CFD MODELING OF THE REGENERATION PROCESS IN DIESEL PARTICULATE FILTER USING FLUENT

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Abstract

Diesel engine particulate filters every year are becoming more popular. The new EURO 5 standard is very restrictive for particulates and this will force the use of particulate filter in every engine. Filters operate very good when they are loaded with small quantity of soot particles and they must be cleaned from time to time by burning out soot inside the filter. This process is called filter regeneration. During regeneration high temperature zones may occur in the filter which may change the properties of porous material and even cause its damage. The regeneration process should be effective at different engine operational conditions in which temperature and oxygen concentration vary. The experimental determination of optimal conditions for regeneration is very difficult and expensive. The simpler and less expensive is computer modeling.

In this paper computer simulation of regeneration process of diesel particulate filter with the use of FLUENT code is described. A two-dimensional model assumes soot and filter wall as a porous materials of different permeability. The influence of soot parameters, filter material, composition and temperature of combustion products as well as activation energy on regeneration process was studied.

Keywords: simulation, soot, air pollution, CFD

1. The of model of particulate filter in Fluent

Real particulate filter is presented as 2D model. In this article only the selected part of filter is modeled. An analysis of the influence of channel position in the filter on the process of regeneration has not been done. It is assumed that all channels behave similarly. They are of the same mass soot deposition before regeneration. Thermal conditions are assumed to be the same. The outside wall is adiabatic, as the result of no radial temperature change. This approach gives the possibility to present the mechanism of regeneration process without enlarging calculation net and prolonging calculation time.

The modeled particulate filter consists of the following parts (Fig.1):
- half inlet channel,
- soot layer deposited on porous wall,
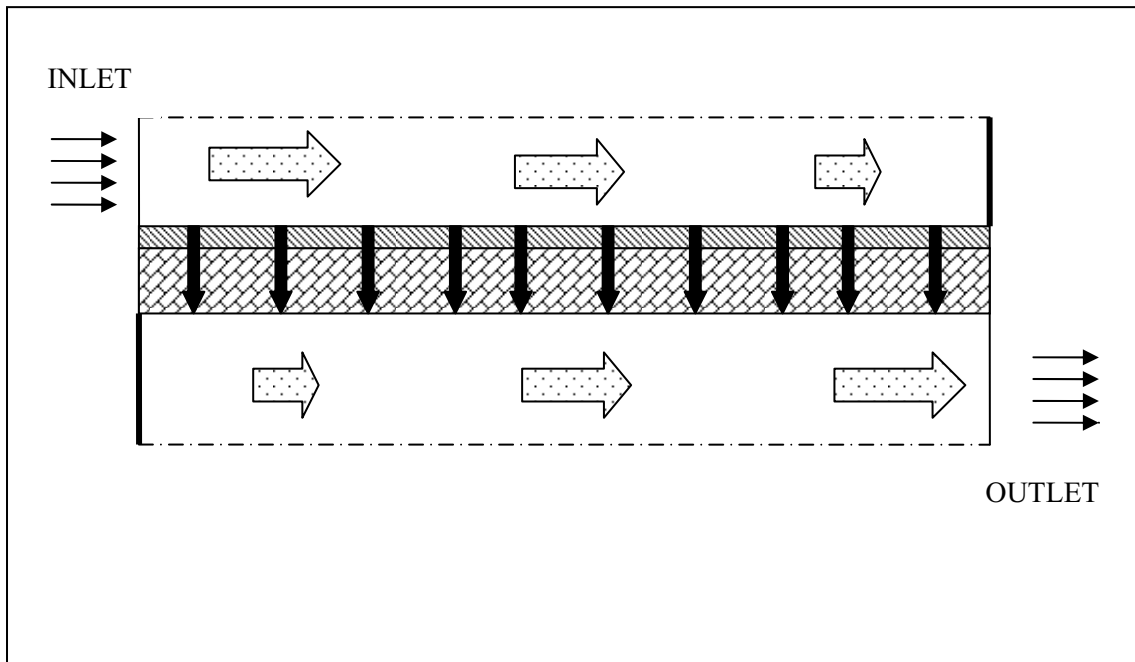- porous wall,
- half outlet channel.

