Model-based Optimization of Advanced SCR Substrates

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ABSTRACT: Innovative high porosity SCR substrates are targeting at optimum utilization of high catalyst amounts without increasing pressure drop. Mathematical modeling of such technologies is challenging, requiring accurate description of both chemistry and mass transfer inside the active material. In this work, a systematic experimental study is conducted towards calibrating a comprehensive commercial simulation model for a Cu-zeolite SCR catalyst. Based on the calibrated model, it is possible to evaluate different substrate technologies with respect to NOx conversion, pressure drop and packaging volume reduction potential.

KEY WORDS: heat engine, selective catalytic reduction, de-NOx catalyst, NOx, modeling, high porosity, substrates, Cu-zeolite (A1)

1. Introduction

Urea-based Selective Catalytic Reduction (SCR) is a well-established technique, enabling efficient control of nitrogen oxides (NOx) from diesel vehicles. NH3-SCR catalytic converters are currently widely used in heavy- and medium-duty applications, with achieved conversion efficiencies higher than 95% 1).

Given the even higher de-NOx efficiency requirements imposed by forthcoming legislation and cost reduction pressures, significant efforts in catalyst development, substrate optimization, urea injection control and system design are necessary 2). Focusing on the former, alternative types of SCR substrates have been proposed. Typical substrates are cordierite honeycomb structures, characterized by a relatively low porosity, in the order of approximately 30%. SCR catalytic material is washcoated on the external surface of the wall and the amount of washcoat is limited by pressure drop induced by the reduction of open frontal area. On the other hand, extruded catalysts can have more active material per reactor volume which results in improved de-NOx performance compared to conventional coated catalysts, especially in the low temperature region 3).

Recently, the technology of high porosity substrates has been proposed. Ceramic materials characterized by porosity as high as 50% allow the introduction of significant amounts of catalytic material inside the porous wall, whereas additional amounts of catalyst can be washcoated on the external surface of the substrate wall. This combination allows the application of increased active material loadings, enhancing NOx conversion 4).

The design of SCR substrate/coating combination has to be undertaken for each specific engine application in order to achieve the desired NOx conversion/NH3 slip targets with minimum costs and optimized packaging. In this respect, it is important for the design engineer to understand thoroughly the underlying physico-chemical phenomena. This is nowadays accomplished by using advanced mathematical models of the transport and reaction phenomena in the SCR catalysts. By using such modeling approaches, it is possible to accelerate the development process, optimize dosing control strategies and minimize the testing costs before start of production.

Numerous mathematical models that describe chemistry, mass transfer, thermal and flow phenomena in SCR systems have been published and validated in the recent literature 5,6,7,8,9). In the present work, we employ a commercial simulation tool (axisuite®) to demonstrate a model-based comparison of different SCR substrate technologies, particularly focusing on conventional washcoated and innovative high-porosity catalysts. Employing synthetic gas bench experiments, performed on a commercial Cu-zeolite based catalyst, a SCR catalyst model was calibrated and validated. Subsequently, the calibrated model was used to evaluate the abovementioned substrate technologies, with respect to de-NOx performance and pressure drop.

2. Mathematical Model

2.1. General

The present simulation study was performed using the commercial axisuite® platform 10). The governing model equations have been presented and discussed in previous publications 11,12,13,14,15,16) and are given here as a reference (equations 1 to 4).

Regarding gas phase, quasi-steady state balance equations for the heat and mass transfer in the channel are shown in equations (1) and (2) respectively:

\[ \rho_g C_p g \frac{\partial T_g}{\partial z} = -h \cdot \frac{H_p}{\varepsilon} \cdot T_g - T_s \]  

(1)
\[
\frac{\partial (v_{j}y_{b,j})}{\partial z} = -k_{j} \cdot \left( \frac{S_{p}}{\varepsilon} \right) \cdot (y_{b,j} - y_{s,j}) \tag{2}
\]

The total surface reaction rate for each species is equal to the external species mass transfer from/to the exhaust gas:

\[
\frac{\rho_{b} - k_{j} \frac{S_{p}}{\varepsilon}}{M_{b}} (y_{b,j} - y_{s,j}) = R_{j} \tag{3}
\]

The following transient energy balance of the solid phase is used to calculate the change of the solid temperature over time:

\[
\rho_{s}C_{p,s} \frac{\partial T_{s}}{\partial t} = \lambda_{s} \frac{\partial^{2} T_{s}}{\partial z^{2}} + S \tag{4}
\]

where the source term \(S\) includes the convective heat transfer due to the gas flow in the channels and the heat release by chemical reactions. Equation (4) is valid for the case of 1-d (single channel) approach, which will be used entirely in the present work.

