A General Approach for Modeling Exhaust Aftertreatment Systems

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AFTERTREATMENT MODELING GOALS

- Physical Mechanisms Included:
  - Flow characteristics in individual monolith channels
  - Global flow characteristics upstream/downstream of monolith (eg. expansion/contraction of exhaust tube)
  - Chemical Kinetics: Catalytic surface reactions and gas phase chemistry using *STAR/Kinetics*
  - Conjugate heat transfer of the entire system
  - Soot Filtration Model for DPF, CSF
- To Model the Entire Aftertreatment Device(s):
  - 3 Way Catalytic Converter
  - Selective Catalytic Reduction (SCR)
  - Sulfur Trap
  - Lean NO_x Trap (LNT)
  - Diesel Particulate Filter (DPF)
  - Catalyzed Soot Filter(CSF,CRT)
  - Multiple Devices

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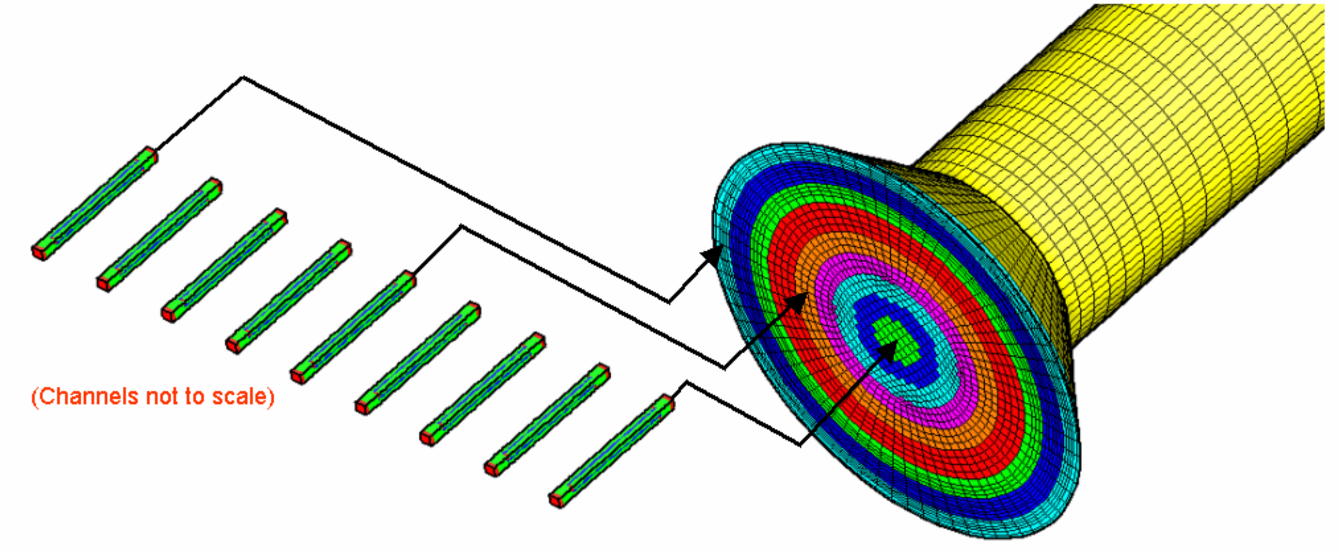
Ceramic “Brick” Monoliths

Representative Channel Coupling

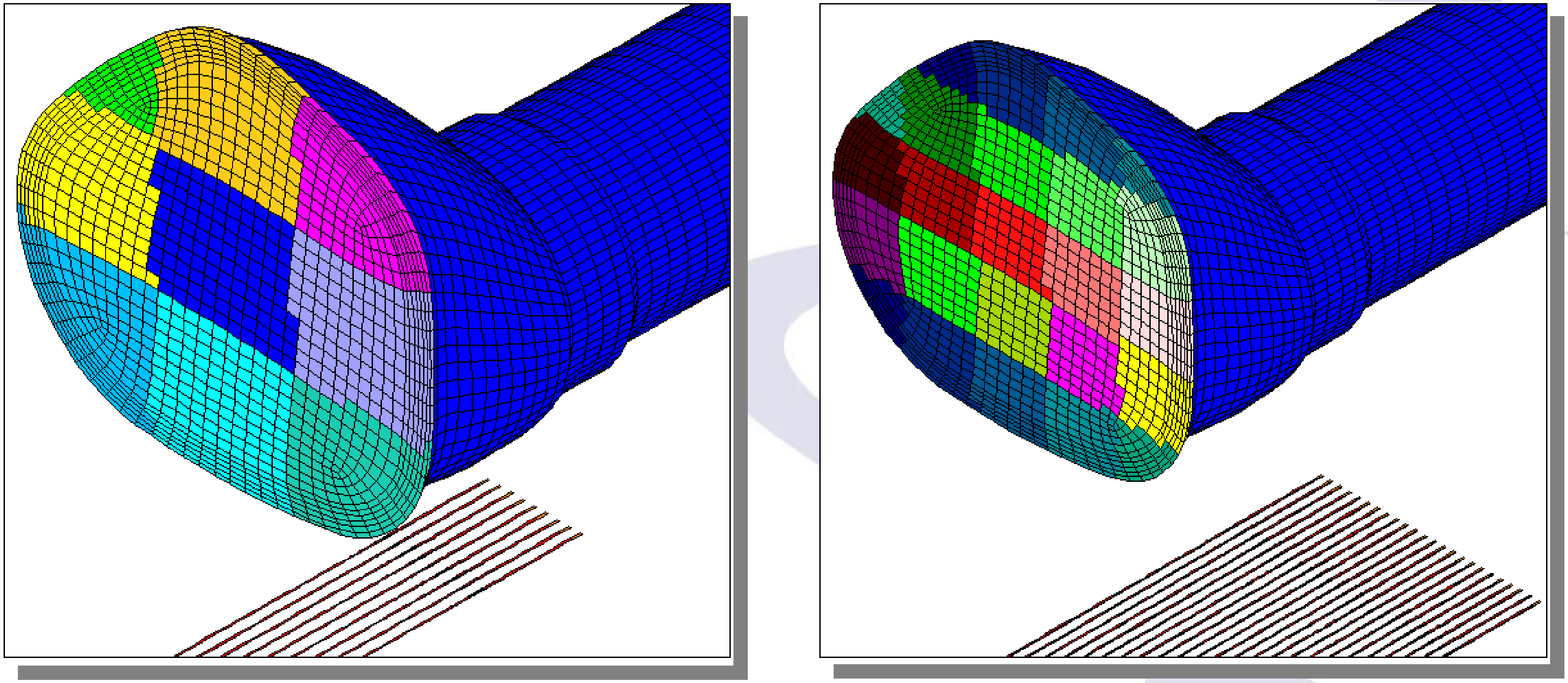
- Velocity, pressure, and all other flow variables are continuously coupled with a new coupling algorithm in STAR-CD (connect average)



