

Modeling of Catalyzed Particulate Filters - Concept Phase Simulation and Real-Time Plant Modeling on HiL

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ABSTRACT

The present work introduces an extended particulate filter model focusing on capabilities to cover catalytic and surface storage reactions and to serve as a virtual multi-functional reactor/separator. The model can be classified as a transient, non-isothermal 1D+1D two-channel model. The applied modeling framework offers the required modeling depth to investigate arbitrary catalytic reaction schemes and it follows the computational requirement of running in real-time. The trade-off between model complexity and computational speed is scalable. The model is validated with the help of an analytically solved reference and the model parametrization is demonstrated by simulating experimentally given temperatures of a heat-up measurement. The detailed 1D+1D model is demonstrated in a concept study comparing the impact of different spatial washcoat distributions. The generic model is further used to describe a diesel particulate filter coated with functionalities for selective catalytic reduction of nitrogen oxide emissions (SDPF). This dedicated model, as a part of a full diesel exhaust line, is combined with a passenger car vehicle and thermodynamic engine model. The whole system model is assessed in office PC simulation regarding result plausibility and computational performance during the New European Drive Cycle and a randomly assembled drive cycle. The real-time capability of the full model is demonstrated by running it on the NI VeriStand real-time simulation environment. The presented type of system model contributes to answer upcoming questions in the context of real driving emissions (RDE) by means of simulation.

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INTRODUCTION

In 2017 the European authorities plan to replace the New European Drive Cycle (NEDC) by the Word Light Duty Cycle (WLTC) and in addition, a gradual introduction of a test procedure for Real Driving Emissions (RDE) is foreseen. The latter will be based on Portable Emission Measurement Systems and driving on public roads with the goal to avoid test cycle specific control device optimization. The technical challenges for engine and car manufacturers are well framed by a recent study of Franco et al. [1] who performed an onroad emission assessment of modern diesel passenger cars in Europe and US. The authors state that "the average on-road emission level of NO_x was estimated at seven times the certified emission limit for Euro 6 vehicles".

The challenge of WLTC and RDE based emission approval tests can be seen in a very pronounced way by comparing the operating points in the engine load-speed-map passed through by the different driving conditions. Following a study on passenger car diesel engines by Striok et al. [2] the NEDC mainly requires engine operation at low loads and speeds, whereas the WLTC and the given RDE reference cycle widen the operating field to significantly higher load and speed points.

The reduction of nitrogen oxides (NO_x) over the lifetime of a vehicle can be seen as a specifically challenging task. On the one hand, more dynamic engine operation will lead to higher NO_x engine out concentrations at higher mass flow rates and temperatures. On the other hand, the goal to reduce also carbon dioxide emissions is addressed by a list of measures leading to lower engine outlet temperatures. The implementation of low pressure exhaust gas recirculation (EGR), advanced boosting systems and electrification raises engine efficiency but reduces considerably the exhaust gas temperature level and delays light-off times [3]. Körfer further states that "active thermal management algorithms will become compulsory" on top of an ameliorated passive thermal management. Passive thermal measures comprise exhaust aftertreatment system (EAS) design optimizations regarding component positioning, insulation, and thermal inertia. The latter is promisingly addressed by combining the abatement functionality of different aftertreatment devices in a single device. By applying e.g. selective catalytic reduction (SCR) coatings within the diesel particulate filter (DPF) the SCR functionality moves closer to the engine and the heat-up time of the unified SCR diesel particulate filter (SDPF) component is additionally shortened proportional to the reduction of the overall thermal inertia. In SDPFs, nitrogen dioxide (NO_2), provided by the diesel oxidation catalyst, does not longer exclusively support the favorable fast SCR reaction but it is

also consumed in a competitive way in the passive oxidation of soot. Czerwinski et al. [4] recently reported that “one of the biggest challenges in research is to identify the optimal trade-off between these activities and to be able to adapt the filter component design for specific engine applications”. Koltsakis et al. [5] show in a simulation study the complexity of layered and zoned filter wall structures. The work also underlines the requirement of understanding in detail the phenomena taking place within the filter to design an efficient and also robust “multi-functional reactor/separator” as classified by Konstandopoulos et al. [6].