Figure 1. Schematic of particulate model

The exhaust gases are poured into the inlet channel. The gases are forced through the soot layer and the porous wall. The exhaust gases leave the wall and flow into the outlet channel. The outlet channel allows them to move in the direction of outlet from the filter.

The real particulate filter channel can be divided by symmetry plane. The model contains only half of the channel. That approach gives some advantages: reduction of model space and simplification of calculation without influence on results. The reduction of calculation space and better-chosen shape of cells allow for the reduction of number of cells. Similar operation is done for outlet channel.

Particulate layer and monolith wall are modeled as porous media. Porous soot layer has similar properties to soot. The soot layer is the most important zone of the model, it is determined by net shape. Monolith is defined as cordierite.

Simulations have been performed using Fluent code. The Fluent gives velocity field, pressure field, it calculates soot combustion process and the exhaust gas composition. The most important parameter calculated by the Fluent code is soot mass depletion. The soot oxidation is done with the use of outsource procedure because the newest Fluent version does not give possibility to define combustion, depletion and porous material together. The outsource procedures are used to calculate the material property of deposited particulate. Property of soot layer is changed according to change of soot mass in the filter. Figure 2 shows the schematic of computations.

2. The mathematical model

Mathematical model was based on Fluent code. The equations for inlet and outlet channels have similar form and they are presented together.

The continuity equation for channels can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \cdot \qquad (1)$$

The momentum conservation equation is described by:

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla (\rho v v) = -\nabla P + \nabla (\bar{\tau}). \qquad (2)$$

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┌─────────────┐
│    Start    │
└─────────────┘
       │
       ▼
┌──────────────────────────────────────┐
│  Calculation of temperature, velocity, │◄────┐
│  pressure field, mass fraction of exhaust │     │
│        gases in The Fluent             │     │
└──────────────────────────────────────┘     │
       │                                       │
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┌──────────────────────────────────────┐     │
│  Soot mass depletion - calculated in outsource │     │
│  procedure                             │     │
└──────────────────────────────────────┘     │
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┌──────────────────────────────────────┐     │
│   Solution of energy equation in       │     │
│          The FLUENT                    │     │
└──────────────────────────────────────┘     │
       │                                       │
       │   ┌──────────────────────────┐       │
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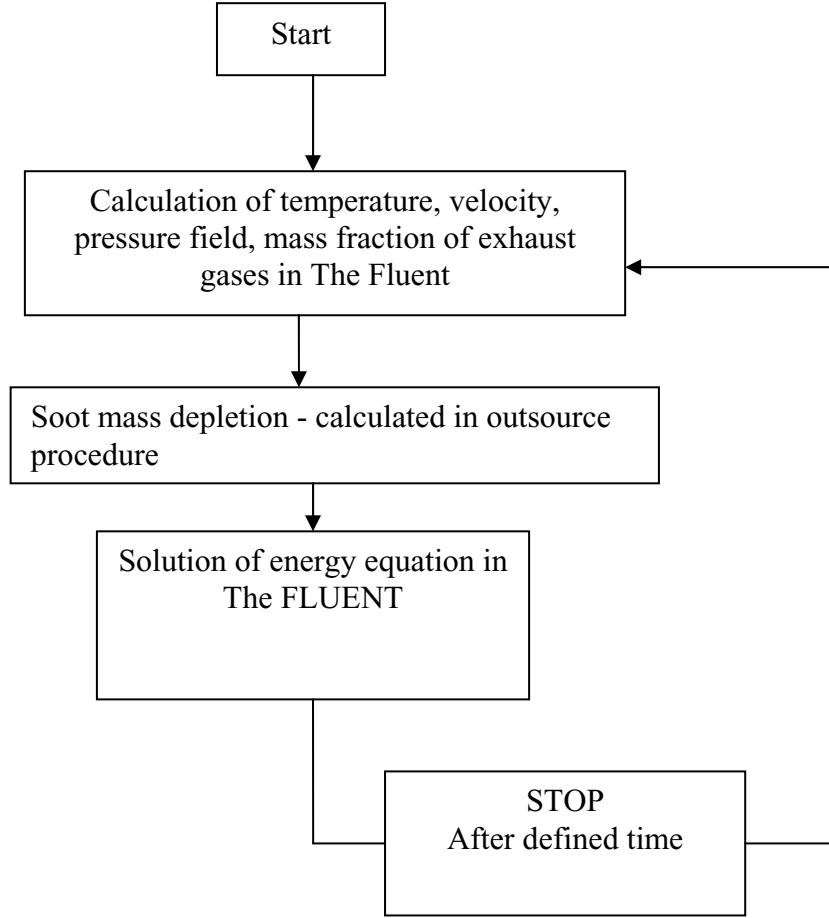
Figure 2. Scheme of calculation