Additional details concerning the derivation of the model equations, their extension to 3-d, the boundary conditions and the solution procedure can be found in the above referenced publications.

It is known that the performance of SCR catalysts at high temperatures and flow rates can be affected by species diffusion in the washcoat (17). Therefore, in order to correctly simulate mass transfer limitations, the species concentrations need to be solved inside the washcoat layer by proper 'intra-layer' discretization and solution of the reaction-diffusion equation:

\[
-D_{w,j} \frac{\partial y_{s,j}}{\partial w^{2}} = \sum_{k} n_{j,k}R_{k} \tag{5}
\]

The boundary conditions for the washcoat layer are:

\[
D_{w,j} \frac{\partial y_{s,j}}{\partial w} \bigg|_{w=-w_{c}} = k_{j} (y_{b,j} - y_{s,j} \bigg|_{w=-w_{c}}) \tag{6}
\]

\[
\frac{\partial y_{s,j}}{\partial w} \bigg|_{w=0} = 0 \tag{7}
\]

where \(w = 0\) corresponds to the wall boundary and \(w = -w_{c}\) to the external surface of the washcoat.

The effective diffusion coefficients in the porous washcoat for the various species were approximated using the “parallel pore” model (18). According to this approach both molecular and Knudsen diffusion are considered for a washcoat with a uniform pore size distribution. Effective diffusivity is calculated as:

\[
\frac{1}{D_{w,j}} = \frac{\tau}{\varepsilon_{pore}} \left( \frac{1}{D_{mol,j}} + \frac{1}{D_{knud,j}} \right) \tag{8}
\]

with the Knudsen diffusivity:

\[
D_{knud,j} = \frac{d_{pore}^{3}}{3} \sqrt{\frac{8RT}{\pi M_{j}}} \tag{9}
\]

The porosity \(\varepsilon_{pore}\) and the mean pore size \(d_{pore}\) can be extracted from the microstructural properties of the washcoat while tortuosity \(\tau\) is an empirical calibrated parameter.

2.2. SCR reaction scheme

A well-accepted global kinetic model, describing the SCR chemistry over Cu-zeolites was used (19). The respective chemical reactions are listed in Table 1.

Table 1 Reactions used in the SCR model.

| Reaction | Equation |
|----------|----------|
| \(\text{NH}_3 \rightarrow \text{NH}_3(l)\) | (a) |
| \(\text{NH}_3(l) \rightarrow \text{NH}_3\) | (b) |
| \(2\text{NO} + \text{O}_2 \rightarrow 2\text{NO}_2\) | (c) |
| \(2\text{NO}_2 \rightarrow 2\text{NO} + \text{O}_2\) | (d) |
| \(4\text{NH}_3 + 4\text{NO} + \text{O}_2 \rightarrow 4\text{N}_2 + 6\text{H}_2\text{O}\) | (e) |
| \(2\text{NH}_3 + \text{NO} + \text{NO}_2 \rightarrow 2\text{N}_2 + 3\text{H}_2\text{O}\) | (f) |
| \(8\text{NH}_3 + 6\text{NO}_2 \rightarrow 7\text{N}_2 + 12\text{H}_2\text{O}\) | (g) |
| \(4\text{NH}_3 + 3\text{O}_2 \rightarrow 2\text{N}_2 + 6\text{H}_2\text{O}\) | (h) |
| \(4\text{NH}_3 + 5\text{O}_2 \rightarrow 4\text{NO} + 6\text{H}_2\text{O}\) | (k) |

\(\text{NH}_3\) adsorption and desorption (reactions a and b) are modeled employing the Dubinin-Radushkevich isotherm (equations 10 and 11).

\[
\ln x_{eq,\text{NH}_3} = \ln (w_{0} \cdot \rho_{\text{NH}_3}) - D_{\text{NH}_3} \left[ \ln \left( \frac{P_{\text{sat,\text{NH}_3}}}{P_{\text{NH}_3}} \right) \right] \tag{10}
\]

\[
D_{\text{NH}_3} = A_{ze} \cdot \left( \frac{R \cdot T}{\beta_{\text{NH}_3}} \right) \tag{11}
\]

