

# Particulate Matter Classification in Filtration and Regeneration-Plant Modeling for SiL and HiL Environment

Johann C. Wurzenberger, Christoph Triebel, Susanne Kutschi, and Christoph Poetsch  
 AVL LIST GmbH

## ABSTRACT

The present work describes an existing transient, non-isothermal 1D+1D particulate filter model to capture the impact of different types of particulate matter (PM) on filtration and regeneration. PM classes of arbitrary characteristics (size, composition etc.) are transported and filtered following standard mechanisms. PM deposit populations of arbitrary composition and contact states are used to describe regeneration on a micro-kinetical level. The transport class and deposit population are linked by introducing a splitting deposit matrix. Filtration and regeneration modes are compared to experimental data from literature and a brief numerical assessment on the filtration model is performed. The filter model as part of an exhaust line is used in a concept study on different coating variants. The same exhaust line model is connected to an engine thermodynamic and vehicle model. This system model is run through a random drive cycle in office simulation. The real-time capability of the model is proven by running the whole model on an ETAS hardware-in-the-loop (HiL) environment. This type of system model and its application on HiL support the assessment of real driving emissions (RDE) by means of simulation.

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## INTRODUCTION

Legal emission regulations of diesel powered passenger cars have been in place for many years with continuously decreasing limits. The upcoming introduction of test procedures for real driving emission (RDE) verification leads to challenging requirements in terms of robust hardware designs and optimized control unit (xCU) calibration. The validation of real vehicles on the road considering all design variants and test scenarios is not affordable. Also the application of climatic chassis dynos required for altitude calibration would be very costly as stated by Fortuna et al. [1]. The authors also conclude that the application of simulation models in software-in-the-loop (SiL) or hardware-in-the-loop (HiL) environments constitutes a promising methodology to address RDE. HiL environments allow the combination of hardware prototypes (sensors, actuators, xCUs...) and simulation models and by that to increase the predictability of the entire simulation. Here, the real-time capability of the plant models is a mandatory pre-requisite for successful HiL applications.

The development of real-time capable vehicle system simulation models is a multi-disciplinary task involving different modeling domains like engine thermodynamics including combustion and pollutant formation, cooling and lubrication, mechanical drivetrain and electrical networks. A crucial area in the context of RDE simulation is an accurate description of the exhaust aftertreatment system. Modern exhaust systems typically contain various pipes, different types of catalysts and particulate filters. The importance of

particulate filter has significantly grown in the past years by upgrading its functionality from a pure filtration device to a component that also provides various catalytic functionalities.

Wall flow filters have been proven as the appropriate technology to meet certification limits of particulate matter (PM) emissions with respect to particulate mass and number. Modern filters serve as multi-functional separators/reactors (see Konstandopoulos et al. [2]) as they combine filtration, PM oxidation and catalytically supported conversion reactions of various types. Here, model based approaches are useful to investigate the filtration efficiency of PM emissions featuring a broad spectrum of particle sizes. Models are also needed to describe and understand PM combustion considering the heterogeneous nature of PM (carbon, condensed liquid hydrocarbons, polynuclear aromatic hydrocarbons) and the interaction with catalysts. Modeling of detailed PM transport and filtration phenomena combined with detailed PM combustion mechanisms is a challenging task per se and even more when adding the requirement of real-time capable simulations.

Modeling studies on particulate filters have been published for more than two decades. Koltsakis et al. [3] summarize various individual modeling aspects in a comprehensive review and underline the above stated need for model based approaches. Simulation studies dealing with combined loading and regeneration models are presented by Huynh et al. [4], Mohammed et al. [5] and Premchand et al. [6] in a series of growing modeling depth. The models are based on the "two-layer approach" presented by Konstandopoulos and Kostoglou

[7] considering two dedicated zones of PM featuring catalyst contact in the wall and no contact in the PM cake. The PM combustion models additionally assume that the PM characteristics over the wall height can be lumped. This enables an analytical pre-processing of the gas species balance equations in the wall and a reduction of computational burdens for the sake of model flexibility.

The filter model presented in this study has been specifically developed to address several requirements. A higher level of physical depth is reached in the area of PM filtration and regeneration by introducing dedicated balance equations for arbitrary PM classes in the gas phase and by considering multiple PM deposit populations. The requirement on real-time capability of the significantly more complex model is maintained by a focused computational implementation. The requirement to support RDE simulations in real-time is shown by connecting the detailed filter model together with other aftertreatment components to an engine and vehicle model.

