Modeling Regeneration in Wall-Flow Diesel Particulate Filters

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Characterization of regeneration modeling:

- Modeling DPF pressure drop: includes *fluid mechanics* only.

- Modeling DPF regeneration:
  - *fluid mechanics.*
  - *heat transfer.*
  - *reaction kinetics.*

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Background:

- First modeling of filter regeneration: Pauli, Lepperhoff, and Pischinger , SAE - 830180, 1983).

- Pioneering work of Bissett (Chem. Eng. Sci., 39, Nos. 7/8, 1233-1244, 1984), Bissett and Shadman, (AIChE, 31.No. 5, 753-758, 1985), further paving the road.

- Continued by
  - Konstandopoulos (Combustion and Flame, 1999, SAE-1999-01-0469, SAE 2000-01-1016, SAE 2001,01-0908, ...).
  - Kandylas, Stamatelos (Indus. Eng. Chem. Res., no. 5, 1866-1876, 1999), ...
  - Opris and Johnson (SAE - 1998 - 980545).
  - MTU team (Johnson's Team -- Awara, Tan, Gadde, … ; several publications).
  - Many recent papers on various regeneration aspects (effect of oscillatory flows, Nox effect, transient effect, ….); mostly in SAE proceedings.
  - (list not exhaustive).

Regeneration Model Formulation:

- Fluid Mechanics:
  - *Conservation of Mass* for inlet channel/ exit channel.
  - *Conservation of Momentum* for channel gas: one balance equation for inlet channel, one for exit channel.

- Heat Transfer:
  - *Conservation of Energy: for gas phase*.
    - One balance for the inlet channel; one for the exit channel.
    - Convective heat exchange between the gas flow and the channel walls (heat added to / removed from the filtration walls)

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Heat Transfer (cont.):

- *Conservation of Energy: for solid phase (filter wall).*
  - Account for convective heat exchange with gas in inlet channel, through wall, in exit channel.
  - Exotherms due to soot combustion.
  - Heat conduction in wall (and in soot layer).
  - Including radiation heat transfer in channel recommended.

  - Key HT mechanism (driver): convection from the gas to the wall. Next: conduction through the wall.

Kinetics:

- Soot combustion and CO selectivity:
  - soot reaction: enthalpy and activation energy consideration.
  - Include additives / catalyst effect / … (if applicable).

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Model Capabilities:

• Simulate “practical” regeneration scenarios (with catalytic coating, fuel borne catalyst, NO2- assisted, ….)

• Simulate 2-d, 3-d simulations / effect of upstream flow non-uniformity on regeneration.

• Model ‘run-time’ should be ‘practical’ (~ minutes for 1-dim., ~ hour for 2-3 dim. simulations).

  • Leaves potential for on-board-diagnostic applications.

• Simulate influence of ash on regeneration (ash production and interactions).

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In addition:

Model should allow

- Effect of hydrocarbon addition / post injection.
- Effect of hydrocarbon adsorption / desorption on particulate reactivity.
- Effect of sulfur content on particulate reactivity
- Effect of catalyst aging
- Effect of ash accumulation on pressure drop and catalyst fouling
- NOx formation during regeneration.

(Perspective from: Konstandopoulos *et al*)

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Model Input -- should be flexible enough to take into account various flow, filter, soot, catalyst, additives, … influencing regeneration:

Model should allow / account for:

- filter *material* (composition) and pore structure (porosity, …) & *filtration characteristics* (mean pore size, porosity, permeability)
- filter *thermophysical properties* (heat capacity, thermal conductivity)
- filter *geometry* (cell density, wall thickness, size, plug length, ring, aspect ratio, bulk mass, ...)
- particulate
  - *growth properties* (cake porosity/ density/ permeability/ structure; SOF, ...) and modes (deep bed following cake layer growth)
  - *composition* (Ash, soot, , HC, …)
- Etc.