NO to \(\text{NO}_x\) oxidation is an important step of the SCR process in Cu-zeolites, since the \(\text{NO}/\text{NO}_x\) ratio affects the rate of \(\text{NO}_x\) reduction. Therefore, both NO oxidation and \(\text{NO}_x\) dissociation were taken into account (reactions c and d). \(\text{NO}_x\) reduction through \(\text{NH}_3\) was modelled through 3 reaction pathways, namely the “Standard”, “Fast” and “\(\text{NO}_x\):” SCR reactions (reactions e,f and g). Finally, the undesired ammonia oxidation was described by two reactions with different product selectivity (reactions h and k), in line with experimental findings reported elsewhere (20).

3. Experimental Section

Experiments presented in this study were performed on a commercial Cu-zeolite catalyst, coated on a monolithic core, provided by NGK. Kinetic studies were performed on a specimen of \(D \times L\) equal to 25.4 mm \(\times\) 50 mm, in order to calibrate and validate kinetic parameters of the reactions shown in Table 1. Additionally, high space velocity experiments were performed,
where it was necessary to use a sample of shorter length (D x L = 25.4 x 25 mm).

The NH₃ storage and space velocity experiments were conducted on synthetic gas bench (Fig. 1) at the Laboratory of Applied Thermodynamics (LAT) of Aristotle University of Thessaloniki, Greece (AUTh). The samples were placed in an electrically heated furnace to control catalyst temperature. Feed gas composition and flow rate were adjusted through a gas mixer (Environics S-2000). H₂O was also included in the gas feed through a saturator. SCR reactivity experiments were performed on synthetic gas bench of NGK (experimental set-up not shown) employing the monolith sample of D x L = 25.4 x 50 mm.

![Fig. 1 Experimental setup for experiments with synthetic gas.](image)

Ammonia adsorption and desorption were investigated first. A mixture of 300 ppm NH₃, 5% H₂O and 1% O₂ with N₂ in balance was isothermally introduced in the catalyst for a certain period, to achieve steady-state conditions at the catalyst exit. Then, ammonia was removed from the feed and the catalyst was heated up from the adsorption temperature up to 550°C, under O₂ and H₂O, in order to thermally release NH₃ adspecies. Ammonia adsorption and desorption tests were repeated at eight different temperatures, in the range of 160-480°C. For the abovementioned experiments, NH₃ was supplied to the catalyst through an external fast responding mass flow controller, to ensure its quick introduction and removal, during the adsorption and desorption phases respectively.

Catalyst SCR reactivity was evaluated through steady-state experiments. The sample was exposed to a mixture of 330 ppm NH₃, 330 ppm NOx, 5% O₂, 8% H₂O and 7% CO₂, whereas N₂ was used as carrier gas. The effects of temperature and NO₂/NOx ratios were also studied, by applying a broad range of temperatures (200-500°C) and three NO₂/NOx ratios (0, 0.5 and 0.75).

Finally, mass transfer limitations in the washcoat were investigated through steady-state SCR experiments, on the specimen with the length of 25 mm. The sample was exposed to 330 ppm NH₃, 330 ppm NOx (NO₂/NOx= 0.5), 5% O₂, 8% H₂O, 7% CO₂ and N₂ in balance. Based on preliminary testing it was deduced that for the abovementioned conditions, maximum NOx conversion was achieved at 350°C. Therefore, it was decided to evaluate the effect of mass transfer limitations at this temperature, where the reaction rates are practically ‘infinite’. Experiments were repeated at various mass flow rates, corresponding to space velocities of: 80, 100, 120, 140 and 160 kh⁻¹.

For all experiments (except for those performed at various mass flow rates) a volumetric flow rate equal to 20 slpm was applied. The experimental protocols applied in the frame of this work are summarized in Table 2.