The energy equation is:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla\left[k_{eff}\nabla T - \left(\sum_i h_i J_i\right) + (\bar{\tau}v)\right] + S_h .\tag{3}$$

where:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2},$$

$$h = \sum_j Y_j h_j,$$

$$h_j = \int_{T_{ref}}^{T} c_{p,j}\,dT,$$

$$k_{eff} = \varepsilon\lambda + (1-\varepsilon)\lambda_w .$$

The particulate layer and monolith wall are described by similar equations. They are defined as porous materials. Thus equations are presented together except for necessary ones.

Assuming isotropic porosity and single phase flow the continuity equation is:

$$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla(\varepsilon\rho\vec{v}) = S_p .\tag{4}$$

At the porous wall $S_p=0$.

The momentum conservation equation is:

$$\frac{\partial(\varepsilon\rho\vec{v})}{\partial t} + \nabla(\varepsilon\rho\vec{v}\vec{v}) = -\varepsilon\nabla P + \nabla\varepsilon\tau - \frac{\mu}{\alpha}\vec{v}.$$ (5)

The energy equation is:

$$\frac{\partial}{\partial t}\left(\varepsilon\rho h(T) + (1-\varepsilon)\rho_w h_w(T)\right) + \nabla\left(\rho\vec{v}h(T) + p\right) = \nabla\left[k_{eff}\nabla T - \left(\sum_i h_i J_i\right) + \left(\overline{\tau}\vec{v}\right)\right] + S_h,$$ (6)

where:

$$k_{eff} = \varepsilon\lambda + (1-\varepsilon)\lambda_w$$

Carbon is put into porous soot layer zone and it is burned there. Chemical reaction has the following form:

$$C + O_2 \rightarrow CO_2.$$ (7)

Chemical kinetics is calculated by Fluent. The Fluent uses the laminar finite-rate model of reactions. The forward rate constant is computed using the Arrhenius expression:

$$k = AT^\beta e^{-E/RT}.$$ (8)

In this model β is assumed as equal to 0.

The soot mass decrease is proportional to deposited mass and the rate of reaction determined by oxidation:

$$\frac{dm}{dt} = -m_s RR,$$ (9)

$$\int_1^2 \frac{dm}{m_s} = -\int_1^2 RR\,dt.$$ (10)

After integration the mass at the next time step is given by:

$$m_2 = m_1 \exp(-RR\Delta t).$$ (11)

The equation of mass depletion is as follows:

$$\frac{dm}{dt} = \frac{-m_1[1-\exp(-RR\Delta t)]}{\Delta t}.$$ (12)

The reaction rate is:

$$RR = A * [O_2] * \exp\left(-\frac{E}{RT}\right).$$ (13)

During soot mass oxidation material properties are changed. The outsource procedures control and change of permeability and porosity. The permeability is changed from initial value to 0 and the porosity from initial value to 1. Final values mean no soot.