## FILTER MODEL

Modeling of particulate filters can be classified as a multiscale task. It requires the description of phenomena on the scale of the entire filter (1e-2 m), of the individual filter channels (1e-3 m), of the filter wall (1e-4 m) including its porous wall structure (1e-5 m) and on the scale of particulate matter (1e-9 m to 1e-6 m). The aim of the filter model presented in this study is to combine models of the different scales, to catch appropriately all relevant phenomena and to preserve real-time capable simulation times. A “1D+1D” model (see Figure 1) is applied where two orthogonal coordinates are defined for one representative pair of inlet and outlet channels connected by the porous wall. The coordinate  $z$  describes the channel along its axial direction and the coordinate  $x$  resolves the filter wall including its porous structure. The 1D+1D approach simplifies the conceptual and computational complexity of multi-dimensional approaches. In the channels, this is based on the assumption of “laminar flow combined with a small transverse component representing the flow to/from the wall system”, Bissett [8]. Figure 1 comprises the different gas phases and cake and wall surface site state variables in a generic manner by  $\phi_{gi}$ ,  $\phi_{gw}$ ,  $\phi_{go}$ ,  $\psi_{sc}$  and  $\psi_{sw}$  respectively.  $T_{sw}$  is the solid wall temperature and  $\dot{F}$  represents all fluxes entering and leaving a finite cell. The fluxes distinguish between convective and diffusive (conductive) transport where the latter is neglected in axial direction (see Haralampous and Koltsakis [9]). Chemical conversion ( $\dot{r}_{conv}$ ) reactions, bi-directional surface storage ( $\dot{r}_{surf}$ ) reactions, one-directional PM deposition ( $\dot{r}_{depo}$ ) rates and gas wall heat transfer ( $\dot{q}_{trans}$ ) are considered in the PM cake layer and in the porous wall. PM depth filtration is considered for the entire thickness of the wall and catalytic reactions are considered in arbitrarily defined wall zones. The formation of PM cake is modeled depending on PM deposit in the wall. Diffusive gas species and conductive heat transfer is considered between the channels and the wall overlaying the convective fluxes through the wall. Diffusive transport phenomena are ignored in the balance equations of particulate matter. This is reasonable as the corresponding diffusion coefficients are typically two orders of magnitude smaller compared to gas species diffusion coefficients (see Konstandopoulos and Johnson [10] and Poling et al. [11]). The temperature of the wall including the PM layer is approximated by a

lumped approach neglecting a temperature variation over the wall thickness (refer to Kostoglou and Konstandopoulos [12], Haralampous and Koltsakis [13]).

In the following section the discussion focuses on the continuity and balance equations of the different PM loading classes in the gas phase and on the balances of different PM deposit populations. Details on transient gas species, momentum and gas and wall enthalpy balances can be found in Wurzenberger et al. [14].

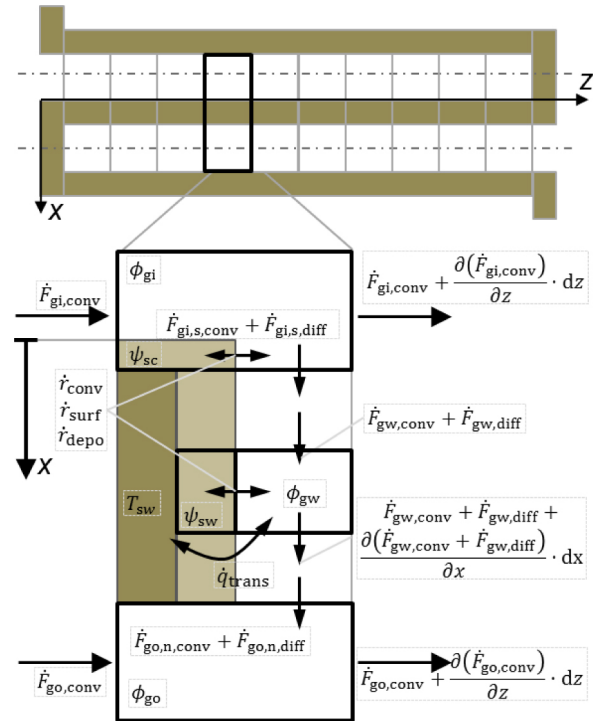


Figure 1. Representative cells of a 1D+1D particulate filter model, states and fluxes.