### Table 2 Summary of experiments and respective conditions.

| Experiment Applied conditions | NH₃ adsorption & desorption experiments | SCR reactivity experiments | Space velocity experiments |
|-----------------------------|----------------------------------------|---------------------------|---------------------------|
| Temp. [°C]                  | 160, 200, 250, 300, 340, 380, 440, 480 | 200, 250, 350, 450, 500   | 350                        |
| NH₃ [ppm]                   | 300                                    | 330                       | 330                       |
| NOx [ppm]                   | -                                      | 330                       | 330                       |
| NO₂/NOx [-]                 | -                                      | 0, 0.5, 0.75              | 0.5                       |
| O₂ [%]                      | 1                                      | 5                         | 5                         |
| H₂O [%]                     | 5                                      | 8                         | 8                         |
| CO₂ [%]                     | -                                      | 7                         | 7                         |
| N₂ [%]                      | Balance                                | balance                   | balance                   |
| GHSV [kh⁻¹]                 | 60                                     | 60                        | 60, 80, 100, 120, 140, 160 |
| Specimen D x L mm           | 25.4 x 50                              | 25.4 x 50                 | 25.4 x 25                 |

For calibrating NH₃ adsorption/desorption, parameters of the Dubinin-Radushkevic model had to be evaluated first. For this purpose, the total amount of stored ammonia was estimated at each temperature, as shown in Fig. 2a. Based on these calculations, experimental points, presented in Fig. 2b (circles) were obtained.

### 4. Results and Discussion

#### 4.1. Model calibration

#### 4.1.1. NH₃ adsorption and desorption

For calibrating NH₃ adsorption/desorption, parameters of the Dubinin-Radushkevic model had to be evaluated first. For this purpose, the total amount of stored ammonia was estimated at each temperature, as shown in Fig. 2a. Based on these calculations, experimental points, presented in Fig. 2b (circles) were obtained.
Increasing the solid phase temperature, lower amounts of \( \text{NH}_3 \) can be stored on the catalyst, which can be assigned to the fact that ammonia adsorbed species, characterized by low thermal stability cannot be formed on the catalytic surface at higher temperatures \(^{(21)} \). Calibrating parameters of the Dubinin-Radushkevic isotherm (equations 10 and 11) we could reproduce experimental results in a quite satisfactory way (Fig. 2b, continuous line).

Subsequently, the kinetic parameters of \( \text{NH}_3 \) storage and release were calibrated, in order to precisely depict the dynamic behavior of adsorbed/desorbed ammonia. Indicative simulations of \( \text{NH}_3 \) storage and release experiments performed at 160, 250, 340 and 440°C, are presented in Fig. 3.

At temperatures as low as 250°C, ammonia is slowly stored on the catalyst, until inlet and outlet \( \text{NH}_3 \) concentrations become equal, indicating complete surface saturation. Nevertheless, this behavior is not the case at higher temperatures, since ammonia outlet concentration level does not reach the level of the inlet one.

The latter is attributed to \( \text{NH}_3 \) oxidation, which reasonably occurs at temperatures higher than 340°C, since \( \text{O}_2 \) is included in the gas feed. Both \( \text{NH}_3 \) adsorption/desorption and oxidation were correctly predicted at different temperatures, by the kinetic model, which proves model robustness.

4.1.2. SCR reaction kinetics calibration

Kinetic parameters for SCR reactions, were evaluated by simulating steady-state reactivity experiments at different temperatures and \( \text{NO}_2/\text{NOx} \) ratios. Respective summarized results are illustrated in Fig. 4.

Kinetic parameters for the “Standard”, “Fast” and “\( \text{NO}_2/\text{SCR} \)” reactions (reactions e-g) were calibrated by simulating SCR experiments, performed at \( \text{NO}_2/\text{NOx} \) ratios equal to 0, 0.5 and 0.75 respectively. Overall, the calibrated model allowed to depict experimental results in a quite satisfactory way, at different temperatures and \( \text{NO}_2/\text{NOx} \) ratios. Nevertheless, some discrepancies were observed in the case of \( \text{NO}_2/\text{NOx}=0.75 \) and particularly in the lower temperature range.
4.1.3. Diffusion in the washcoat

Finally, the intralayer model had to be calibrated, and particularly washcoat tortuosity (τ). The effect of this parameter on NOX conversion was investigated as shown in Fig. 5. At mass flow rates corresponding to GHSV up to 120 km⁻¹, NOX conversion is kinetically limited and only minor changes up to 2%, in de-NOX efficiency are observed (within the range of experimental error). Nevertheless, at higher mass flow rates, NOX conversion yield attenuates up to 6%, as a result of mass transfer limitations in the washcoat. From a modeling point of view, if washcoat diffusion was not taken into consideration (blue line), the calibrated kinetic model would not be capable of predicting this effect at high mass flow rate regimes. The latter underlines the necessity of implementing an additional intra-layer model for considering species diffusion in the washcoat. Calibrating tortuosity equal to 1 (black line), a quite satisfactory simulation of experimental curves was achieved, throughout the whole range of applied conditions.