3. Results

For all simulations the initial conditions were similar. The filter temperature is 600 K, mass fraction of nitrogen is equal to 100%. The regeneration process is determined by initial conditions, the temperature of inlet gases, the mass of deposited soot, the mass fraction of oxygen in inlet gases.

3.1 The influence of monolith physical properties on regeneration process

Monolith properties are defined mainly by porosity, thermal conductivity, density and specific heat. The porosity and the thermal conductivity have been set up at the level of 50% and 2 W/m/K, respectively.

The values of specific heat and density are presented in table 1.

Table 1. The monolith properties

No.	Density [kg/m^3]	Specific heat [J/kg/K]
1	2000	750
2	1250	750
3	1250	1100
4	2000	1100

The first row of table 1 contains values taken from [2]. The third row contains the most popular values presented in the literature. Density and specific heat in second and fourth rows are the combination of above-mentioned values. Porosity depends on density. In a few cases density is depended on an average pore diameter (www.dieselnet.com).

The parameters which characterize our regeneration process are collected in table 2.

Table 2. The parameters of regeneration at different material properties

	Case number			
	1	2	3	4
The first cell without soot [s]	310	200	290	440
Advanced regeneration process [s]	430	270	380	570
End of regeneration [s]	540	380	510	740
Max. temperature of regeneration [K]	2093	2471	2224	1747
Max. temperature of advanced process [K]	1810	1910	1840	1510

The thermal capacity is a multiplication of specific heat and mass (mass = density*volume; volume is constant in all examples). If the thermal capacity is too small, the regeneration process is too rapid and temperature is too high. High temperature is not recommended for particulate filter, it can damage the filter. The rapid regeneration is difficult to simulate. When the regeneration process is faster, the time step size should be shorter. If the time step size is not short enough, solution is not converged. Short time step requires long calculation time. It should be noted, that object files are saved every 10 seconds.

The following figures are presented for better explanation of the influence of monolith properties. The data for the figures were noted at 290 second of the process. This time is determined as the time of first burnt cells of soot for the third example.

The characteristics of the regeneration process is given in table 4. The following data are given: the soot fraction in cells, the mass fraction of oxygen and the temperatures.