### Inlet and Outlet Channel

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

$$\begin{aligned} \frac{\partial(m_{gi})}{\partial t} &= -\frac{\partial(\dot{m}_{gi})}{\partial z} \cdot dz - \dot{m}_{gis} \\ \frac{\partial(m_{go})}{\partial t} &= -\frac{\partial(\dot{m}_{go})}{\partial z} \cdot dz + \dot{m}_{gon} \end{aligned} \quad (1)$$

where  $m_{gi}$  and  $m_{go}$  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  $\dot{m}_{gi}$  and by  $\dot{m}_{go}$ , reduced or augmented by an additional wall flow source term, respectively. This flow through the PM cake and further through the porous wall from the inlet to the outlet channel is described by the terms  $\dot{m}_{gis}$  and  $\dot{m}_{gon}$ , 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 PM loading conservation equation in the inlet and outlet channel can be written as

$$\begin{aligned} \frac{\partial(m_{gi} \cdot X_{gi,j})}{\partial t} &= - \frac{\partial(\dot{m}_{gi} \cdot X_{gi,j})}{\partial z} \cdot dz - \dot{m}_{gis} \cdot X_{gis,j} \\ \frac{\partial(m_{go} \cdot X_{go,j})}{\partial t} &= - \frac{\partial(\dot{m}_{go} \cdot X_{go,j})}{\partial z} \cdot dz + \dot{m}_{gon} \cdot X_{gon,j} \end{aligned} \quad (2)$$

where the variables  $X_{gi,j}$ ,  $X_{go,j}$ ,  $X_{gis,j}$  and  $X_{gon,j}$  represent the mass loading of the PM class  $j$  in the inlet and outlet channels and at the south side of the inlet and the north side of the outlet channel, respectively. The PM loadings in the gas are transported in a passive manner without backlash to the gas flow. Their transient change depends on convective transport in axial direction and the transverse transport into and from the wall, respectively. The PM classes can differentiate between arbitrary individual characteristics such as particle diameter, number of particles per class or PM composition.

### Wall Gas Phase, Cake and Substrate

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

$$\begin{aligned} \frac{\partial(m_{gw})}{\partial t} &= - \frac{\partial(\dot{m}_{gw})}{\partial x} \cdot dx + dx \cdot A_w \\ &\cdot \left[ \begin{aligned} &+ \sum_l MG_l \cdot v_{c,i,l} \cdot \sum_i \dot{r}_{c,i} (T_{sw}, w_{gw}, \psi_c) \\ &+ \sum_l MG_l \cdot v_{w,i,l} \cdot \sum_i \dot{r}_{w,i} (T_{sw}, w_{gw}, \psi_w) \end{aligned} \right] \end{aligned} \quad (3)$$

where  $m_{gw}$  represents the mass of the gas phase in the cake / porous wall and  $\dot{m}_{gw}$  is the mass flow through the cake / wall. The second and third term on the right side describe mass sources due to chemical reactions taking place in the PM cake and the wall, respectively. PM regeneration or surface adsorption and desorption reactions lead to continuity sources.  $MG_l$  is the molar mass of species  $l$  and  $A_w$  is the cross section available for the gas flow through the cake and wall. It is assumed to be constant in all wall balance equations. This simplification is made as the cross section is only used to evaluate local flow velocities as input for empirical heat and mass transfer correlations. The variables  $\dot{r}_{c,i}$  and  $\dot{r}_{w,i}$  represent a volume specific mole rate of reaction  $i$  in the cake and the wall, respectively. The rates are evaluated as a function of the wall substrate temperature  $T_{sw}$  and, depending on the type of reaction, they are typically a function of the gas composition  $w_{gw}$ , the PM cake and wall state  $\psi_c, \psi_w$ , including different PM deposit populations and surface species. The variables  $v_{c,i,l}$  and  $v_{w,i,l}$  represent the stoichiometric coefficient of species  $l$  in the  $i$ 'th cake or wall reaction, respectively. The boundary condition of the spatial mass flow derivative

at  $x = 0$  is given by the mass flow  $\dot{m}_{gis}$  of the inlet channel (Eq.1). The mass flow source  $\dot{m}_{gin}$  of the outlet channel (Eq.1) is fed by the mass flow leaving the wall.