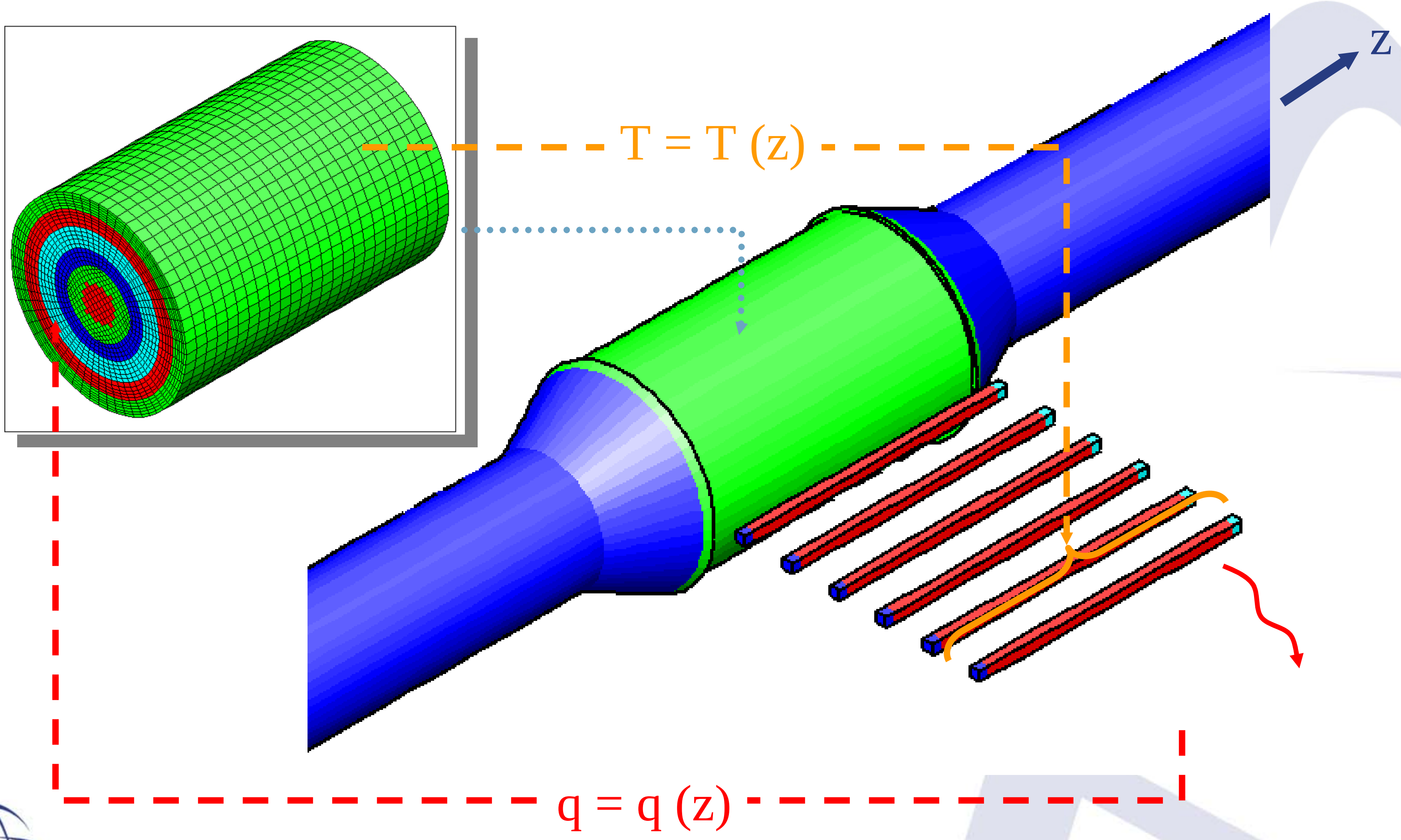
- Coupling insures average flux continuity across discrete pairs of boundary regions
- In this example, each channel is associated with a different radial zone of the inlet and outlet pipes

REPRESENTATIVE CHANNEL COUPLING

- Cartesian Based Subdivision



Conjugate Heat Transfer Coupling



Conjugate Heat Transfer Coupling Assumptions

- Temperature in wall between channels is almost constant across the wall
- Channel to channel temperature variations are small
- Thermal properties of solid are the homogenized properties (effective properties of a solid with voids)

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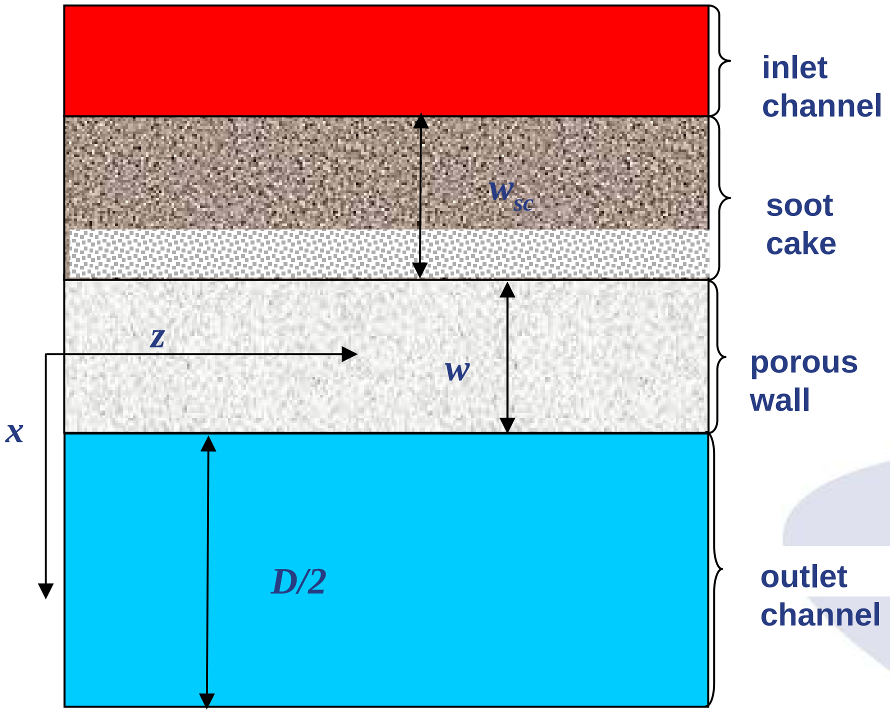
SIMPLE Transient
Solver for Multiple Time Scale Physics