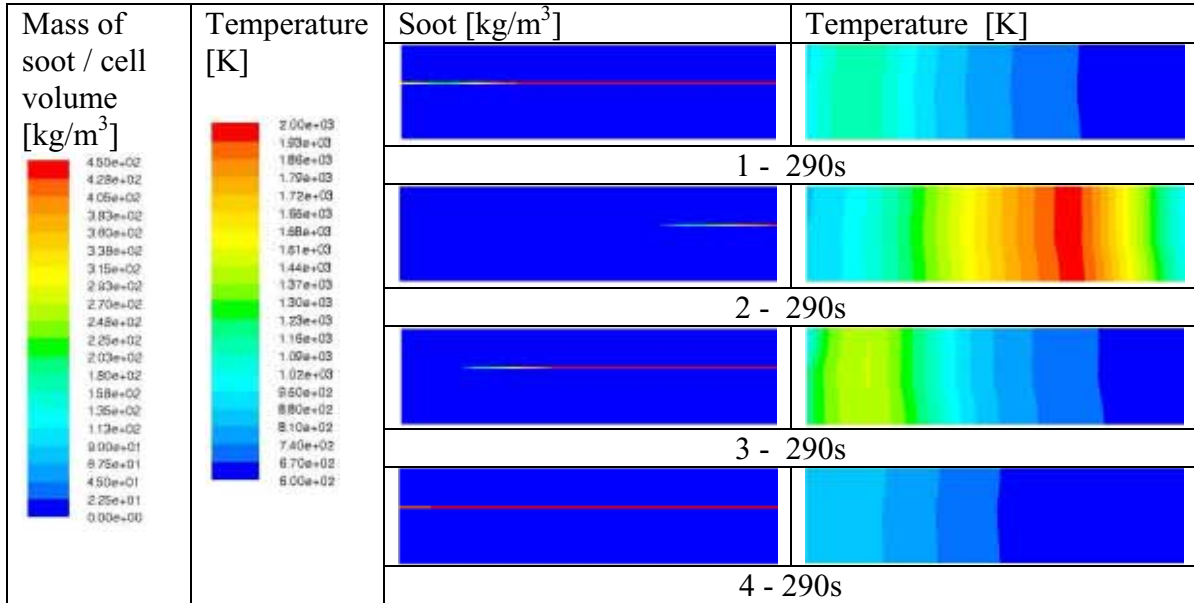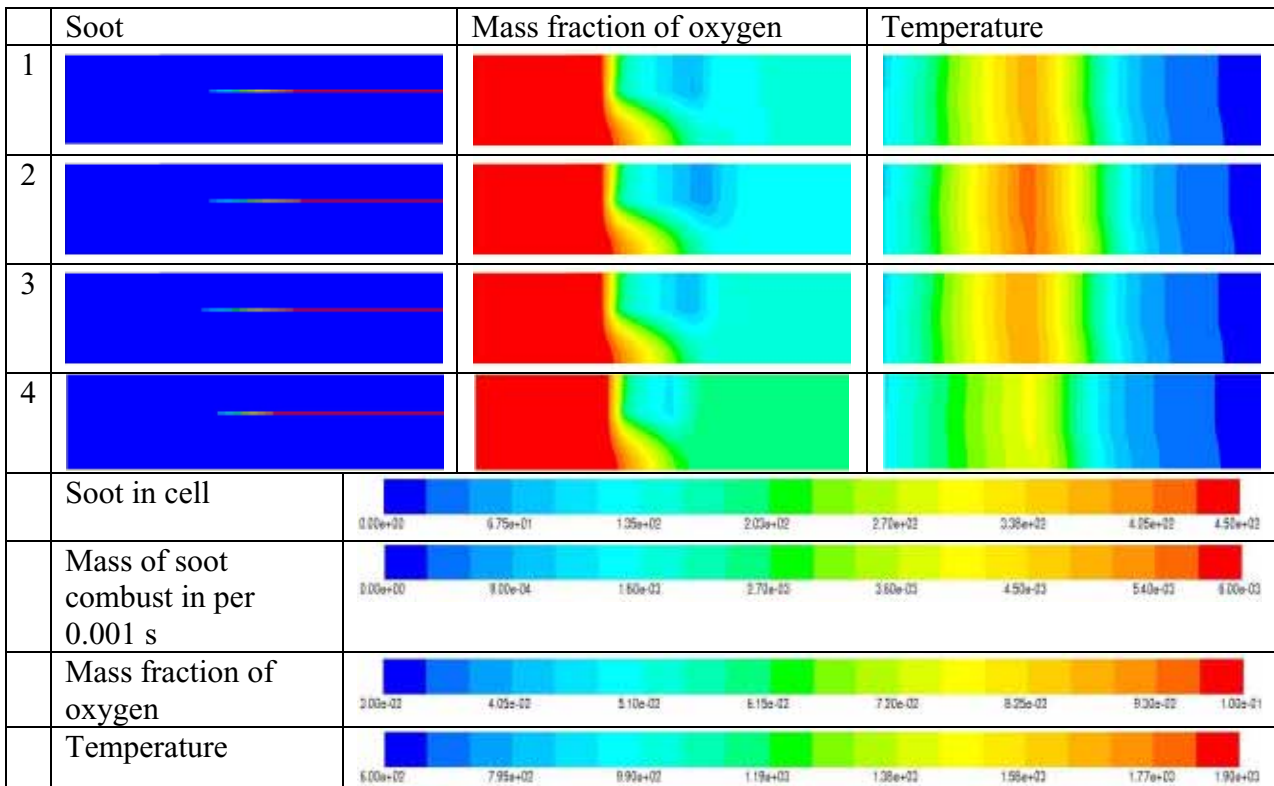*Table 3. Diagram at the same time.*