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Model output -- should yield both spatial and temporal data (various locations / time) due to regeneration

- Filter wall temperature / temperature gradient
- Gas temperature (inlet to exit)
- Pressure drop evolution during regeneration
- Particulate layer: deposited and remaining (details in time and space) during regeneration (particulate oxidation is typically non-uniform in space and time).
- Species: O_2, CO, CO_2, NO, NO_2, HC, H_2O ,
- Transient input conditions.
- Etc.
- Output should be importable into other platforms for other applications (e.g., thermal stress modeling.)

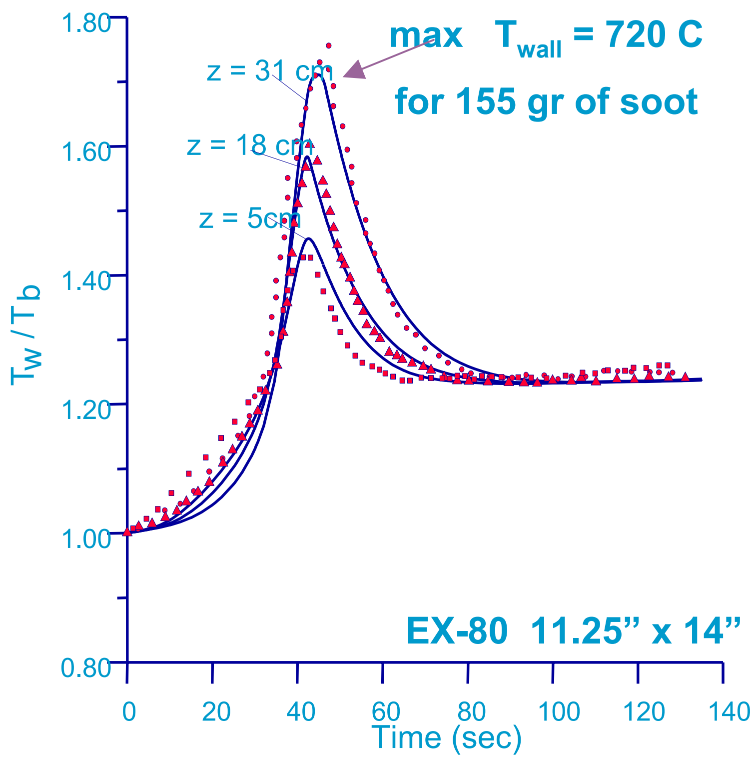
Other:

- It’s wise to build data base of
  - kinetics information,
  - mechanical (porosity, density, permeability, …) and thermal (thermal conductivity, heat capacity, …) properties of soot deposit layer.
  - Similarly relevant information.

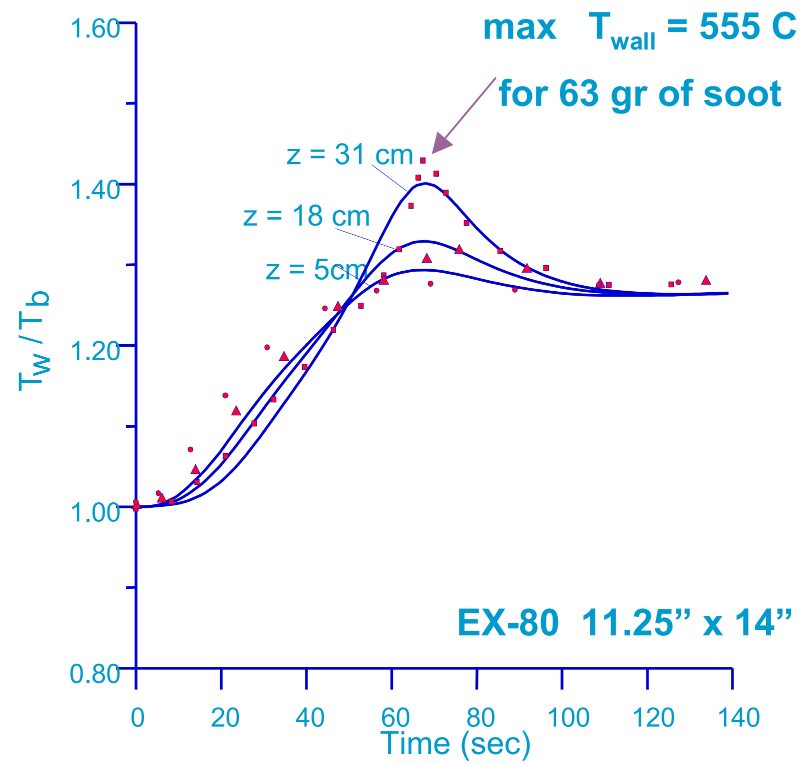
Example -- Simulation Results*

FILTER TEMPERATURE RISE DURING REGENERATION

Model vs. Experiment (data from: Tan et al. SAE 960136)