The PM loading balance in the wall is represented by

$$\begin{aligned} \frac{\partial(m_{gw} \cdot X_{gw,j})}{\partial t} &= - \frac{\partial(\dot{m}_{gw} \cdot X_{gw,j})}{\partial x} \cdot dx \\ &- \dot{m}_{gwn} \cdot X_{gwn,j} \cdot E_{dep,j} \end{aligned} \quad (4)$$

where  $X_{gw,j}$  represents the mass loading of PM class  $j$  in the gas phase of the wall. The transient mass change of each class depends on convective transport and on a PM deposition rate. The deposit rate depends on the incoming PM mass flow and macroscopic filtration efficiency  $E_{dep,j}$ , Tien [15]. The filtration efficiency is noted with the index  $j$  as it is a function of the particle size and it also changes depending the spatial position differentiating between PM cake and wall deposit layer. The boundary conditions of the PM loading balance are connected to the inlet and outlet channel (Eq.2) in analogy to the continuity equation.

The conservation equation of PM deposit considers sources due to PM filtration and sinks due to PM regeneration reactions. Following the approach of multiple PM states presented by Konstandopoulos et al. [16], the overall PM balance is split into individual population/ state balance equations. The different populations represent different components of diesel engine PM such as volatile organic compounds, amorphous disordered and graphitic soot. Additionally, the populations feature different contact states to, if present, catalytically active sites and individual kinetic rate parameters. The balance equations are given by

$$\begin{aligned} \frac{dm_{sw,l}}{dt} &= \sum_j \dot{m}_{gwn} \cdot X_{gwn,j} \cdot E_{dep,j} \cdot \theta_{l,j} \\ &- k_l \cdot m_{sw,l} + \xi_l \cdot k_l \cdot m_{sw,l} \\ \frac{dm_{sw,k}}{dt} &= \sum_j \dot{m}_{gw} \cdot X_{gw,j} \cdot E_{dep,j} \cdot \theta_{k,j} \\ &- k_k \cdot m_{sw,k} - \xi_{k-1} \cdot k_{k-1} \cdot m_{sw,k-1} + \xi_k \cdot k_k \cdot m_{sw,k} \\ \forall k &= 2, n-1 \\ \frac{dm_{sw,n}}{dt} &= \sum_j \dot{m}_{gw} \cdot X_{gw,j} \cdot E_{dep,j} \cdot \theta_{n,j} \\ &- k_n \cdot m_{sw,n} - \xi_{n-1} \cdot k_{n-1} \cdot m_{sw,n-1} \end{aligned} \quad (5)$$

where  $m_{sw,k}$  represents the mass of the  $k$ 'th PM population in the wall or cake. The PM deposit onto each population is given by the sum over the deposition rates of the individual PM classes in the gas phase. Here,  $\theta_{k,j}$  is a dimensionless distribution factor ( $\sum_k \theta_{k,j} = 1$ ) covering the split of the PM classes onto the deposit populations. For the time being,  $\theta_{k,j}$  is  $1/n$  for reasons of simplicity. It can be refined based on a more detailed characterization of the composition of the different PM classes. The regeneration of the different populations is

described by the population mass  $m_{sw,k}$  multiplied with  $k_k$ , a generic rate constant. The mobility between the populations is represented by the interaction parameter  $\xi_k$ . It describes the partial replacement of PM in population  $k$  by PM from the next higher ( $k+1$ ) state by physical motion. Konstandopoulos et al. [16] presented a second mobility mechanism describing the fragmentation of populations. This is left out here, as the authors conclude from their experimental data fitting that the contribution of fragmentation is insignificant. The PM regeneration rates on the right hand side seem to use first order approaches with respect to the available PM mass. This can change, see later in the section, since the individual rate constants additionally incorporate dependencies on PM mass.

The overall PM deposit mass  $m_{sw}$  is given by:

$$m_{sw} = \sum_n m_{sw,k} \quad (6)$$

This mass is later used when evaluating the local filtration characteristics depending on the available PM deposit.