Table 4 Diagram at the same position of oxidation front

Tables 3 and 4 show the influence of thermal capacity on regeneration process. Table 4 presents in columns: mass of soot and mass fraction of oxygen present at the reaction zone. The space of reaction is the largest at the second configuration. Similarly the temperature of reaction is

the highest. The density and the specific heat are the smallest in the second example. The opposite configuration (4) is characterized by the lowest temperature of reaction and the smallest reaction zone. The third and the first row present similar characteristics.

The specific heat of 1100 J/kg/K and the density of 1250 kg/m^3 were used.

3.2 The influence of exhaust gas temperature

Regeneration begins only at inlet temperature of the appropriate value. So, the exhaust gases have to be hot enough. The following tables show simulation examples with 0.1 inlet mass fraction of oxygen.

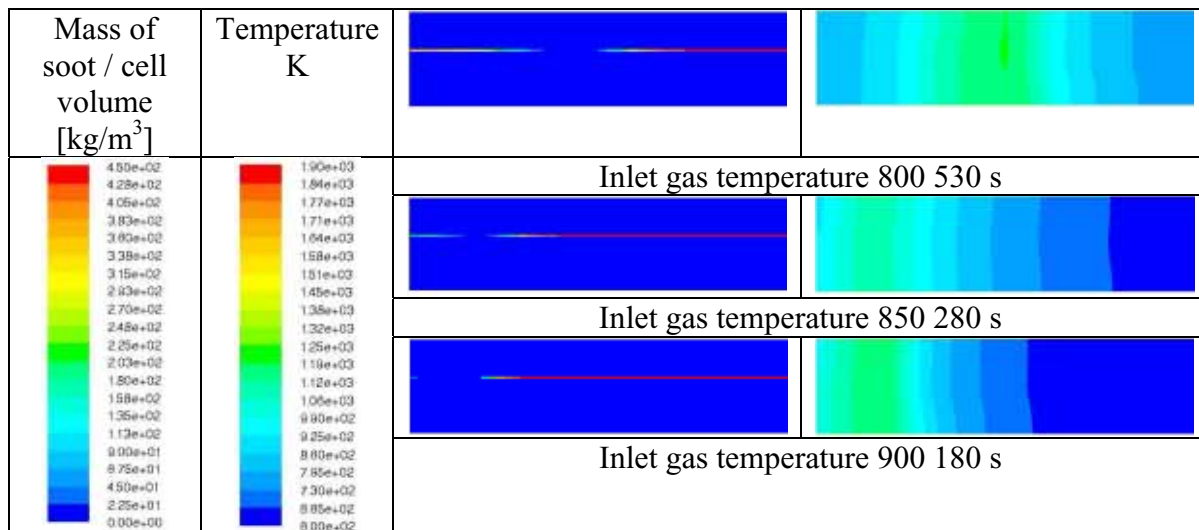*Table 5. The parameters of regeneration at different inlet gas temperature*

	Inlet temperature [K]			
	750	800	850	900
The first cell without soot [s]	-	530	280	180
Advanced regeneration process [s]	-	-	330	250
End of combustion [s]	-	630	440	370
Max Temperature of regeneration [K]	-	1460	1450	1460
Max temperature of advanced oxidation [K]	-	1200	1281	1279

No values at 750 K column means, that determination of the sought parameters is difficult. That example has taken 1100 seconds of simulation time (3-4 days of calculation on Xeon 2.8 GHZ).

Despite of the long time of simulation the cells with burnt soot were not observed. There are some sights of regeneration. The temperature of filter is higher than the inlet gas temperature. Maximum temperature is observed at the end of filter and is equal to 835 K. The similar sight is given by mass fraction of oxygen inside filter. At the end of filter the mass fraction of oxygen is about 9.6 %, the inlet mass fraction of oxygen is 10 %. Probably, the first burnt soot cell would be at the end of filter. The assumption is based on above-mentioned observations and lower fraction of soot in the soot layer at the end of the filter.