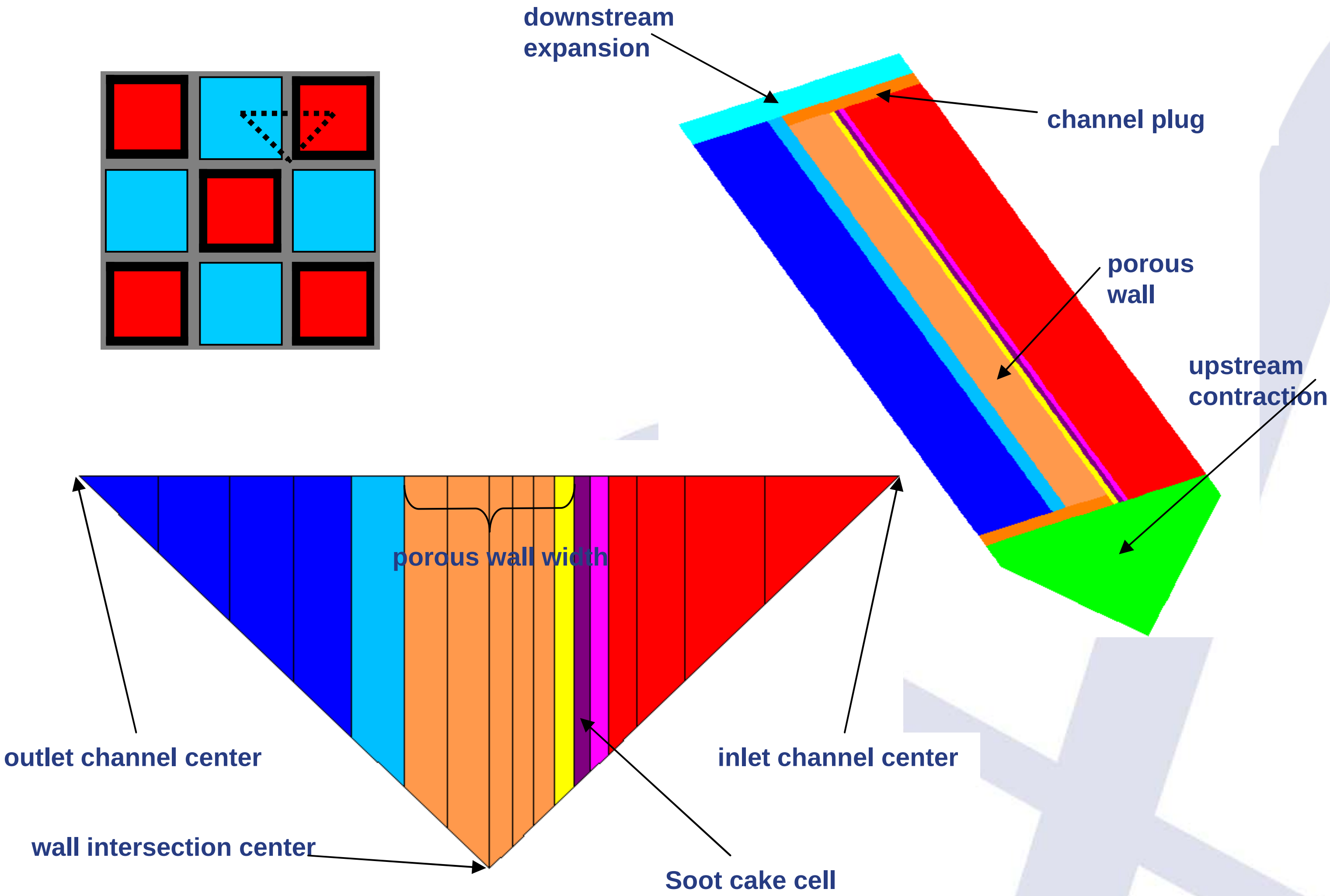
- Multiple Time Scale Physics
  - Conduction heat redistribution time on order 10’s minutes
  - Catalyst adsorption/desorption time on order of minutes
  - Thermal warm-up/light-off time on order of minutes
  - Fluid channel resident time on order of 10-100ms
  - Chemical equilibrium time on order of 1ms
- Fluid & chemistry is in a quasi-steady state relative to the warm-up, adsorption, and heat diffusion time scale
- SIMPLE transient with CHEMKIN Coupling
  - Completely implicit, stable at any time step size
  - Stable for time steps on the thermal time scale and yet accurate representation of the fluid and chemistry quasi-steady states
  - >1000 fold increase in performance over PISO

DPF Model Development



- Development follows work at Michigan Tech University (MTU) and Aerosol & Particle Technology Laboratory (APTL)
- 1-D deep bed filtration pore unit cell model
- Particle size dependent filtration
- Deep-bed to soot cake transition model
- Porous wall permeability depends on retained soot mass
- Heat transfer from gas to soot cake and porous wall
- Thermal and catalytic oxidation on "2-layer" model

DPF Representative Channel



downstream
expansion

channel plug

porous
wall

upstream
contraction

porous wall width

outlet channel center

inlet channel center

wall intersection center

Soot cake cell

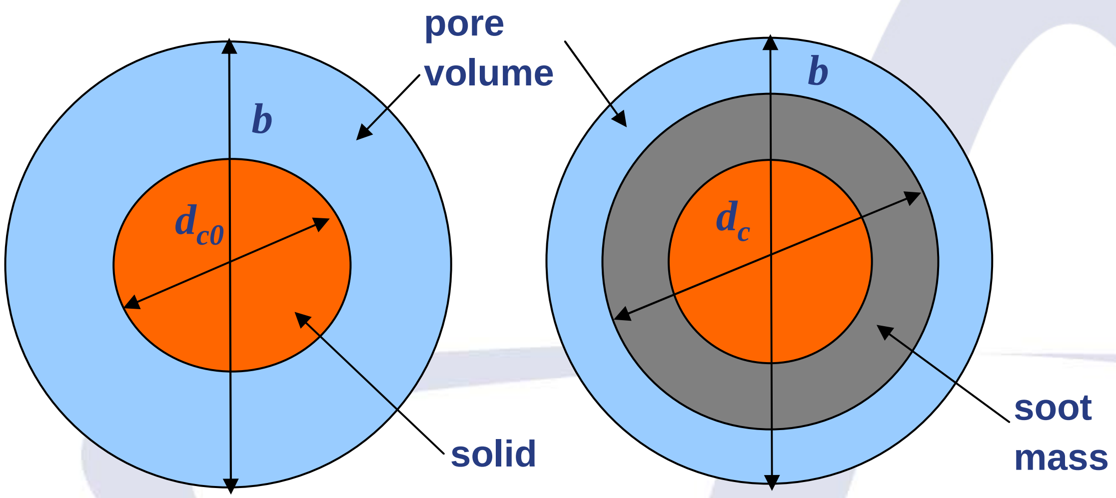
Porous Wall Filter

Conservation of gas phase soot mass in wall

$$\frac{\partial \bar{\rho}_{pm}}{\partial t} + \frac{\partial v \bar{\rho}_{pm}}{\partial x} = -\frac{v \bar{\rho}_{pm}}{l_f}$$

source (sink)

$$\varepsilon = \varepsilon_0 - \frac{\bar{\rho}_s}{\rho_{pw}}$$



Conservation of retained soot mass in wall

$$\frac{\partial \bar{\rho}_s}{\partial t} = v \sum_{m=1}^{M} \frac{\bar{\rho}_{pm}}{l_f\left(\varepsilon, v, d_m\right)} - S_s$$

source

soot oxidation sink

spherical unit collector:

