-mentioned optimization methods.

4.1 Comparison of obtained data and industrial-case geometries

In order to get a sense of how well the optimization tool discussed in the previous section performs, the authors compared its outputs to several existing catalytic converters connected in series. Although these converters have been designed before wide-spread availability of CFD and other numerical tools requiring substantial computing power, all design decisions were then made according to both experience and extensive prototype testing to ensure as good a performance as possible while retaining low overall pressure drop.

Catalytic bed of the first converter was required to be 14.5 m^3 in volume and have inner diameter of 0.65 m. Characteristic size of particles making up the packed bed was 1.9 mm. Mass flow rate of the

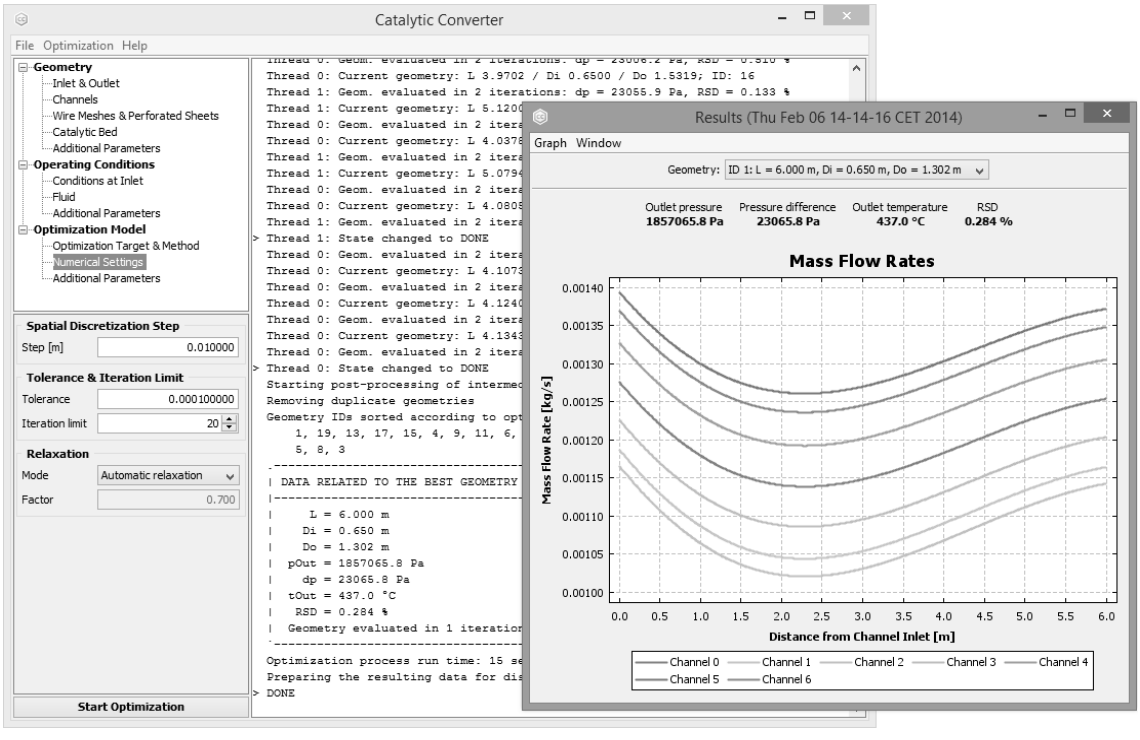

Figure 3: Screenshot of the developed geometry optimization tool with sample results being displayed

hydrocarbon mixture being converted was 52.44 kg s^{-1} and – according to the operator – its temperature dropped from 505 °C to 437 °C in the converter. The second converter in the series contained packed bed with volume of 36.3 m^3 that consisted of the same type of particles and had the same inner diameter as in case of the first apparatus. Here, temperature of the stream dropped from 505 °C (after re-heating) to 470 °C. As for the third converter, its catalytic bed was required to be 72.5 m^3 in volume. Again, the same type of particles was used as packing and identical inner diameter of the bed was required. Temperature drop in this case, however, was even smaller – from 505 °C to 495 °C.

Results yielded by the optimization tool are shown in Table 1 alongside data provided by the operator of the three converters mentioned above. It can be seen that there is a good agreement between the data sets. Of course, this is not sufficient as a model validation (for that an extensive testing is planned) but it hints that the model might perform rather well in its present state.

It should also be noted that relative standard deviation from uniform flow distribution, being a measure of uniformity of flow distribution along the catalytic bed, is quite low for all three converters. The catalyst inside the packed beds should therefore be aging uniformly.

Table 1: Comparison of data obtained with the geometry optimization tool and data provided by the operator of the catalytic converters

	Converter I		Converter II		Converter III	
	opt. tool	operator	opt. tool	operator	opt. tool	operator
Catalytic Bed						
inner diameter	0.650 m		0.650 m		0.650 m	
outer diameter	2.034 m	2.060 m	2.882 m	2.920 m	3.083 m	3.100 m
length	4.967 m	4.830 m	5.854 m	5.700 m	10.163 m	10.050 m
Operating conditions						
inlet temperature	505 °C		505 °C		505 °C	
outlet temperature	437 °C		470 °C		495 °C	
inlet pressure	1,834.0 kPa		1,692.0 kPa		1,571.0 kPa	
outlet pressure	1,801.9 kPa	1,803.7 kPa	1,666.7 kPa	1,667.5 kPa	1,548.4 kPa	1,550.1 kPa
pressure drop	32.1 kPa	30.3 kPa	25.3 kPa	24.5 kPa	22.6 kPa	20.9 kPa
RSD*	0.30 %	N/A	0.15 %	N/A	1.16 %	N/A

*Relative standard deviation from uniform flow distribution

5. Future work

Although according to preliminary tests it seems that the presented model performs quite well, it still needs to be validated properly. In other words, until performance of the model is validated against a large-enough set of experimental data or at least data obtained via CFD evaluations, it cannot be considered to be production-ready.

6. Conclusions

A simple mathematical model allowing easy and very fast evaluation of catalytic converter pressure drop and flow distribution uniformity has been described. According to preliminary tests, the model seems to be quite accurate but proper validation is still necessary before it is production-ready. Also, a user-friendly geometry optimization tool developed in Java has been presented. The tool takes advantage of modern multi-core processors and splits each optimization task to an optimum number of cores to shorten optimization time as much as possible.

Once a validated model is available, chemical engineers will be able to use the respective optimization tool to quickly and effortlessly design radial catalytic converters with low pressure drops and as uniform flow distributions along catalytic beds as possible. Not only that such converters will be cheaper to operate because of lower pumping costs, they will also require less maintenance due to more uniform catalyst ageing.

Nomenclature

A cross-sectional area of a channel, m^2
c_p specific heat capacity at constant pressure, J kg^{-1} K^{-1}
c_v specific heat capacity at constant volume, J kg^{-1} K^{-1}
D_h hydraulic diameter, m
E energy, J
F_F friction, N
g standard gravity, m s^{-2}
l length, m

p pressure, Pa
R specific gas constant, J kg^{-1} K^{-1}
T thermodynamic temperature, K
v flow velocity, m s^{-1}
δ amount of fluid that leaves control volume through a wall, kg m^{-1} s^{-1}
ζ coefficient of hydraulic resistance, –
κ heat capacity ratio, –
λ Darcy friction factor, –
ρ density, kg m^{-3}
φ angle of inclination of a segment from the direction of g, °

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