In a case study on model based development Fortuna et al. [7] conclude that the application of hardware in the loop or software in the loop (HiL/SiL) environments constitutes a cost efficient and quality increasing methodology to address RDE emissions. HiL combines simulation with hardware prototypes of the control units, sensors, and actuators and therefore is one step closer to the real system compared to pure simulation. This efficiency gain in the development will be compulsory because of two further reasons. The validation of all design variants and test cases would not be affordable in the real vehicle on the road. Also the application of climatic chassis dynos required for altitude calibration would be very costly. Model based development on HiL in the context of RDE requires real-time capable models comprising the domains vehicle, engine and EAS. Physical based plant models have been identified as a promising attempt (see Kordon et al. [8]) to fulfill the increasing requirements on control development and calibration. The modeling of SDPFs is seen as a specifically challenging task as it requires an appropriate modeling depth at real-time capable simulation times.

Modeling of DPFs has been done for decades and numerous studies focusing on specific aspects and application areas lead to a broad spectrum of different approaches. Koltsakis et al. [9] discuss and compare many different approaches in a comprehensive review. Here, previous studies focusing on fast running models supporting reactor/separator functionalities shall be briefly discussed. Assuming that the radial distributions within the inlet and outlet channel can be lumped, a 1D channel model (see Bissett [10]) can be combined with a 2D description of the wall. York et al. [11] emphasize in a study on oxidation catalyzed DPFs that a 2D wall model is essential to cover non-uniform aging effects and to optimize zone coating. The 2D model can be further simplified by neglecting diffusive effects in axial direction and by lumping the wall into individual layers (see Konstandopoulos and Kostoglou [12]), representing the soot cake and the wall. Premchand et al. [13, 14, 15] apply this type of model in a series of modeling and verification studies on catalyzed soot filters. The model combines a transient description of the wall temperature with steady-state balance equations for the gas phase. The species conservation equations of the zone next to the inlet channel additionally applies a diffusive transport term considering a concentration driven drag of species from the inlet channel into the reactive wall. The concept of lumping effects is also applied by Kladopoulou et al. [16] and Depcik et al. [17] in a net of axial and radial zones where the gas phase energy and species conservation do not distinguish between inlet and outlet channel. The lumped balances exchange energy and species sources with the wall

describing heat up and soot conversion. In a consecutive effort, Depcik [18] refines the previously applied approach of “dynamic incompressibility” and combines the lumped energy and species model with the classical two-channel model (see Konstandopoulos et al. [19]) for the pressure drop calculation. The author highlights the real-time capability (even in non-compiled form as interpreted code) and also concludes that further details on chemical reactions require the classical two channel modeling approaches. The difference between 1D and real-time 0D models are evaluated by Nicolin et al. [20] who run both approaches in combination with a map based engine model and conclude that with an appropriate calibration of the soot oxidation kinetics also the 0D model shows good agreement with experimental data. Similarly, Cloudt et al. [21] state that “more modeling depth does not necessarily imply more accurate models” when presenting a real-time capable DPF model executed in a HiL environment. How to hold a high level of physical depth combined with well interpretable parameters and most efficient computational speed is demonstrated by Konstandopoulos and Kostoglou [22], who derived analytical expressions for the steady-state concentration profiles in the channels and the wall considering advection, diffusion, and first order reactions in isothermal operation.

The particulate filter model presented in this work has been specifically developed to support model based development. The modeling part of the study focuses on extending the modelling depth of DPFs required to describe specific phenomena relevant for SDPFs. In the simulation part of the study validation and application simulations are shown. A full vehicle, engine and EAS model is assessed in office simulation and executed on a HiL environment.