Filter wall temperature (T_w) for 155 gr of soot loading under controlled regeneration (T_b = 583 K) [1]



Filter wall temperature (T_w) for 63 gr of soot loading under controlled regeneration (T_b = 583 K) [1]

(* from Walter© Regeneration Simulator, Konstandopoulos *et al*)

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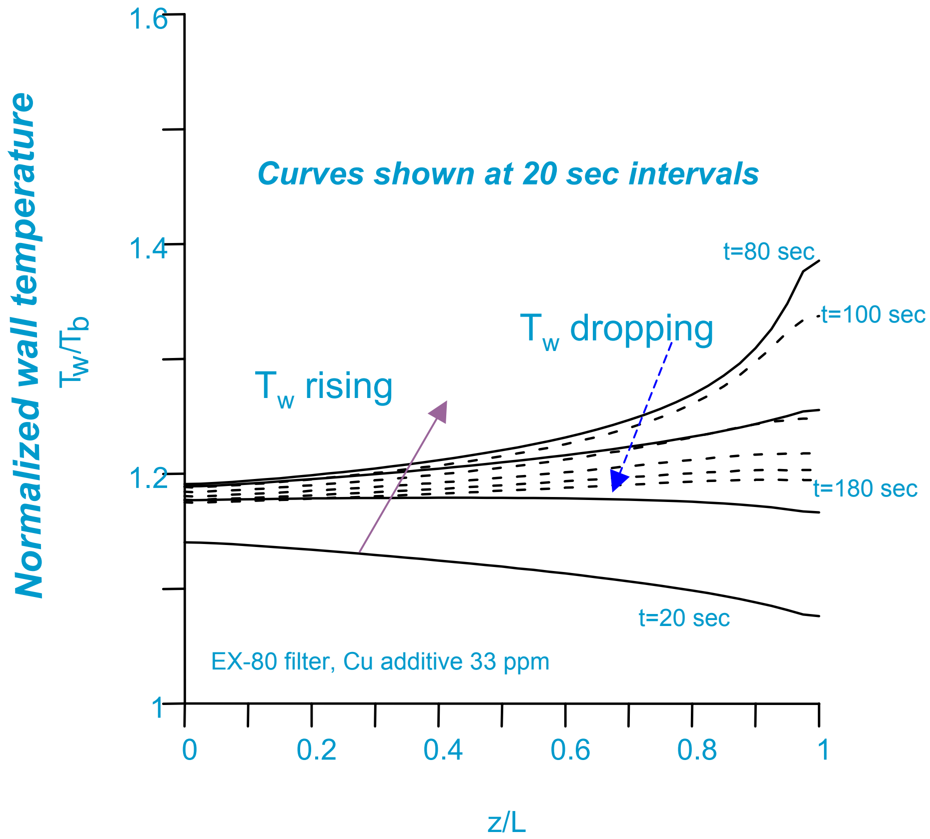
Example -- Simulation Results

Simulation results for

- ***spatial and temporal profiles of filter wall temperature***
- ***maximum filter wall temperature gradient (T_{exh} = 330 C)***