- filter length scale l_f
- porosity
- permeability

Soot Cake Growth

- Conservation of retained soot mass in soot cake

$$w_{grid}\frac{d\bar{\rho}_s}{dt} = \rho_{sc}\frac{dw_{sc}}{dt} = \Phi v\sum_m \rho_{pm} - \int_0^{w_{sc}} S_s dx$$

source

soot oxidation sink

- Deep-bed to soot cake partition from spherical unit collector:

pores open $0 < \Phi < 1$ pores complete closed

$$\Phi = \frac{d_c^2\left(\varepsilon(x=-w/2)\right) - d_{co}^2}{\left(\Psi b\right)^2 - d_{co}^2}$$

DPF Chemistry (Thermal Oxidation)

$$[C] + \left(1 - \frac{f^{th}}{2}\right)[O_2] \rightarrow f^{th}[CO] + \left(1 - f^{th}\right)[CO_2]$$

- s_p : specific surface area (m^2/m^3) !!!
- Y_{O_2} , X_{O_2} : mass and mole fraction of oxygen
- k_0^{th} : pre-exponential frequency factor (m/s/°K)
- E^{th} : activation energy (J/mole)

$$S_{O_2} = -\left(1 - \frac{f^{th}}{2}\right) \boxed{\rho_g s_p k_0^{th}} T \exp\left(\frac{-E^{th}}{RT}\right) Y_{O_2} \ \text{(kg/m}^3\text{/s)}$$

- CO selectivity $$f^{th} = \frac{1}{1 + k_f^{th} X_{O_2}^{\mu_{th}} \exp\left(\frac{-E_f^{th}}{RT}\right)}$$

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User Customizations

- subroutine porous_wall_properties
  - sets the local porous wall properties:
  - porosity,permeability,filter efficiency, specific area, ..
- subroutine soot_cake_properties
  - sets the local porous wall properties:
  - porosity,permeability,filter efficiency, specific area, ..
- subroutine reactwall
  - sets the local reactions rates within the porous wall
- subroutine reactsc
  - sets the local reactions rates within the soot cake

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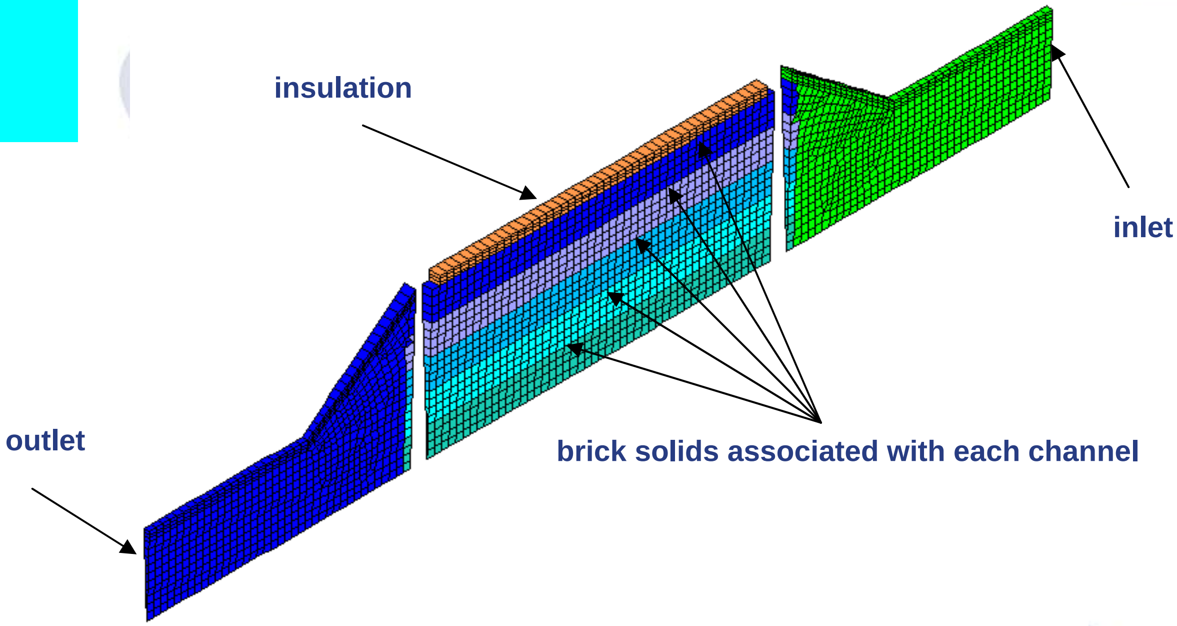
Test Dataset and Geometry