FILTER MODEL

The filter model presented in this study attempts to combine the required physical depth to investigate soot conversion and catalytically driven reactions in transient non-isothermal operations with the requirement of real-time capability and flexibility to apply spatial coating variants and arbitrary reaction chemistry. Following the literature review this applied approach is referred to as transient, non-isothermal 1D+1D two-channel model. Figure 1 shows the inlet channel, the porous wall, the outlet channel and also indicates a finite volume discretization in two orthogonal directions along the channel (represented by the coordinate z) and along the wall thickness (represented by the coordinate x). The state variables (i.e. species fractions, internal energy, velocity) in the gas phase are given by ϕ and ψ is a generic surface state representing local soot masses or species surface coverages. T_{sub} is the solid substrate temperature. The fluxes entering and leaving the finite cells are represented by $\dot{F}$ where the leaving fluxes are expressed by a first order Taylor series expansion in the given coordinate direction, respectively. The fluxes also distinguish between convective and diffusive (conductive) transport. Diffusive transport is considered along the wall direction and neglected in axial direction (see also Haralampous and Koltsakis [23]). This distinction is based on the Péclet numbers of the wall flow that are typically three orders of magnitude smaller than given in axial flow direction. Chemical

conversion ($\dot{r}_{\text{conv}}$) reactions, surface storage ($\dot{r}_{\text{surf}}$) reactions and gas wall heat transfer ($\dot{q}_{\text{trans}}$) are considered only in the porous wall. Here, no further mass and heat transfer limiting steps are taken into account between gas phase and wall. Diffusive (conductive) transfer is also considered between the channels and the wall overlaying the convective fluxes through the wall.

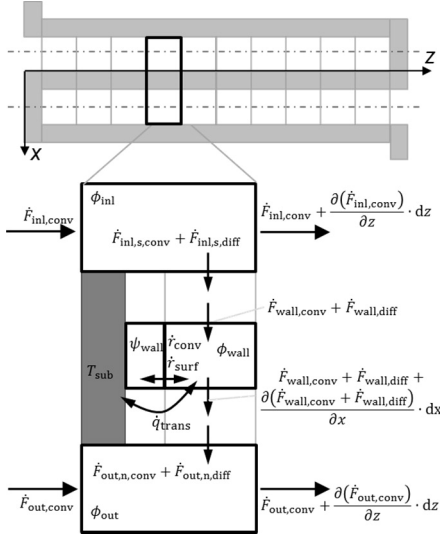


Figure 1. Representative cells of a 1D+1D particulate filter model, states and fluxes.

Based on the schematic of Figure 1 the transient balance equations describing the different state variables are discussed in the following section.

Inlet and Outlet Channel

The transient mass conservation equation in the inlet and outlet channel is given by

$$\begin{aligned} \frac{\partial(m_{\text{inl}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{inl}})}{\partial z} \cdot dz - \dot{m}_s \\ \frac{\partial(m_{\text{out}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{out}})}{\partial z} \cdot dz + \dot{m}_n \end{aligned} \quad (1)$$

where m_{inl} and m_{out} represent the gas phase mass in the inlet and outlet channel, respectively. In a 1D consideration the time (t) derivative of these masses equals the spatial (z) derivative of the mass fluxes represented by $\dot{m}_{\text{inl}}$ and by $\dot{m}_{\text{out}}$, reduced or augmented by an additional wall flow source term, respectively. This flow through the porous wall from the inlet to the outlet channel is described by the terms $\dot{m}_s$ and $\dot{m}_n$, representing the mass fluxes leaving the inlet channel at its “south” side and entering the outlet channel at its “north” side. Assuming that chemical conversion reactions leading to continuity sources take place only within the wall no further source terms are applied in this equation.