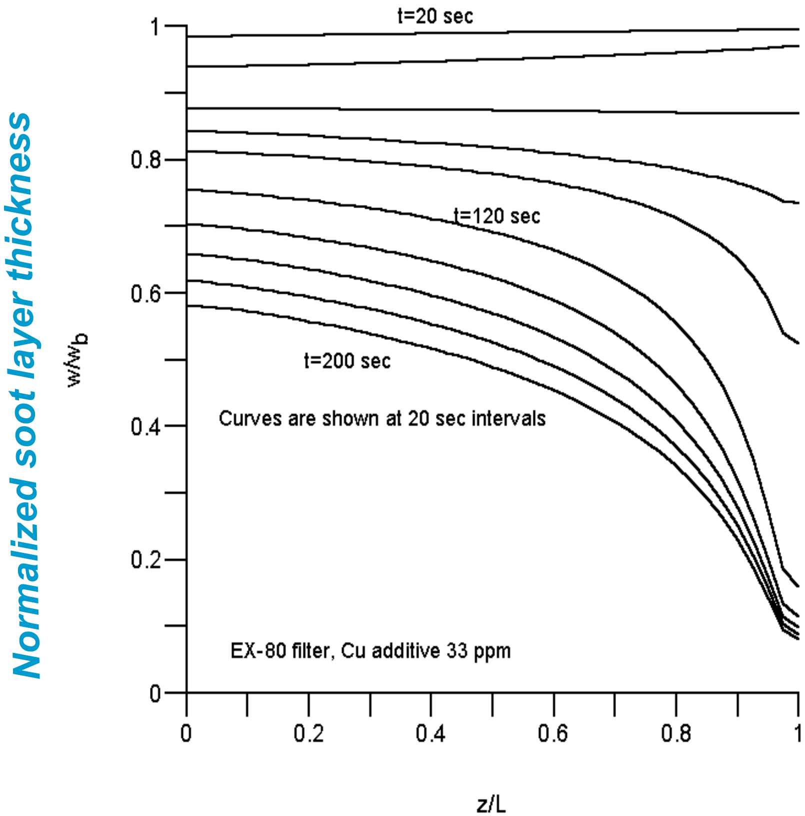


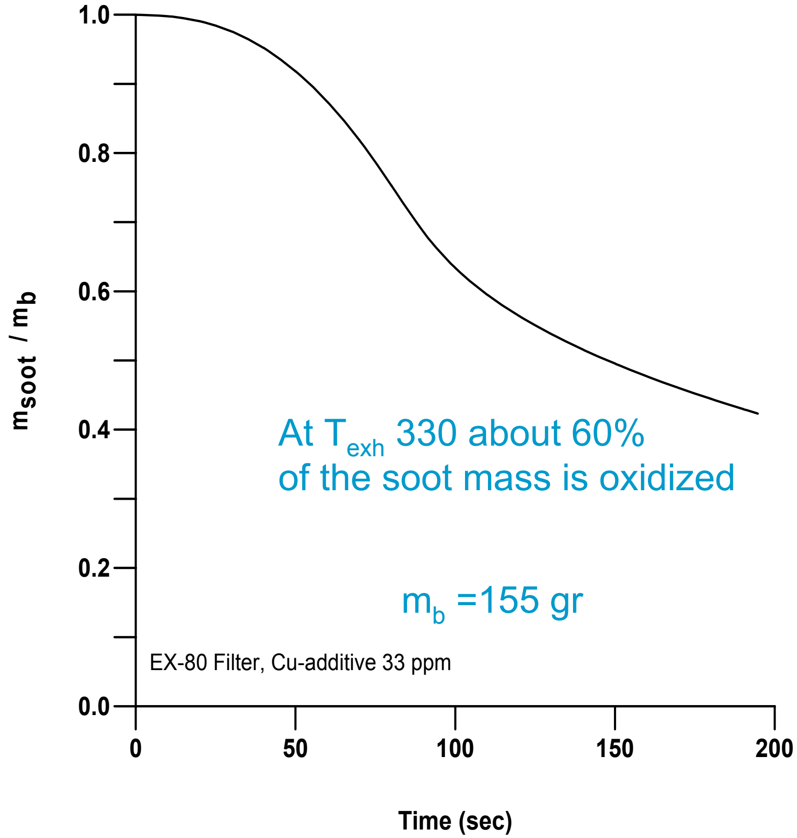
(from Walter© Regeneration Simulator, Konstandopoulos *et al*)