### Particulate Matter Deposition

Research of particle filtration in porous media goes back to the sixties of the last century, Tien and Payatakes [17]. In the context of automotive applications, Konstandopoulos and Johnson [10] adopted in an early publication the concept of unit bed collectors to describe the deep bed filtration in wall flow filters. Since then the model has been widely used in literature (see reviews in Koltsakis et al. [3] and Huang [18]). It is based on two ideas. First, the filter wall is split into a series of unit bed elements that are considered to be made up of “unit collectors”. Second, the geometry of the single collector is simple enough (i.e. spherical) to get an analytical solution for the flow trajectories, Mackie et al. [19].

Following Tien [15], the macroscopic wall filtration efficiency  $E_{dep,j}$  used in Eq.(4) can be related to the filtration efficiency of a single collector by

$$E_{dep,j} = 1 - \exp\left(-\frac{3}{2} \cdot (1 - \varepsilon_w) \cdot \frac{\eta_{DR,j}}{d_c} \cdot \frac{U_\infty}{u_{gw,sl}} \cdot \Delta x\right), \quad (7)$$

where  $\varepsilon_w$  represents the porosity of the wall,  $d_c$  is the diameter of a single unit collector and  $\eta_{DR,j}$  is the filtration efficiency of PM class  $j$  in a single collector. The collector approach velocity is given by  $U_\infty$  and  $u_{gw,sl}$  is the superficial wall velocity. The quotient of these two velocities is typically represented by reciprocal wall porosity.  $\Delta x$  represents the thickness of the considered wall slab. Assuming that Brownian diffusion and direct interception are the dominant filtration mechanisms (gravity, inertia or electrostatic forces are comparably small, Ohara et al. [20]) the single collector efficiency of PM class  $j$  combines both according to

$$\eta_{DR,j} = \eta_{D,j} + \eta_{R,j} - \eta_{D,j} \cdot \eta_{R,j}, \quad (8)$$

where  $\eta_{D,j}$  and  $\eta_{R,j}$  represent the diffusive and interceptive collection efficiency, respectively. Table 1 summarizes different filtration approaches from literature and a slightly adapted version is alternatively used in this study. The diffusive collection efficiency is mainly a function of the Péclet number that is defined via interstitial velocity ( $u_{gw,sl}/\varepsilon_w$ ), the collector diameter and the particle diffusion coefficient. The latter is calculated depending on the particle Knudsen number considering a Stokes-Cunningham slip-flow correction. The function  $g(\varepsilon_w)$  covers the impact of the flow field representing Kuwabara's hydrodynamic factor. The interceptive collection efficiency depends on the ratio of particle diameter to collector diameter and also Kuwabara's function.

Table 1. Diffusive and interceptive collection efficiencies.

| #  | Approach                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Reference                        |
|----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------|
| D1 | $\eta_{D,j} = 3.5 \cdot g(\varepsilon_w) \cdot \text{Pe}_j^{-\frac{2}{3}}$                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Konstandopoulos and Johnson [10] |
| D2 | $\eta_{D,j} = 8 \cdot \text{Pe}_j^{-\frac{2}{3}} \quad   \quad (\text{Re} \rightarrow 0)$<br>$\eta_{D,j} = 2.1 \cdot \text{Pe}_j^{-\frac{1}{2}} \quad   \quad (\text{Re} \rightarrow \infty)$                                                                                                                                                                                                                                                                                                                                | Ohara et al. [20]                |
| D3 | $\eta_{D,j} = 0.7 \cdot \text{Pe}_j^{-\frac{2}{3}}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | This study                       |
| R1 | $\eta_{R,j} = 1.5 \cdot \frac{N_{R,j}^2}{(1 + N_{R,j})^3} \cdot g(\varepsilon_w)^3$                                                                                                                                                                                                                                                                                                                                                                                                                                          | Konstandopoulos and Johnson [10] |
| R2 | $\eta_{R,j} = 16 \cdot N_{R,j}^2 \quad   \quad (\text{Re} \rightarrow 0)$<br>$\eta_{R,j} = 16 \cdot N_{R,j} \quad   \quad (\text{Re} \rightarrow \infty)$                                                                                                                                                                                                                                                                                                                                                                    | Ohara et al. [20]                |
| R3 | $\eta_{R,j} = 1.5 \cdot N_{R,j} + 1e - 7 \cdot N_{R,j}^2$                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | This study                       |
|    | $\text{Pe}_j = \frac{u_{gw}}{\varepsilon_w} \cdot \frac{d_c}{D_{p,j}}, N_{R,j} = \frac{d_{p,j}}{d_c}$<br>$s = (3 - 2 \cdot \varepsilon_w) / (3 \cdot \varepsilon_w)$<br>$g(\varepsilon_w)^3 = \frac{\varepsilon_w}{2 - \varepsilon_w - \frac{9}{5} \cdot (1 - \varepsilon_w)^{\frac{1}{3}} - \frac{1}{5} \cdot (1 - \varepsilon_w)^2}$<br>$f(\varepsilon_w) = \frac{2}{9} \cdot \frac{2 - \varepsilon_w - \frac{9}{5} \cdot (1 - \varepsilon_w)^{\frac{1}{3}} - \frac{1}{5} \cdot (1 - \varepsilon_w)^2}{1 - \varepsilon_w}$ | Konstandopoulos and Johnson [10] |