The transient species mass conservation equation in the inlet and outlet channel can be written as

$$\begin{aligned} \frac{\partial(m_{\text{inl}} \cdot w_{\text{inl},j})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{inl}} \cdot w_{\text{inl},j})}{\partial z} \cdot dz \\ &- \dot{m}_s \cdot w_{s,j} - \rho_s \cdot A_{\text{wall}} \cdot \beta_{\text{inl}} \cdot (w_{\text{inl},j} - w_{s,j}) \\ \frac{\partial(m_{\text{out}} \cdot w_{\text{out},j})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{out}} \cdot w_{\text{out},j})}{\partial z} \cdot dz \\ &+ \dot{m}_n \cdot w_{n,j} + \rho_n \cdot A_{\text{wall}} \cdot \beta_{\text{out}} \cdot (w_{n,j} - w_{\text{out},j}) \end{aligned} \quad (2)$$

where the variables $w_{\text{inl},j}$, $w_{\text{out},j}$, $w_{s,j}$ and $w_{n,j}$ represent the mass fraction of species j in the inlet and outlet channels and at the south side of the inlet and the north side of the outlet channel, respectively. Both equations feature two source terms covering convective and diffusive mass fluxes exchanged between the channel and the gas flow going through the wall. Here ρ_s and ρ_n represent the gas density at the south face of the inlet channel and the north face of the outlet channel, respectively. The species mass fractions of the convective fluxes and the densities in the diffusive fluxes are noted as face values for reasons of generality. In the numerical solution of the 1D channel model, these face values are approximated by cell center values, i.e. the channel fraction/density of the inlet channel and the fraction/density of the wall bottom cell, respectively. The application of the inlet channel fraction is in line with Koltsakis et al. [9] who, beyond this, discuss possibilities of resolving the boundary layer and cell face values in more detail. A_{wall} is the cross section available for the gas flow through the wall. It can be derived from the geometrical surface area of the filter considering also the cell size given by the axial discretization and the porosity of the wall. β_{inl} and β_{out} represent mass transfer coefficients. The diffusive terms in each channel apply one density, respectively. This ignores the impact of different temperatures in the inlet channel and on the wall surface leading to different densities and different diffusive velocities. A rigorous analysis of diffusive velocities and a discussion on the applied assumption of diluted mixture diffusion can be found in Depcik [24]. The diffusive terms are typically negligible at high mass flows, though they become dominant at medium and low mass flows. The importance of capturing both convective and diffusive transport effects in the wall is underlined in a simulation study from Votsmeier et al. [25] running a 2D, steady-state fluid dynamic model.

The energy conservation equation of the gas in the inlet and outlet channels is given by

$$\begin{aligned} \frac{\partial(m_{\text{inl}} \cdot u_{\text{inl}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{inl}} \cdot h_{\text{inl}})}{\partial z} \cdot dz \\ &- \dot{m}_s \cdot h_s - A_{\text{wall}} \cdot \alpha_{\text{inl}} \cdot (T_{\text{inl}} - T_s) \\ \frac{\partial(m_{\text{out}} \cdot u_{\text{out}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{out}} \cdot h_{\text{out}})}{\partial z} \cdot dz \\ &+ \dot{m}_n \cdot h_n + A_{\text{wall}} \cdot \alpha_{\text{out}} \cdot (T_n - T_{\text{out}}) \end{aligned} \quad (3)$$

where u_{inl} , u_{out} represent the mass specific internal energy in the inlet and outlet channel. h_{inl} , h_{out} , h_s and h_n are the mass specific enthalpies in the inlet and outlet channels and on the south side of the inlet and the north side of the outlet channel, respectively. In

both equations the convective enthalpy flow through the wall is superimposed by heat transfer. Here α_{inl} and α_{out} are heat transfer coefficients and T_{inl} , T_s , T_n , T_{out} represent the temperature at the above mentioned cell faces.

The momentum balance equation in the inlet and outlet channel is given by

$$\begin{aligned} \frac{\partial(m_{\text{inl}} \cdot v_{\text{inl}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{inl}} \cdot v_{\text{inl}})}{\partial z} \cdot dz - A_{\text{inl,C}} \cdot \frac{\partial p_{\text{inl}}}{\partial z} \cdot dz \\ &- F_{\text{inl}} \cdot \mu \cdot v_{\text{inl}} \cdot dz - v_{\text{inl}} \cdot \dot{m}_s \\ \frac{\partial(m_{\text{out}} \cdot v_{\text{out}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{out}} \cdot v_{\text{out}})}{\partial z} \cdot dz - A_{\text{out,C}} \cdot \frac{\partial p_{\text{out}}}{\partial z} \cdot dz \\ &- F_{\text{out}} \cdot \mu \cdot v_{\text{out}} \cdot dz \end{aligned} \quad (4)$$