Test data: DPF-CRT

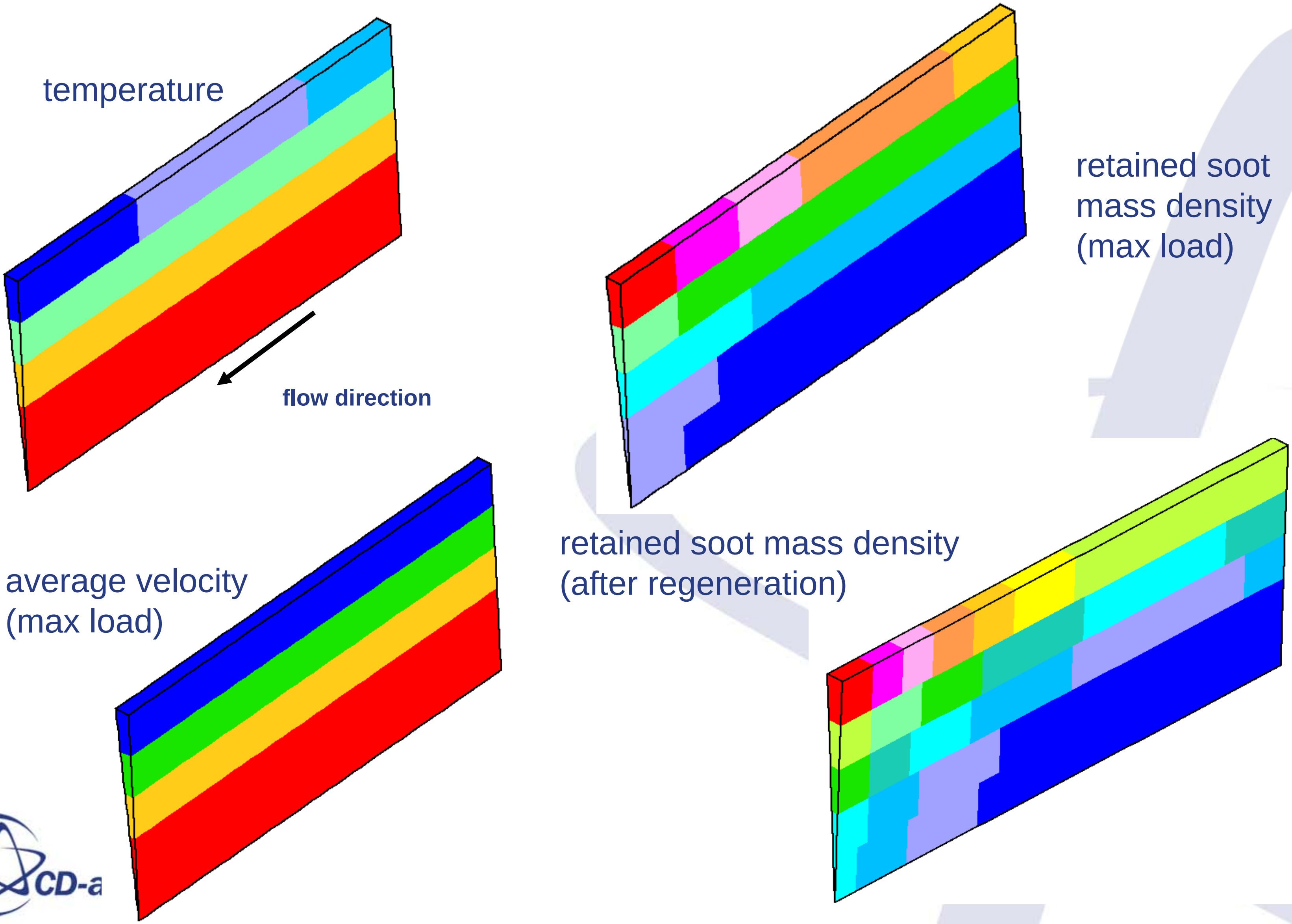
- 7 data sets of loading and regeneration over wide range
- exhaust flow rates
- exhaust PM concentration
- exhaust NO and NO_2 concentration
- presumed uniform inlet conditions

Numerical model:

- 5 representative channels
- axisymmetric
- heat loss on manifold and can
- uniform or non-uniform inlet temperature



Heat Loss Effects



Model Limitations

- microstructural variations of soot cake properties especially during forced or continuous regeneration
- porous wall permeability , porosity evolution requires small soot packing densities
- Characterization of catalytic chemistry for a wash coat

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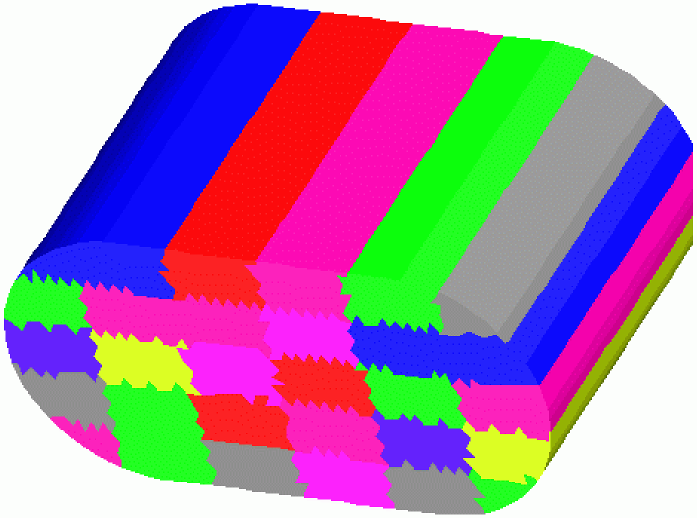
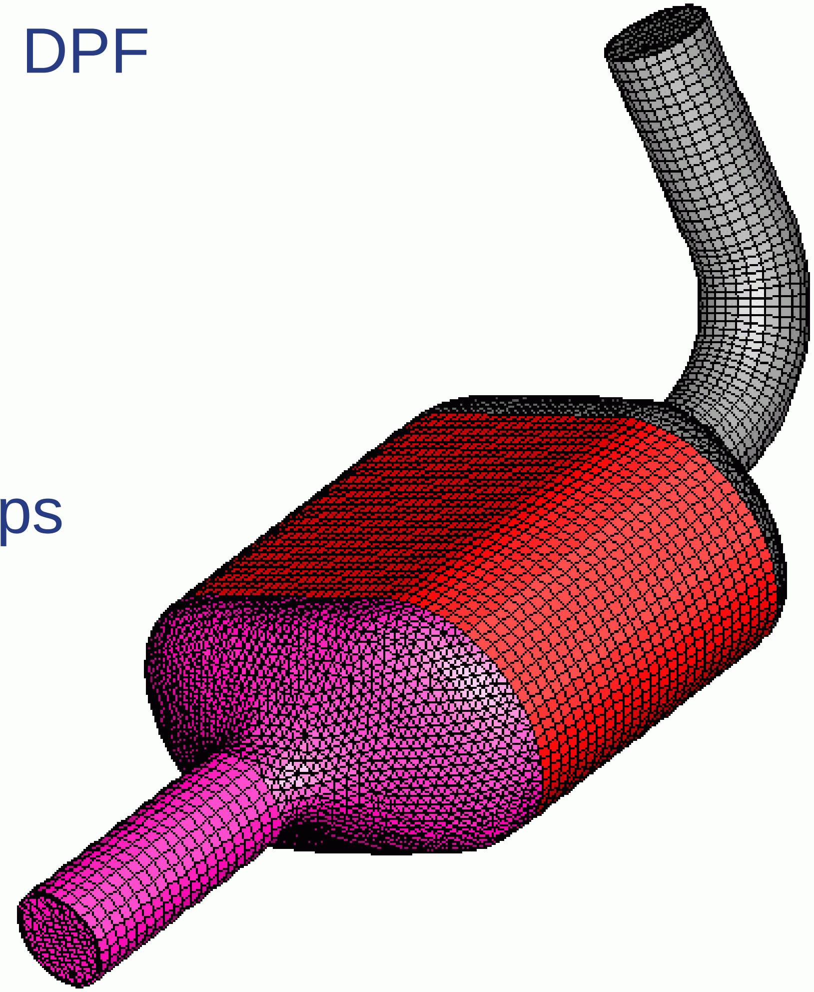
Loading with Complex Geometry