The unit collector diameter and the wall porosity used in Eq. (7) and in Table 1 change while loading a filter and growing PM deposit in the wall structure. Konstandopoulos et al. [21] proposed, considering a spherical growth of the unit collector, the following correlation

$$d_c = 2 \cdot \left[ \frac{3}{4 \cdot \pi} \cdot \frac{m_{sw}}{\rho_{sw}} + \left( \frac{d_{c,0}}{2} \right)^3 \right]^{1/3}, \quad (9)$$

where  $m_{sw}$  is the total PM mass, see Eq.(4), given at any position over the wall height, and  $\rho_{sw}$  is the corresponding PM density in the wall. This value is based on pressure drop measurements, Konstandopoulos et al. [21]. The collector diameter of a clean filter is given by  $d_{c,0}$ . It depends on wall porosity and pore diameter and can be approached using simple geometrical assumptions, Huang [18]. Similar, the local porosity is given by



$$\varepsilon_w = 1 - \left( \frac{d_c}{d_{c,0}} \right)^3 \cdot (1 - \varepsilon_{w,0}), \quad (10)$$

where  $\varepsilon_{w,0}$  represents the clean filter porosity, a value that is typically given by filter manufacturer data sheets.

The impact of the collected PM mass on the filter wall permeability and pressure drop is expressed, following Konstandopoulos and Johnson [10], by

$$k_f = k_{f,0} \cdot \left( \frac{d_c}{d_{c,0}} \right)^2 \cdot \frac{f(\varepsilon_w)}{f(\varepsilon_{w,0})}, \quad (11)$$

where  $k_{f,0}$  is the permeability of the clean filter wall and  $f(\varepsilon_w)$  represents Kuwabara's flow function (see Table 1) for a bed of spherical particles. It is evaluated using the permeability of the clean and loaded filter wall.

The transition of the deep bed filtration model to the cake filtration model is described by the partition factor  $\Phi$ . It represents the fraction of available free flow area to the maximum free area. It is given by

$$\Phi = \frac{d_c^2 - d_{c,0}^2}{(\psi \cdot b)^2 - d_{c,0}^2}, \quad (12)$$

where  $b$  is the diameter of the unit collector and  $\psi$  is the percolation factor. It is used for model parameterization purposes. The partition factor is evaluated for the top most computational cell when numerically discretizing the wall.

### Particulate Matter Regeneration

The regeneration of PM in particulate filters can be described as heterogeneous, gas-solid reaction of oxygen and nitrogen dioxide on the gas side and on the solid side of different types of volatile hydrocarbons adsorbed at an inhomogeneous structure of carbon micro-particles. The complexity of diesel PM conversion behavior has been experimentally investigated by many studies (i.e. Neeft et al. [22], Darcy et al. [23] and Konstandopoulos et al. [16]) where the following rate equation can be identified as a common basis

$$\dot{r} = k_0 \cdot \exp\left(\frac{-E_a}{R_{\text{mol}} \cdot T_{\text{sw}}}\right) \cdot p_x^{o_x} (1 - \zeta)^{o_\zeta}. \quad (13)$$