where v_{inl} , v_{out} and p_{inl} , p_{out} are the flow velocity and the pressure in the inlet and outlet channel. $A_{\text{inl,C}}$ and $A_{\text{out,C}}$ represent the inlet and outlet channel flow cross sections and F_{inl} and F_{out} are the corresponding friction coefficients applied together with the dynamic viscosity μ of the gas. The last term in the inlet channel momentum balance considers a momentum sink (see Hinterberger et al. [26]) due to a mass sink in order to comply with the second law of thermodynamics, see Wurzenberger and Kutschi [27]. The sink term is only applied in the inlet channel featuring separating flow characteristics compared to the outlet channel featuring joining flow conditions. The term is small compared to the friction losses along the channel, therefore it is often dropped. Similar, the left hand side of the momentum balance is often dropped assuming that the flow field builds up significantly faster than e.g. temperature changes take place.

Wall Gas Phase and Substrate

The transient mass conservation equation of the gas flow through one slice (see Figure 1) of the porous wall is given by

$$\begin{aligned} \frac{\partial(m_{\text{wall}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{wall}})}{\partial x} \cdot dx \\ &+ A_{\text{wall}} \cdot dx \cdot \sum_j v_{i,j} \cdot \text{MG}_j \cdot \sum_i \dot{r}_i (T_{\text{sub}}, w_{\text{wall}}, \psi) \end{aligned} \quad (5)$$

where m_{wall} represents the mass of the gas phase in the porous wall and $\dot{m}_{\text{wall}}$ is the mass flow through the wall. The second term on the right side describes a mass source due to chemical reactions. Here, soot regeneration or surface adsorption and desorption reactions lead to continuity sources. The variable $\dot{r}_i$ represents a volume specific mole rate of reaction i . It is evaluated as a function of the wall substrate temperature T_{sub} and, depending on the type of reaction, it is typically a function of the gas composition w_{wall} and the surface coverage, ψ . The variable $v_{i,j}$ represents the stoichiometric coefficient of species j in reaction i and MG_j is the molar mass of species j . The boundary condition of the spatial mass flow derivative at $x=0$ is given by the mass flow $\dot{m}_s$ of the inlet channel (Eq.1). The mass flow source $\dot{m}_n$ of the outlet channels (Eq.1) is fed by the mass flow leaving the

wall. The cross section available for the gas flow through the wall (A_{wall}) is assumed to be constant in the wall continuity, gas species and enthalpy balance. This simplification is made as the cross section is mainly used to evaluate conduction/diffusion areas and local flow velocities. These flow velocities are used to evaluate empirical heat and mass transfer correlations. A more rigorous model approach can be found in Koltsakis et al. [9] who also point out the difficulties of measuring heat transfer coefficients.

The gas species balance in the wall is represented by

$$\begin{aligned} \frac{\partial(m_{\text{wall}} \cdot w_{\text{wall},j})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{wall}} \cdot w_{\text{wall},j})}{\partial x} \cdot dx \\ &+ D_{\text{eff}} \cdot \rho_{\text{wall}} \cdot A_{\text{wall}} \cdot \frac{\partial\left(\frac{dw_{\text{wall},j}}{dx}\right)}{\partial x} \cdot dx \\ &+ A_{\text{wall}} \cdot dx \cdot \text{MG}_j \cdot \sum_i v_{i,j} \cdot \dot{r}_i \end{aligned} \quad (6)$$

where $w_{\text{wall},j}$ represents the mass fraction of species j in the gas. D_{eff} is the effective pore diffusion coefficient and ρ_{wall} is the gas density in the wall. Both parameters are taken out of the spatial derivative to hold the overall mass conservation. The effective pore diffusion coefficient depends on the wall porosity and tortuosity, see Edelbauer et al. [28]). The boundary conditions of the species balance link to the inlet and outlet channel (Eq.2) in analogy to the continuity equation. In addition, the species balance also couples the diffusive fluxes.