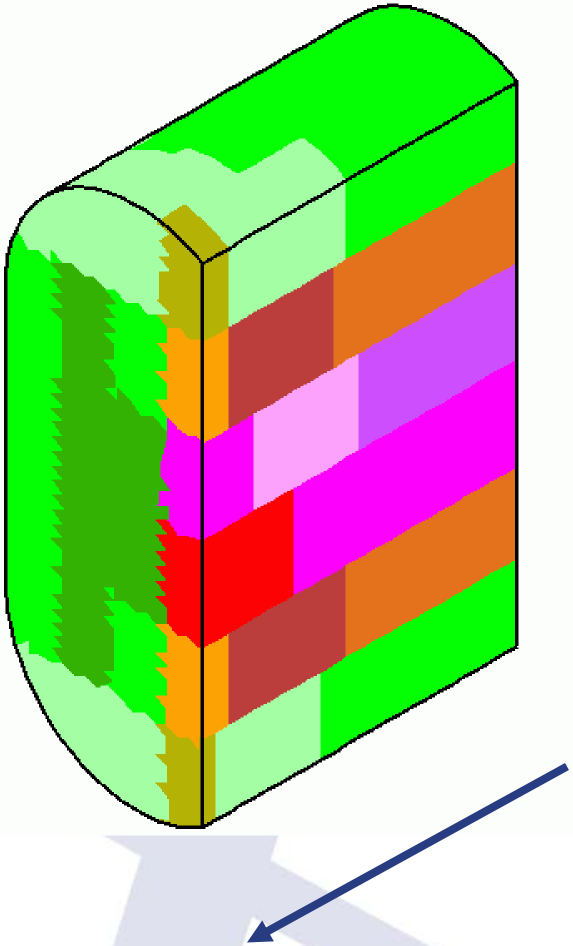
- Inlet Elbow, Non Cylindrical DPF
- Poor upstream distribution
- Isothermal Loading
- constant inlet conditions
- 6x5 channels
- 3 hr loading, 1.5 minute steps



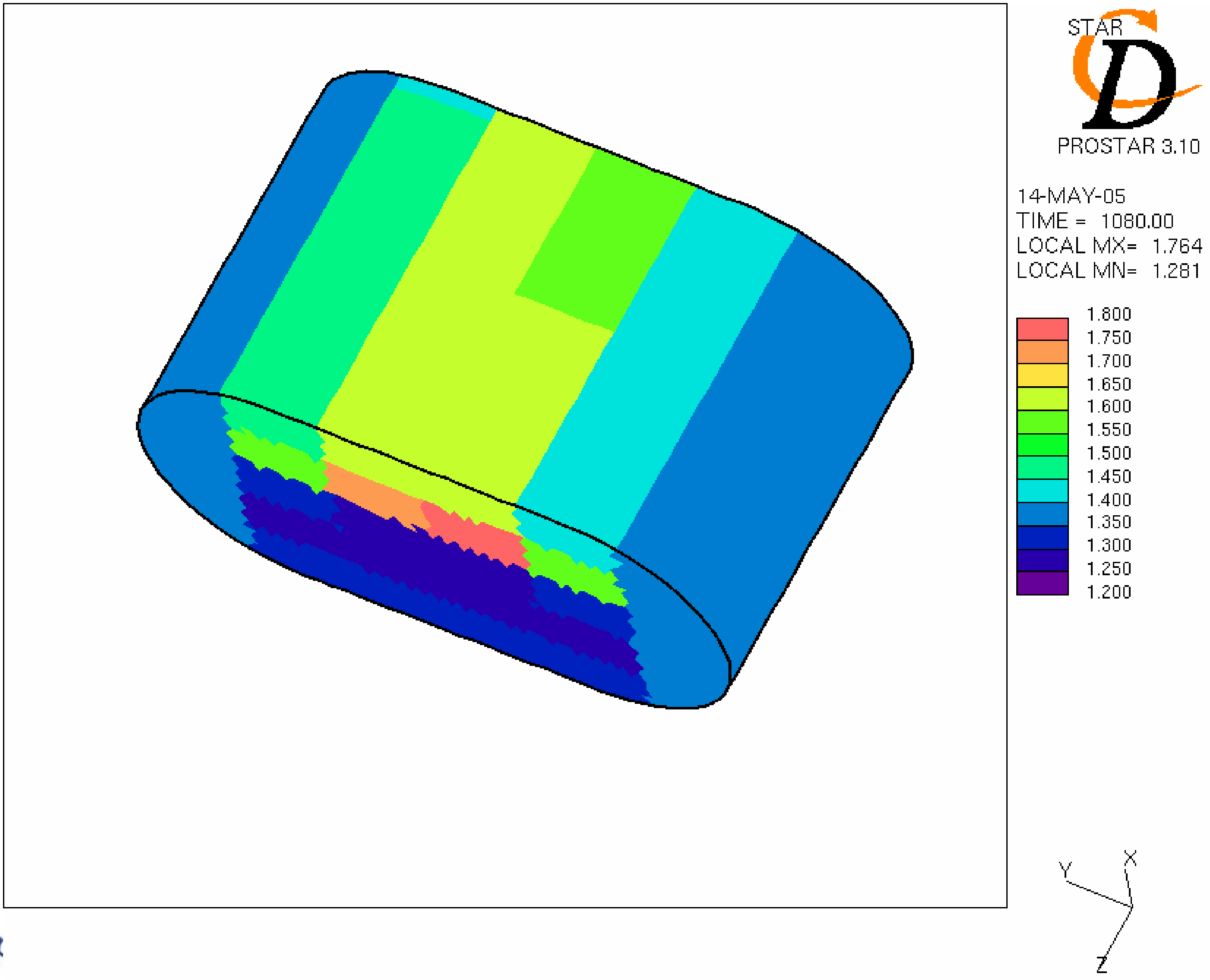


Retained soot mass density

- uneven distribution of the collected soot within the DPF
- strong later variations
- somewhat weaker axial variations with more soot downstream