4.2. Model-based comparison of substrate technologies

High NOX conversion performance and low pressure drop are the main requirements for the new generation SCR catalysts. However, a trade-off between these two requirements exists for current conventional coated SCR catalysts, since pressure drop increases with increasing catalyst amount. In this respect, advanced substrates such as high porosity ones could combine high de-NOX performance with minimum fuel penalty.

The main factors that limit de-NOX performance are illustrated in Fig. 6. At low temperatures, SCR activity is kinetically limited and can be increased with the addition of higher washcoat loading. On the other hand, at mid and high temperatures, the conversion efficiency is limited by mass-transfer and can be improved by increasing the available surface area through higher cell density (external mass transfer) and/or by decreasing diffusion resistance in the active layer (internal mass transfer). Finally, at even higher temperatures, NH3 oxidation becomes significant, hence limiting NOX conversion.

Pressure drop depends on the channel hydraulic diameter and consequently it is adversely affected by higher washcoat loading, increasing cell density and/or higher wall thickness.

In this section, a model-based comparison of high porosity SCR substrates, with respect to conventional coated ones, will be presented. The calibrated Cu-zeolite SCR catalyst model, discussed in the previous section, is used as a basis for the simulation exercise. The simulated SCR substrates include the standard porosity coated (SP 4/400 x1.0), the high porosity-standard cell density (HP 6/400 x1.5) and the high porosity-high cell density substrate (HP 5/600 x1.5). The above standard naming conventions will be used throughout the presentation of simulations results. For example, in HP 5/600 x1.5, ‘HP’ stands for high porosity, 5/600 is the cell structure and x1.5 denotes the ratio of active washcoat amount with respect to the reference amount of the conventional SP catalyst. The geometrical and structural properties used in the simulations (see Table 3) were selected based on the literature (3).
Table 3 Geometrical and structural properties of the simulated catalysts.

| Property               | Catalyst  | SP 4/400 x1.0 | HP 6/400 x1.5 | HP 5/600 x1.5 |
|------------------------|-----------|---------------|---------------|---------------|
| Diameter [m]           |           | 0.266         | 0.266         | 0.266         |
| Length [m]             |           | 0.152         | 0.152         | 0.152         |
| Cpsi                   |           | 400           | 400           | 600           |
| Wall thickness [mils]  |           | 4             | 6             | 5             |
| Substrate porosity [%] |           | 35            | 60            | 60            |
| Catalyst amount [g/l]  |           | 150           | 225           | 225           |
| Catalyst on layer [%]  |           | 100           | 33            | 33            |
| Catalyst in wall [%]   |           | 0             | 67            | 67            |

4.2.1. Steady-state NOx conversion

Initially, the steady-state de-NOx performance of the different catalysts was examined at 3 temperatures (Fig. 7). The inlet gas consisted of 400ppm NO, 100ppm NO\textsubscript{2} and 600ppm NH\textsubscript{3} at a GHSV of 120000 h\textsuperscript{-1}.

At 200°C, the HP 6/400 x1.5 exhibits an increased conversion efficiency of about 5%, compared to the reference SP 4/400 x1.0 coated catalyst, which can be mainly attributed to the higher active material mass per unit volume. At mid and high temperatures, the HP 6/400 x1.5 shows the same or even slightly lower performance than the conventional catalyst. The increased washcoat amount cannot be properly exploited since NOx conversion at these temperatures is limited by internal mass transfer resistance. The combination of high washcoat loading with high surface area for the HP 5/600 x1.5 substrate results in the best de-NOx performance for all temperatures.

4.2.2. Internal mass transfer resistance

Steady-state NOx conversion at two space velocities was investigated in order to quantify the effect of internal mass transfer resistance for each SCR substrate. Simulations were performed at 350°C, where a de-NOx performance, close to 100%, is achieved (section 4.1.2). An inlet gas feed of 400ppm NO, 100ppm NO\textsubscript{2} and 600ppm NH\textsubscript{3} was applied.

