

A New CFD Model for Understanding and Managing Diesel Particulate Filter Regeneration

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# **DPF Technology Development**

- Understand Regeneration
  - When?
  - How?
- Characterize Soot Loading and Pressure Drop vs. Time
- System Control
  - Model-Based Feed-Forward Adaptive Control
- Component Development
- Flow Distribution and Thermal Management



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# **Why Model Regeneration?**

- Goal: Achieve Quick, Complete and Safe Regeneration with Minimal Fuel Penalty
- Regeneration is Very Complex
- Experiments are Difficult and Costly
- Modeling Allows Us to Optimize System and Regeneration Strategy



# **Regeneration Is Complex**

- 3-D, Transient Flow
- Three Modes of Heat Transfer
- Porous Layers: Substrate and Soot
- Soot Combustion / Catalyst Effect
- Variable Properties: Porosity, Permeability, etc.
- Sensitive to Operating Parameters:
  - Exhaust flow rate, gas temperature, soot load, oxygen, filter design, etc.



## **Filter Failure: Want to Avoid**

#### • Ring-off Cracking of Cordierite





# **Regeneration Model: I/O**

Input:

- Filter configuration: dimensions, cell density, wall thickness
- Soot loading / distribution
- Regeneration condition: inlet gas temp, exhaust flow rate, O<sub>2</sub>
- Substrate property: porosity, permeability, thermal, etc.
- Soot property: packing density, permeability, etc.
- Soot reaction kinetics and catalyst effect

Output:

- Spatial and temporal profiles of key variables
  - Temperature, velocity, oxygen, reaction rate, etc.
- Soot distribution (regen efficiency) vs. time
- A tool for parametric and what-if studies



## **Regeneration Modeling: State of the Art**

- Ongoing, lots of good efforts to date
- Mostly 2-D, some 3-D (multiple 2-D channels)
- Lack details at channel level
- Simplified flow equations / Many assumptions
- Single temperature field for all phases: gas, substrate and soot



## **Features in The New Model**

- 3-D for one inlet/outlet channel unit
- Porous medium model for substrate and soot layer
- Generic conservation equations for whole domain
- Capable of separate temperature fields for gas and solid via a heat transfer coefficient
- Arrhenius soot reaction with catalytic effect
- Custom CFD code



## **Computational Domain**



## **Conservation Equations**

#### Continuity equation:

 $\frac{1}{\beta}\frac{\partial}{\partial t}(\beta\rho) + \frac{1}{\beta}\frac{\partial}{\partial x_i}(\beta\rho u_i) = \dot{m}'''$ 

Momentum equations:

$$\frac{1}{\beta}\frac{\partial}{\partial t}(\beta\rho u_k) + \frac{1}{\beta}\frac{\partial}{\partial x_i}(\beta\rho u_i u_k) = \frac{1}{\beta}\frac{\partial}{\partial x_i}\left(\beta\mu\frac{\partial u_k}{\partial x_i}\right) - \frac{\partial p}{\partial x_k} + S_k$$

Energy equation (single temperature):

$$\frac{(\rho c_P)}{\beta} \frac{\partial T}{\partial t} + \frac{\beta \rho c_{P,f}}{\beta} u_i \frac{\partial T}{\partial x_i} = \frac{1}{\beta} \frac{\partial}{\partial x_i} \left( k_{eff} \frac{\partial T}{\partial x_i} \right) + S_E$$

Species continuity equation:

$$\frac{1}{\beta}\frac{\partial(\beta\rho Y)}{\partial t} + \frac{1}{\beta}\frac{\partial(\beta\rho u_i Y)}{\partial x_i} = \frac{1}{\beta}\frac{\partial}{\partial x_i}\left(\beta\rho D\frac{\partial Y}{\partial x_i}\right) + S$$



## **Required Model Input:** Soot Reaction Kinetics by TGA





### **Required Model Input:** Soot Cake Shape and Porosity by SEM





#### **Model Validation:** Step 1. Heat-up w/o Regeneration

Heat Up at 160 liter/min - Cordierite





### **Model Validation: Step 2. Regeneration**

800 700 600 Temperature (C) - Measured at 3" down 500 - Measured at 6" down 400 -Measured at 9" down 300 200 180 0 60 120 240 300 Time (sec)

**Temperature Measurements at 3 Axial Locations** 



### **Model Validation: Step 2. Regeneration**

800 700 600 Temperature (C) -Measured at 3" down 500 - Modeled at 3" down -Measured at 6" down Modeled at 6" down Measured at 9" down 400 Modeled at 9" down 300 200 60 120 180 240 300 0 Time (sec)

**Comparing Measurement and Model at 3 Axial Locations** 



## **Model Results:** Velocity and Temperature Fields



#### Colored by Temperature

Cross-sectional View





## **Model Results:** Velocity and Pressure Field

#### Colored by Pressure



Side view – Gas Zone



### **Model Results:** Temperature and Oxygen Distribution



### **Model Results:** Reaction Rate and Soot Distribution



# **Parametric Study:**

#### **Effect of Flow Rate**





### **Parametric Study:** Effect of Soot Loading





## **Parametric Study:** Effect of DPF Inlet Temperature





### **Parametric Study:** Effect of Oxygen





### What-If Study: Runaway Regeneration?

![](_page_25_Figure_1.jpeg)

![](_page_25_Picture_2.jpeg)

# Summary

- A new regeneration model was developed and validated
- Features include: (1) 3-D; (2) A porous model; and (3) Generic equations solved
- The model provides detailed prediction of spatial and temporal distributions of key parameters such as temperature, as well as regeneration efficiency
- The model was shown to be effective in parametric and what-if studies
- A good model is useful in the design and operation of DPF systems, hence shortening development cycle

![](_page_26_Picture_6.jpeg)