Three different dependency groups can be distinguished. The temperature dependency follows Arrhenius with  $k_0$  and  $E_a$  representing the frequency factor and activation energy, respectively. Second, the gaseous reaction educt  $X$  influences the rate via its partial pressure including a reaction order  $o_x$ . Here, the influence of other gas species is not considered. This is reasonable e.g. for water in its typical concentration range of 3 % and higher, Neeft et al. [22], Messerer et

al. [24]. Third, the dependency on PM mass is considered by its conversion  $\zeta$  to the power of a reaction order  $o_\zeta$ . This reaction order can be analytically estimated ( $o_\zeta = 2/3$ ) applying the shrinking core model (Levenspiel [25]) for mass transfer limited operating conditions and the assumption that heterogeneous reactions strongly depend on the available reaction surface. Deviations from the two-third order can be attributed to the fact that PM is not an ideal sphere with a homogeneous porosity where the reaction takes only place at the surface. Following Darcy et al. [23], the analytic reaction order fits reasonably well in the conversion range between 15 % and 90 %. The poor fit at low and high conversion is overcome by introducing multiple PM populations featuring individual rate constants, Konstandopoulos et al. [16]. The influence of catalytic active sites, fuel born or wash coat, is covered by the multiple population model where different catalytic activities are reflected by different Arrhenius parameters. The simulation cases presented later in this work rely on two sets of reaction parameters taken from literature. Table 2 shows the reaction constants and reaction orders used to calculate catalytically supported PM oxidation at three different temperatures. The reaction order of 2/3 is chosen following several hints on the shrinking core model in the given reference. The reaction order one is chosen as alternative to reveal the impact of different reaction orders. Here the rate constants of the 2/3 approach have been adapted with to goal of getting a close match with the published data.

Table 2. Reaction parameters for the two population models based on Konstandopoulos et al. [16].

| T<br>(°C) | $k_1$<br>(variable/s) | $k_2$<br>(variable/s) | $o^x$<br>(-) | $o^\zeta$<br>(-) |
|-----------|-----------------------|-----------------------|--------------|------------------|
| 560       | 5.97e-2               | 5.95e-4               | 1            | 1                |
| 560       | 2.93e-3               | 5.06e-5               | 1            | 2/3              |
| 590       | 6.83e-2               | 6.30e-4               | 1            | 1                |
| 590       | 3.35e-3               | 5.36e-5               | 1            | 2/3              |
| 620       | 8.95e-2               | 9.55e-4               | 1            | 1                |
| 620       | 4.39e-3               | 8.12e-5               | 1            | 2/3              |

Table 3. Reactions for the single population model.

| Approach                                                                                 | Component | Reference                                                                     |
|------------------------------------------------------------------------------------------|-----------|-------------------------------------------------------------------------------|
| $\text{C(s)} + 1/2 \text{O}_2 \rightarrow \text{CO}$                                     | DPF, cDPF | Premchand et al. [26]                                                         |
| $\text{C(s)} + \text{O}_2 \rightarrow \text{CO}_2$                                       | DPF, cDPF | Premchand et al. [26]                                                         |
| $\text{C(s)} + \text{NO}_2 \rightarrow \text{NO} + \text{CO}$                            | DPF, cDPF | Premchand et al. [26]                                                         |
| $\text{C(s)} + 2 \text{NO}_2 \rightarrow 2 \text{NO} + \text{CO}_2$                      | DPF, cDPF | Premchand et al. [26]                                                         |
| $\text{CO} + 1/2 \text{O}_2 \rightarrow \text{CO}_2$                                     | cDPF, DOC | Premchand et al. [26]                                                         |
| $\text{C}_3\text{H}_6 + 9/2 \text{O}_2 \rightarrow 3 \text{CO}_2 + 3 \text{H}_2\text{O}$ | cDPF, DOC | Premchand et al. [26], adapted from $\text{C}_{12}\text{H}_{24}$ , this study |
| $\text{NO} + 1/2 \text{O}_2 \leftrightarrow \text{NO}_2$                                 | cDPF, DOC | Premchand et al. [26]                                                         |

A second set of reaction is given in Table 3. It comprises PM oxidation reactions following a single population model and catalytically supported oxidation reactions of several gas species. PM oxidation takes place in the presence of oxygen and nitrogen dioxide