Example -- Simulation Results

Simulation results for

- ***Particulate layer thickness changing in time during regeneration.***
- ***Total particulate mass in the trap.***





(from Walter© Regeneration Simulator, Konstandopoulos *et al*)

Sample publications on modeling regeneration in DPF

- Pauli, E., Lepperhoff, G., Pischinger, F., "The Description of the Regeneration Bahavior of Diesel Particulate Traps with the Aid of a Mathematical Model," SAE - 830180, 1983.
- Bissett, E.J., "Mathematical Model of the Thermal Regeneration of a Wall-Flow Monolith Diesel Particulate Filter," Chem. Eng. Sci., 39, Nos. 7/8, 1233-1244, (1984).
- Bissett, E.J., Shadman, F., "Thermal Regeneration of Diesel-Particulate Filters," AIChE, 31, No. 5, 753-758, (1985).
- Kandylas, I., Stamatelos, A.M., "Modeling Catalytic Regeneration of Diesel Particulate Filters, Taking into Account Adsorbed Hydrocarbon Oxidation," Indus. Eng. Chem. Res., vol. 38, no. 5, 1866-1876, (1999).
- Konstandopoulos, A.G., and Kostoglou, M. (1998) “A Mathematical Model of Soot Oxidation on Catalytically Coated Ceramic Filters”, in *Proc. Advances in Vehicle Control and Safety* (AVCS’98), (Eds. Rachid A. and Meizel, D.), p.137, July 1-3, 1998, Amiens, France.
- Konstandopoulos, A.G., and Kostoglou, M. (1999) “Periodically Reversed Flow Regeneration of Diesel Particulate Traps”, *SAE Tech. Paper* 1999-01-0469. Also in Diesel Exhaust Aftertreatment 1999.
- Konstandopoulos, A. G., Skaperdas, E., Warren, J. and Allanson, R. (1999) “Optimized Filter Design and Selection Criteria for Continuously Regenerating Diesel Particulate Traps”, *SAE Tech. Paper* 1999-01-0468. Also in Diesel Exhaust Aftertreatment 1999.
- Kandylas, I., Stamatelos, A.M., "Modeling Catalytic Regeneration of Diesel Particulate Filters, Taking into Account Adsorbed Hydrocarbon Oxidation," Indus. Eng. Chem. Res., vol. 38, no. 5, 1866-1876, (1999).
- Koltsakis, G.C. and A.M. Stamatelos: Modeling Thermal Regeneration of Diesel Particulate Traps AIChE Journal, Vol.42, No.6, pp.1662-1672, June 1996.

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Sample publications (cont.)

- Versaevel, P., Colas, H. Rigaudeau, C., Noirot, R., Koltsakis, G.; Stamatelos, A.:Some Empirical Observations on Diesel Particulate Filter Modeling and Comparison between Simulations and Experiments. SAE 2000 International Congress, Detroit, U.S.A., March 2000. Paper 2000-01-0477
- Konstandopoulos, A.G., and Kostoglou, M. (1999) “Reverse Flow Soot Oxidation in Ceramic Filters”, *Proc. Med. Combustion Symp*., (Beretta, Ed.), CNR, Naples, p.456
- Konstandopoulos, A.G. and Kostoglou, M. (2000) “Reciprocating Flow Regeneration of Soot Filters”, *Comb. and Flame, 121 (3) pp.488-500.*
- *Konstandopoulos, A.G., Skaperdas, E., Masoudi, M., "Microstructural Properties of Soot Deposits in Diesel Particulate Traps," SAE-2002 Congress; in review.*
- Awara, A.E., Opris, C.N., Johnson, J.H., "A Theoretical and Experimental Study of the Regeneration Process in a Silicon Carbide Particulate Trap Using a Copper Fuel Additive," SAE - 1997 - 970188.
- Rumminger, M.D., Zhou, X., Balakrishnan, K., Edgar, B.L., Ezekoye, O.A. "Regeneration Behavior and Transient Thermal Response of Diesel Particulate Filters," SAE - 2001 – 01 – 1342.

List not exhaustive; ‘sample’ publications shown; no preference or endorsement.

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