The gas phase energy conservation equation in the wall is given by

$$\begin{aligned} \frac{\partial(m_{\text{wall}} \cdot u_{\text{wall}})}{\partial t} &= -\frac{\partial(\dot{m}_{\text{wall}} \cdot h_{\text{wall}})}{\partial x} \cdot dx \\ &+ \lambda_{\text{eff}} \cdot A_{\text{wall}} \cdot \frac{\partial\left(\frac{\partial T_{\text{wall}}}{\partial x}\right)}{\partial x} \cdot dx \\ &+ A_{\text{wall}} \cdot dx \cdot \text{GSA}_{\text{sub}} \cdot \alpha_{\text{sub}} \cdot (T_{\text{wall}} - T_{\text{sub}}) \\ &- A_{\text{wall}} \cdot dx \cdot \sum_i \text{MG}_j \cdot \Delta h_{R,i} \cdot \sum_i v_{i,j} \cdot \dot{r}_i \end{aligned} \quad (7)$$

where u_{wall} , h_{wall} , T_{wall} represent the mass specific internal energy, the enthalpy and the temperature of the gas mixture in the wall, respectively. The equation covers transport terms for convective and conductive transfer in analogy to the species balance equation. The term considering cross diffusion (enthalpy transport due to diffusive transport) is neglected here for reasons of simplicity. The heat exchange of the gas phase with the solid substrate is described by a geometric heat transfer area GSA_{sub} , a corresponding heat transfer coefficient α_{sub} and the difference between the gas (T_{wall}) and substrate temperature T_{sub} . The last term on the right side describes the sum of all heat of reactions where $\Delta h_{R,i}$ is the i 'th heat of reaction. The term is subtracted from the gas phase energy balance, because it is assumed that the heat is released in the energy balance of the solid substrate and because any heat of reaction is implicitly covered by

applying thermal properties including latent heats. The boundary conditions of the enthalpy balance link to the inlet and outlet channel enthalpy balance (Eq.3) in analogy to the species balance equation, covering convective and conductive fluxes.

The wall substrate energy conservation equation is applied using a lumped consideration in wall direction (see Figure 1). This leads to

$$\begin{aligned} m_{\text{sub}} \cdot c_{p,\text{sub}} \frac{\partial T_{\text{sub}}}{\partial t} = & \\ + A_{\text{wall}} \cdot GSA_{\text{sub}} \cdot \int_0^{\delta_{\text{wall}}} \alpha_{\text{wall}} \cdot (T_{\text{wall}} - T_{\text{sub}}) dx & \\ + A_{\text{wall}} \cdot \int_0^{\delta_{\text{wall}}} \sum_i MG_j \cdot \Delta h_{R,i} \cdot \sum_i v_{i,j} \cdot \dot{r}_i dx & \\ + A_{\text{front}} \cdot \lambda_{\text{sub}} \cdot \frac{\partial \left(\frac{dT_{\text{sub}}}{dz} \right)}{\partial z} \cdot dz + \dot{Q}_{\text{loss}} & \end{aligned} \quad (8)$$

where m_{sub} is the mass of substrate, $c_{p,\text{sub}}$ is its heat capacity and T_{sub} is the substrate temperature. Following the lumped consideration of the substrate, it exchanges heat with the gas along its integral way through the wall thickness, δ_{wall} . In the same way, the spatial integral of all heat of reaction is applied as a source term to the substrate energy balance. The solid substrate exchanges heat via conduction in axial direction where the heat transfer area A_{front} is evaluated as a function of wall thickness and cell density of the substrate. The last term in the equation represents a generic heat loss to the ambient via convection and radiation. The impact of radial temperature distributions over the converter is neglected in this approach. More details on how to model this can be found in Depcik et al. [17].