4.2.3. Pressure drop

The pressure drop comparison was performed considering a full-load operating point with an exhaust temperature of 450°C and a mass flow rate of 2500 kg/h. The HP 6/400 x1.5 catalyst exhibits the same pressure drop level as the reference catalyst, despite its higher total washcoat amount (see Fig. 9). The HP 6/400 x1.5 is characterized by higher catalyst amount inside the substrate and lower on the coating layer which is favorable for pressure drop. However, this benefit is compensated from the higher wall thickness (6mils compared to 4mils of the reference catalyst) resulting finally in equivalent pressure drop. The HP 5/600 x1.5 catalyst which has higher cell density and higher wall thickness, with respect to the conventional catalyst, has the highest pressure drop.
4.2.4. Downsizing

Packaging volume reduction, maintaining similar performance levels is challenging for modern complicated aftertreatment systems. One approach to meet this challenge is to increase catalyst mass per unit volume and shorten catalyst substrate length. The volume reduction potential for the high cell density HP 5/600 x1.5 was investigated. This substrate is characterized by 50% higher washcoat amount per unit volume compared to the reference SP 4/400 substrate. Simulation results indicate that a 30% smaller HP 5/600 x1.5 catalyst can maintain equivalent de-NOx efficiency and pressure drop behavior as the reference SP catalyst, as illustrated in Fig. 10.

![Graph showing NOx conversion and pressure drop](image)

Fig. 10 (a) de-NOx efficiency (Inlet: NO=400ppm, \(NO_2=100ppm\), \(NH_3=600ppm\), \(SV=120000\) h\(^{-1}\)) and (b) pressure drop (\(T=450°C\), flow=2500 kg/h) of downsized SCR catalyst.

5. Conclusion

Experimental studies combined with simulation were employed in the present work in order to evaluate alternative SCR substrates. Based on synthetic gas bench experiments, a SCR catalyst model was calibrated and successfully validated, applying a broad range of experimental conditions. Overall, \(NH_3\) storage and release, NOx conversion, as well as mass transfer limitations at high space velocities were correctly depicted.

Employing the calibrated SCR model, a model based comparison was performed between conventional coated SCR catalysts and innovative high porosity substrates. Simulation enabled to evaluate advantages and disadvantages of each technology with respect to NOx conversion and pressure drop, whereas, possibilities of catalyst downsizing were analyzed.

From a methodology point of view, we demonstrated a possible contribution of modeling and simulation for evaluating innovative SCR substrate technologies. Different geometries, experimental conditions as well as application cases (eg. mid and heavy duty vehicles) could be evaluated, employing model based analysis. This topic is under consideration for future work.

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Nomenclature

| A. Latin letters |  |
|------------------|--|
| $C_p$ | specific heat capacity | $J/(kg\cdot K)$ |
| $d_h$ | hydraulic diameter of a channel | m |
| $D_{Knud}$ | Knudsen diffusivity | $m^2/s$ |
| $D_{mol}$ | molecular diffusivity | $m^2/s$ |
| $d_{pore}$ | mean pore size | m |
| $D_{w}$ | effective diffusivity | $m^2/s$ |
| $h$ | heat transfer coefficient | $W/(m^2\cdot K)$ |
| $k_j$ | mass transfer coefficient | m/s |
| $M$ | molecular weight | kg/mol |
| $R$ | universal gas constant | $J/(mol\cdot K)$ |
| $R_j$ | reaction rate | mol/(m$^3\cdot$s) |
| $S$ | heat source term | $w/m^3$ |
| $S_F$ | monolith specific surface area | $m^2/m^3$ |
| $T$ | temperature | K |
| $t$ | time | s |
| $v$ | velocity | m/s |
| $w$ | dimension perpendicular to wall surface | - |
| $w_c$ | washcoat layer thickness | m |
| $y_j$ | molar fraction | - |
| $z$ | axial coordinate along monolith | m |

| B. Greek letters |  |
|-------------------|--|
| $\varepsilon$ | macroscopic void fraction | - |
| $\varepsilon_{pore}$ | porosity of the washcoat | - |
| $\lambda$ | thermal conductivity | $W/(m\cdot K)$ |
| $\rho$ | density | $kg/m^3$ |
| $\tau$ | tortuosity | - |

| C. Subscripts and Superscripts |  |
|-------------------------------|--|
| $g$ | exhaust gas |  |
| $j$ | species index |  |
| $k$ | reaction index |  |
| $s$ | solid |  |
| $w$ | substrate wall |  |