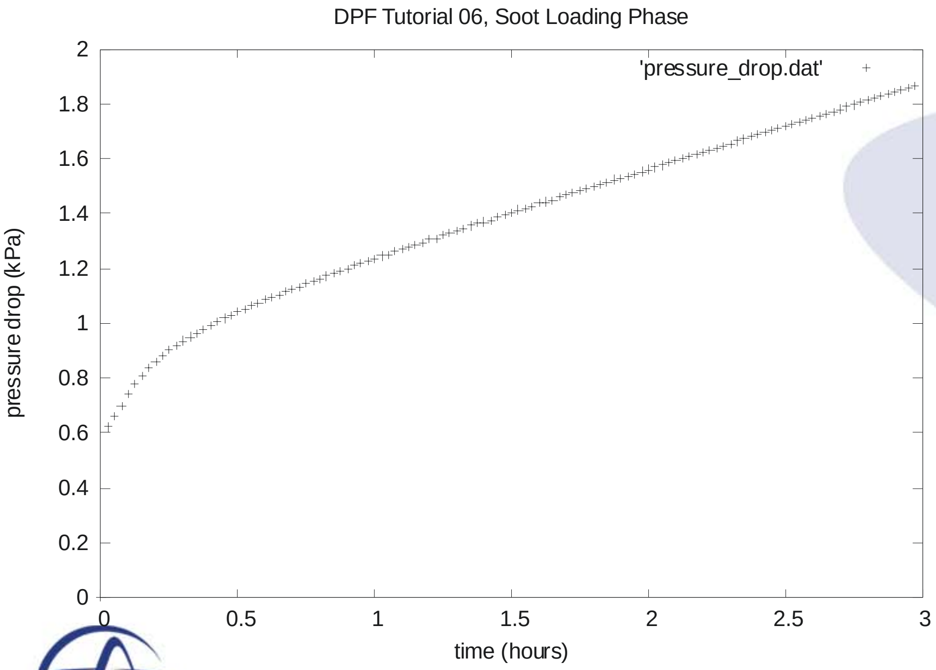
Velocity Redistribution

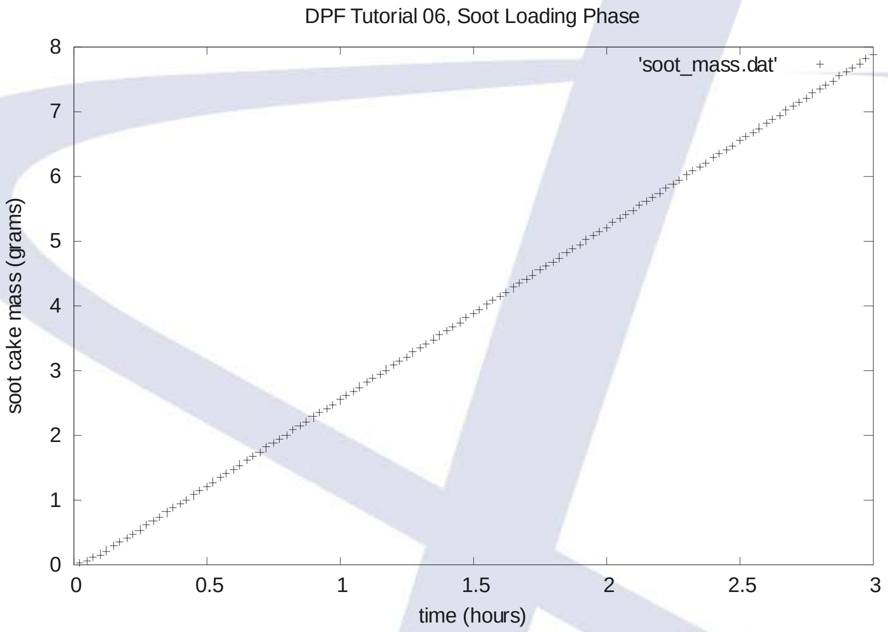


Post Processing: History Files

- pressure drop history across DPF

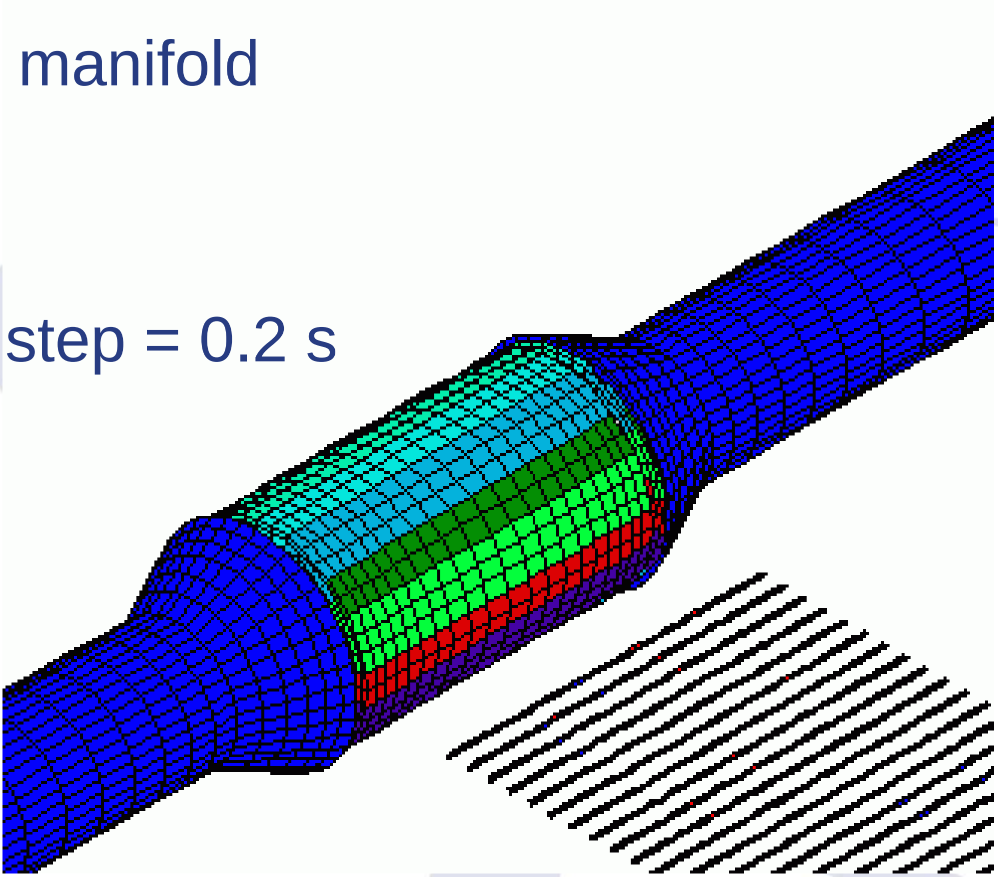
- retained soot mass history





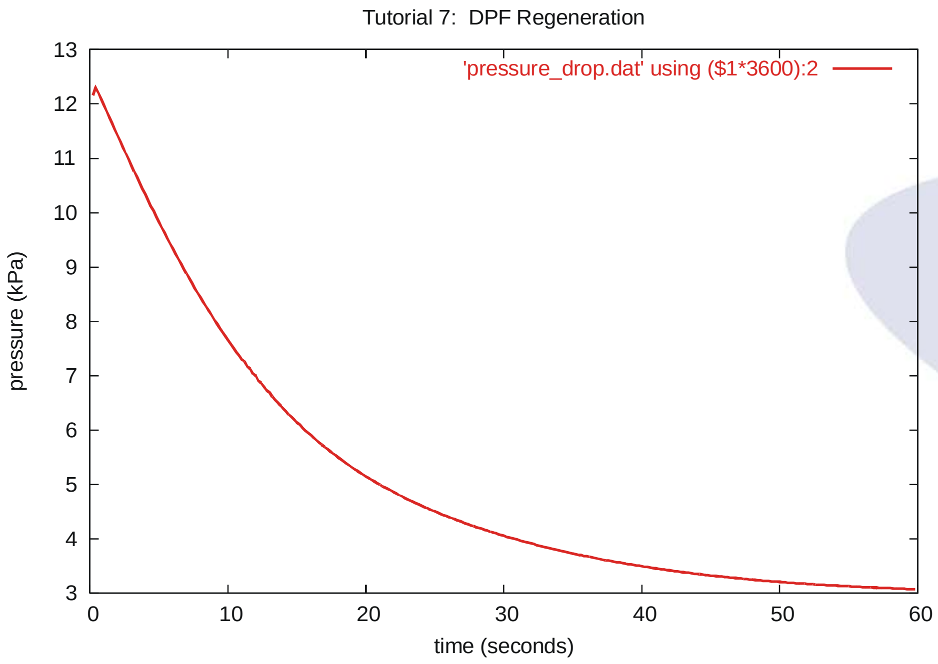
DPF Regeneration

- Initially loaded DPF with 9 grams of soot (5 g/liter)
- Initially at thermal equilibrium with an inlet temperature of 600 °C
- heat losses on inlet/outlet manifold
- Thermal oxidation only
- Flow rates held constant
- Burns in < 1 minute, time step = 0.2 s
- 5x5 channels

