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Gas-solid mass transfer coefficients in channels of automotive converters

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Highlights

- Evaluation of mass transfer coefficients for automotive converter performing CFD calculations.
- Correlation of mass transfer coefficients with the channel length and dimensionless numbers Sh, Sc and Re.
- Satisfactory fitting of the correlation to the calculated mass transfer coefficients.

1. Introduction

In literature, many models have been proposed for the simulations of the monolith converters. The most widely used simplification is the representation and simulation of the whole structure by a single channel, with the assumption of no interaction between the monolith cells. This simplification is indicated by the uniform flow rate across the inlet face and the adiabatic behaviour of the monolith. [1],[2] The use of simplified approaches incorporating mass transfer correlations in channels has a wide use due to their simplicity. However, these approaches sometimes have low validity and prediction capabilities due to ambiguous mass transfer correlations which mainly derive from heat transfer correlations.

The objective of this work is the estimation of mass transfer coefficients of species in the automotive exhaust gases from the bulk of the gas phase to channel wall according to thin film theory within a wide range of velocities and conditions in lab-size and real size monoliths. Mass transfer rates were derived from developing and running a 2-D isothermal CFD model in Comsol Multiphysics which describes in detail the fluid flow and the mass transport along a monolith channel. A technical kinetic model of the reactions taking place in an automotive converter was used. The mass transfer coefficients were correlated using relations of the dimensionless numbers Sh, Re and Sc and the monolith length. The effectiveness of an 1-D simplified model that couples PFR with mass transport effects was also tested.

2. Methods

A 2D geometry with axial symmetry was used for the geometric representation of the monolith channel in the CFD model. A channel diameter 1.1 mm was used. The CFD model incorporates in detail the momentum and mass transport through the monolith channel. For the momentum transport the Incompressible Navier Stokes was used to describe the laminar and isothermal flow of the gas mixture. A Convective and Diffusive model according to Fick's law was used to describe mass transport in the gas phase as the diffusing species were dilute with respect to N_2. No homogeneous reactions were considered in the bulk of the gas phase and the heterogeneous reaction on the channel walls predominates.

The investigation of the mass transfer limitations and the calculations of the mass transfer coefficients were performed at isothermal conditions and temperatures 300, 400 and 500 °C. Thirty in total interstitial velocities (ten velocities at each temperature) within the range 0.028-7.2 m/s covering the total range of the working conditions with a laboratory and real size monolith and two gas feed compositions lean and rich were tested. A total cell length of 1 cm and 3cm was tested for the low velocities (u_{int}<1.3 m/s) and 12 cm for the high velocities (u_{int}>1.3 m/s). The gas-solid mass transfer coefficients for 6 species NO, CO, O_2, CH_4, C_3H_6 and C_3H_8 were calculated along the channel length according to the thin film theory using the 1-D equation:

$$(-R_i'')_z = (K_{gs,i})_z((C_{i,b})_z - (C_{i,s})_z) \quad (1)$$

where $(-R_i'')_Z$ is the reaction rate at the position z of the cell length coordinate expressed per square meter of washcoat wall in contact with the gas phase. $(C_{i,s})_Z$ corresponds to the component's i concentration at the position z of the cell length coordinate on the catalytic surface. As bulk concentration $(C_{i,b})_Z$ at the position z of the cell length coordinate the mean concentration of component i along the channel radius was considered.

The mass transfer coefficients were correlated and the derived correlation was used to couple the 1-D simplified isothermal PFR model with the mass transport and test the validation of this approach.

3. Results and discussion

The mass transfer coefficient changes with the channel length. Near the entrance, the mass transfer coefficient has a high value which steeply decreases at the first mm from the cell entrance. After some mm reaches a plateau, and remains constant for the rest of the length.

The mass transfer coefficients were correlated along the monolith cell length using dimensionless numbers of Sherwood, Schmidt and Reynolds according to the following equation.

$$Sh(z) = a + b \cdot (z^* \cdot 10^3)^c \exp(d \cdot z^*) \quad (2)$$

where :

$$z^* = \frac{z}{l_{cell}} \frac{1}{Re \cdot Sc} \quad (3)$$

z : length coordinate, distance from the cell inlet [m]
l_{cell} : characteristic length of the monolith cell [m]
a, b, c, d : correlation's parameters

In Figure 1 a typical diagram of the calculated mass transfer coefficient K_{gs} for CO along the channel length is presented along with correlation fitting.

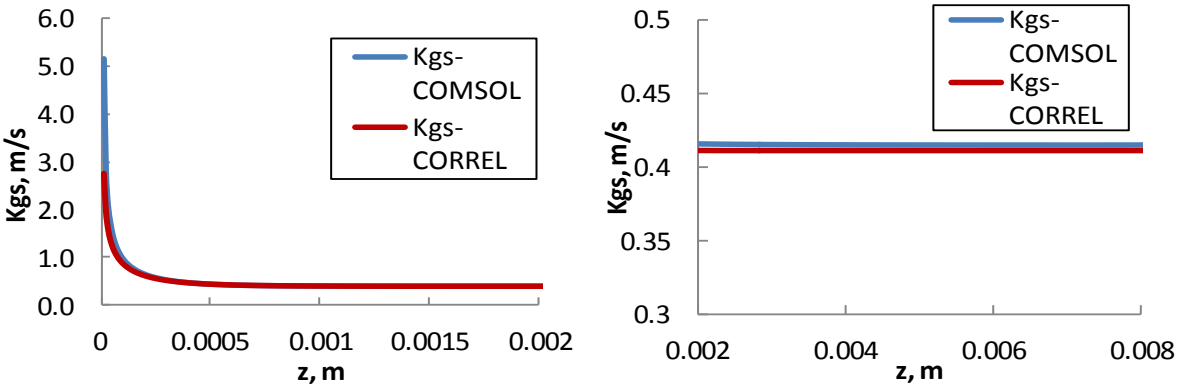

Figure 1. Typical diagram of calculated and correlated mass transfer coefficient Kgs for NO. T=400 °C. Interstitial velocity u_{int}=0.261 m/s.

4. Conclusions

A very good fitting of the correlation to the calculated mass transfer coefficients of the gas phase species was achieved. The 1-D simplified model that couples PFR with mass transport effects using the derived correlation is an effectively approach of the reactor performance obtained by the CFD model.

References

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Keywords
Automotive converter; mass transfer coefficients; correlation of mass transfer coefficients; CFD calculations