The momentum balance of the wall flow is described by the steady-state Darcy correlation assuming that the pressure drop is a linear function of the local flow velocity. Assuming quadratic channels and non-negligible soot cake heights, the following correlation can be derived.

$$\begin{aligned} p_{\text{inl}} - p_{\text{out}} = & \frac{\dot{m}_{\text{wall}}}{\rho_{\text{wall}} \cdot A_{\text{wall}}} \cdot \mu \cdot \frac{d_{\text{inl}} - 2 \cdot \delta_{\text{cake}}}{d_{\text{inl}}} \cdot \\ & \left[\frac{\delta_{\text{wall}}}{k_{\text{wall}}} + \frac{d_{\text{inl}}}{2 \cdot k_{\text{cake}}} \cdot \ln \left(\frac{d_{\text{inl}}}{d_{\text{inl}} - 2 \cdot \delta_{\text{cake}}} \right) \right] \end{aligned} \quad (9)$$

Here, d_{inl} is the diameter of the inlet channel, δ_{wall} and δ_{cake} are the wall and soot cake thickness and k_{wall} and k_{cake} represent the corresponding permeability of the two “layers”. More details on the impact of asymmetrical channel geometries can be found in Wurzenberger and Kutschi [27].

Conversion Reactions

The initially required flexibility to easily adapt and exchange reaction schemes is realized by decoupling the implementations of the numerical solution procedure and the coding of rate formulations.

The latter is framed by a separate tool. A graphical user interface (see Figure 2) guides through all required inputs of a rate formulation up to a compile step for multiple execution platforms. The compiled and encapsulated rate model is loaded into the solver framework of the DPF and contributes source terms in the various balance equations.

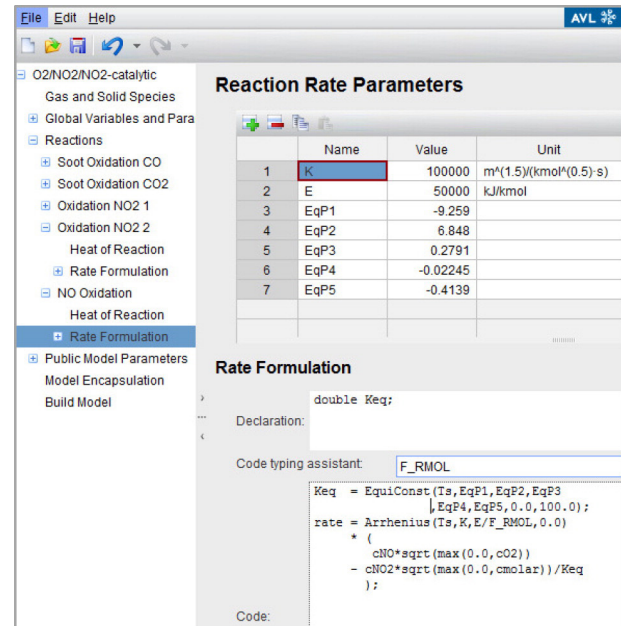


Figure 2. Reversible NO oxidation reaction in setup in AVL User Coding Interface.

In this study different reaction mechanisms are used and each of them is discussed in the corresponding results section.

Heat and Mass Transfer

The heat and mass transfer within the wall between the gas phase and the surface of the substrate is assumed to be negligible. This is modeled by applying the local gas concentrations in the chemical reaction rates without considering an additional adsorption/desorption step to active reaction centers. The heat transfer coefficient in the wall is chosen by a reasonable high number making sure that gas and wall temperature do not deviate significantly.

The heat and mass transfer coefficients for the diffusive/conductive drag between the channel and the gas phase in the wall are derived from Sherwood correlations taken from Konstandopoulos and Kostoglou [22]. It is given by

$$Sh = 2.72 + 0.35 \cdot Re_{\text{wall}} \quad (10)$$

where Re_{wall} represents the Reynolds number evaluated with the wall velocity. Typically this is a very small number bringing little influence. The fact that the boundary layer in the given wall flow constellation does not compare to the boundary layer in a flow-through catalyst is neglected, as well as the observation that the mass transfer coefficients might be different in inlet and outlet channel.