The inlet temperature determines the place of the first burnt cells. When temperature increases, the place of first burnt cells moves to the inlet. It is shown at the following tables.

Table 6. Place of the first burnt cells

Mass of soot / cell volume [kg/m^3]	Temperature K		
		Inlet gas temperature 800 530 s	
		Inlet gas temperature 850 280 s	
		Inlet gas temperature 900 180 s	

At low inlet gas temperature, time between the start of simulation and the beginning of oxidation is longer. But when inlet gas temperature is higher, the gas generates earlier reaction, which takes place at the inlet.

The regeneration process is divided into two parts: heating up time and soot oxidation time. The heating up time is longer when the inlet temperature is lower, nevertheless, the whole filter is heated up. If the temperature of filter is higher, the oxidation time is shorter. The part of released energy used to heat-up the filter is smaller. The higher temperature begins earlier but the oxidation is longer. It means that significant part of released energy is used to heat up the reaction zone.

3.3 The influence of deposited soot mass and mass fraction of oxygen

The next interesting parameters are mass fraction of oxygen and mass of soot deposited on porous wall. An analysis of Arrhenius equation indicates linear relation between mass fraction of oxygen and reaction rate.

Tables 7 and 8 show an influence of these parameters on regeneration process.

Table 7. Parameter of regeneration at different mass of deposited soot and mass fraction of oxygen.

Kg of soot / m3 of cell	200		300	450	
Mass fraction of oxygen	10 %	23%	10%	10 %	23%
The first cell without soot [s]	280	180	290	290	170
Advanced regeneration process[s]	330	250	360	370	230
End of combustion [s]	440	370	480	510	330
Max Temperature of regeneration [K]	1450	1309	1773	2224	1853
Max temperature of advanced oxidation [K]	1281	1147	1487	1818	1407

Table 8. Regeneration at the same position of oxidation flame.

"Oxygen" 10 "soot" 200 "time" 330s

"Oxygen" 23 "soot" 200 "time" 230s

"Oxygen" 10 "soot" 300 "time" 360s

"Oxygen" 10 "soot" 450"time" 370s
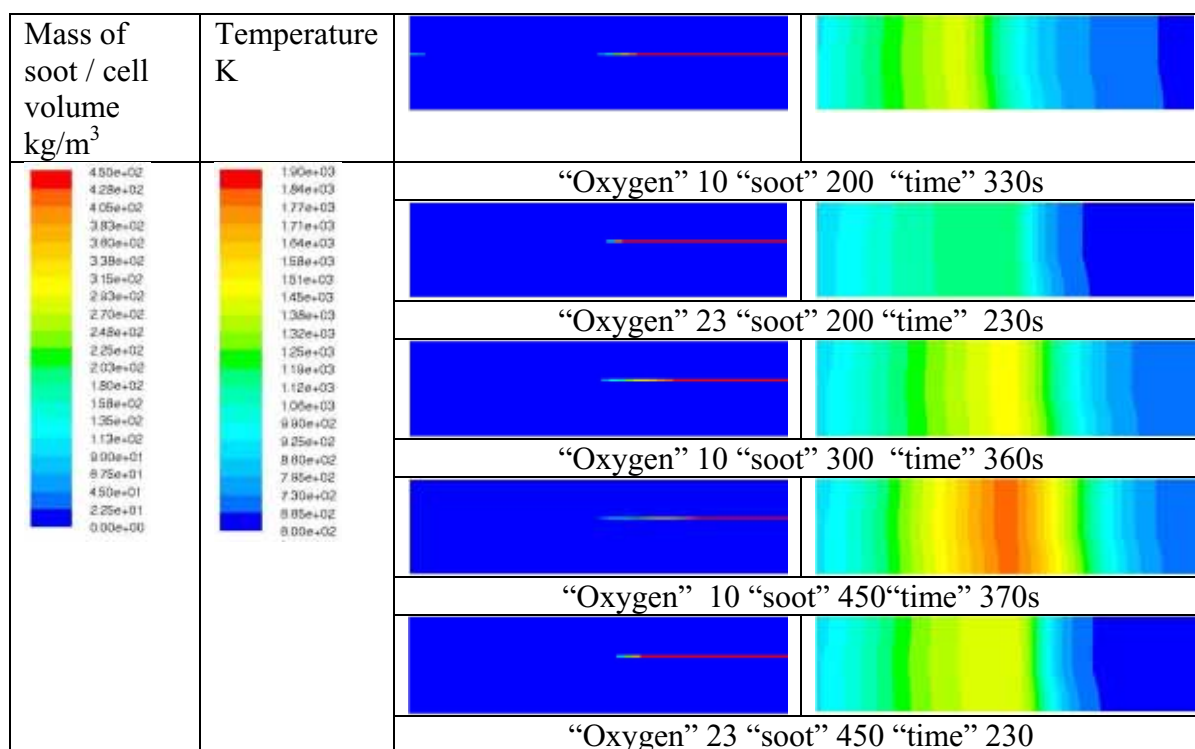
"Oxygen" 23 "soot" 450 "time" 230

Table 8 compares simulations of advanced oxidation at the same time of regeneration. Temperature plots on the diagram are useful for an explanation of surprising data in table 7. The higher temperature at 10% mass fraction of oxygen could explain stronger influence of inlet gas temperature on reaction zone. It is shown via comparison of temperature diagram for 10% oxygen fraction, 200 kg/m^3 soot fraction with temperature diagram for 23% oxygen fraction, 200 kg/m^3 soot fraction. Similar conclusion is given by a comparison of temperature diagram for 10% O$_2$, 450kg/m^3 soot and temperature diagram for 23% O$_2$, 450 kg/m3 soot. Upper temperature range is larger at 10% of O$_2$ than 23% of O$_2$.

The lower temperature in the example with 23 % mass fraction of oxygen is caused by the filter which is not hot enough. Part of the energy release during combustion is consumed to heat up the wall. Because the filter warm-up time is longer for the example with 10 % mass fraction of oxygen and time of oxidation is shorter and the local temperature is higher. When the front of combustion moves to the end of channel, the hot wall gives back the heat to the gas, what boosts the reaction.

An increase of mass deposited on the filter wall provides the soot layer with more energy. The energy is released, when the soot is burned. The release of larger energy is the reason of higher temperature of filter. Temperature during regeneration is higher when mass of deposited soot is higher. This shows how important is the release energy for regeneration process.

4. Conclusions

1. Inlet gas temperature, mass fraction of oxygen, mass of soot layer influence the rate of energy release during the regeneration process. Density and specific heat determine the value of thermal capacity.
2. Higher thermal capacity protects the filter from high temperature, which can damage the filter monolith.
3. An appropriate combination of inlet temperature, oxygen mass fraction and soot deposit controls regeneration process. This combination should be adequate for the specified density and the specific heat.
4. Combustion initial time and oxidation period are dependent of all parameters.

Symbols

A   pre-expotential factor
E   activation energy
h   gas enthalpy
h$_w$ porous media enthalpy
k$_{eff}$ effective thermal conductivity
S$_h$ fluid enthalpy source term
J$_i$ mass flux of species i
h   gas enthalpy
h$_i$ enthalpy of species i
[O$_2$]   mole fraction of oxygen
P   pressure
R   universal gas constant
v   velocity
S$_p$ source term
S$_h$ enthalpy source term
α thermal diffusivity of porous media

β	temperature exponent
ε	porosity
λ	gas thermal conductivity
λ_w	porous media thermal conductivity
μ	dynamic viscosity
ρ	density of fluid
ρ_w	porous media density
$\overline{\tau}$	stress tensor

References

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