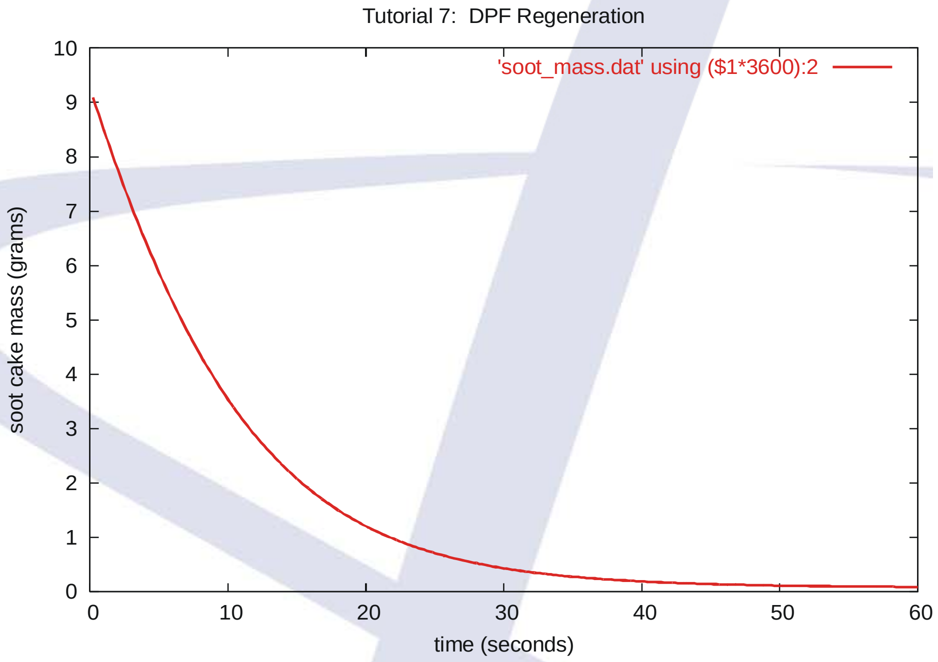


DPF Regeneration: Post Processing

pressure drop

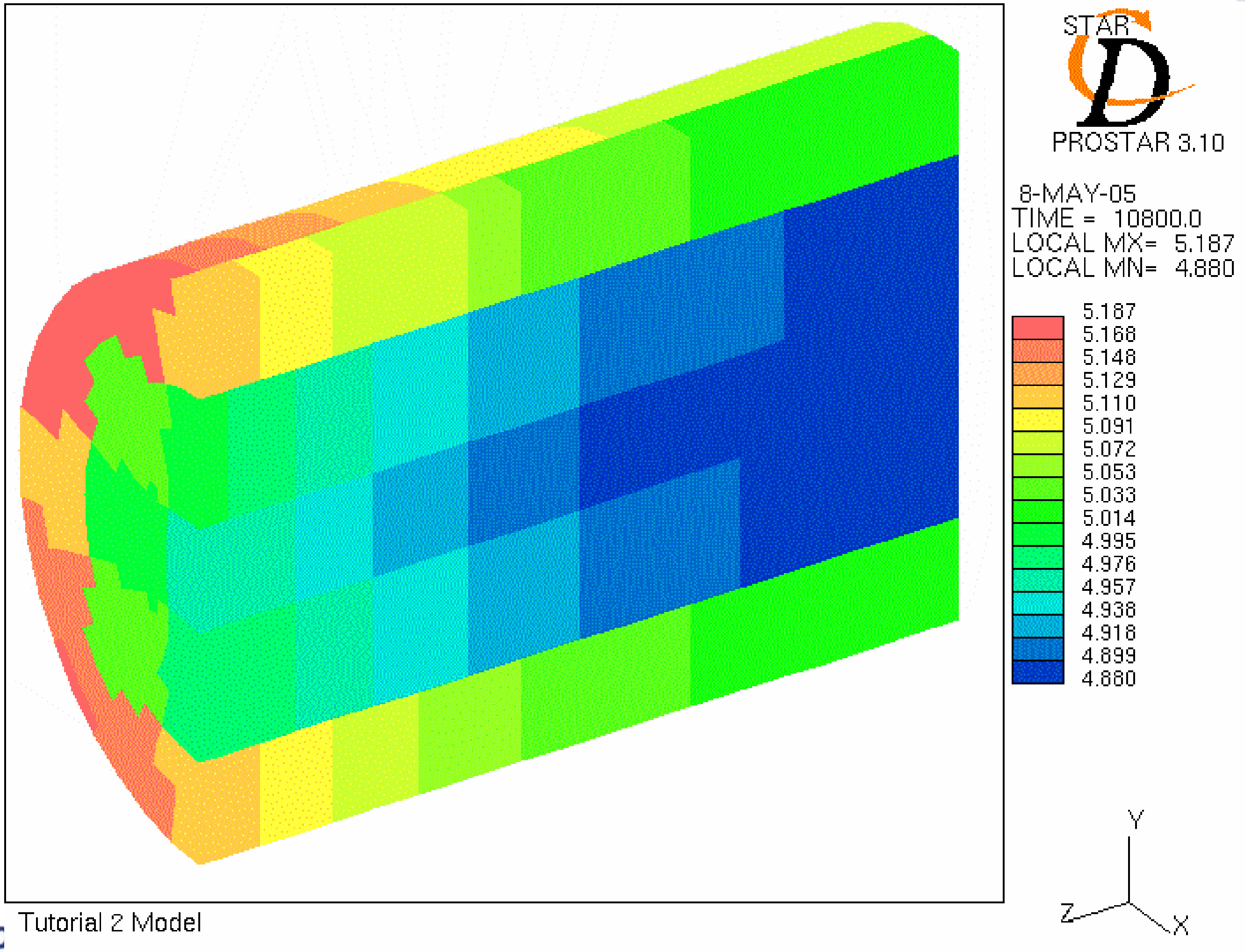


retained soot mass



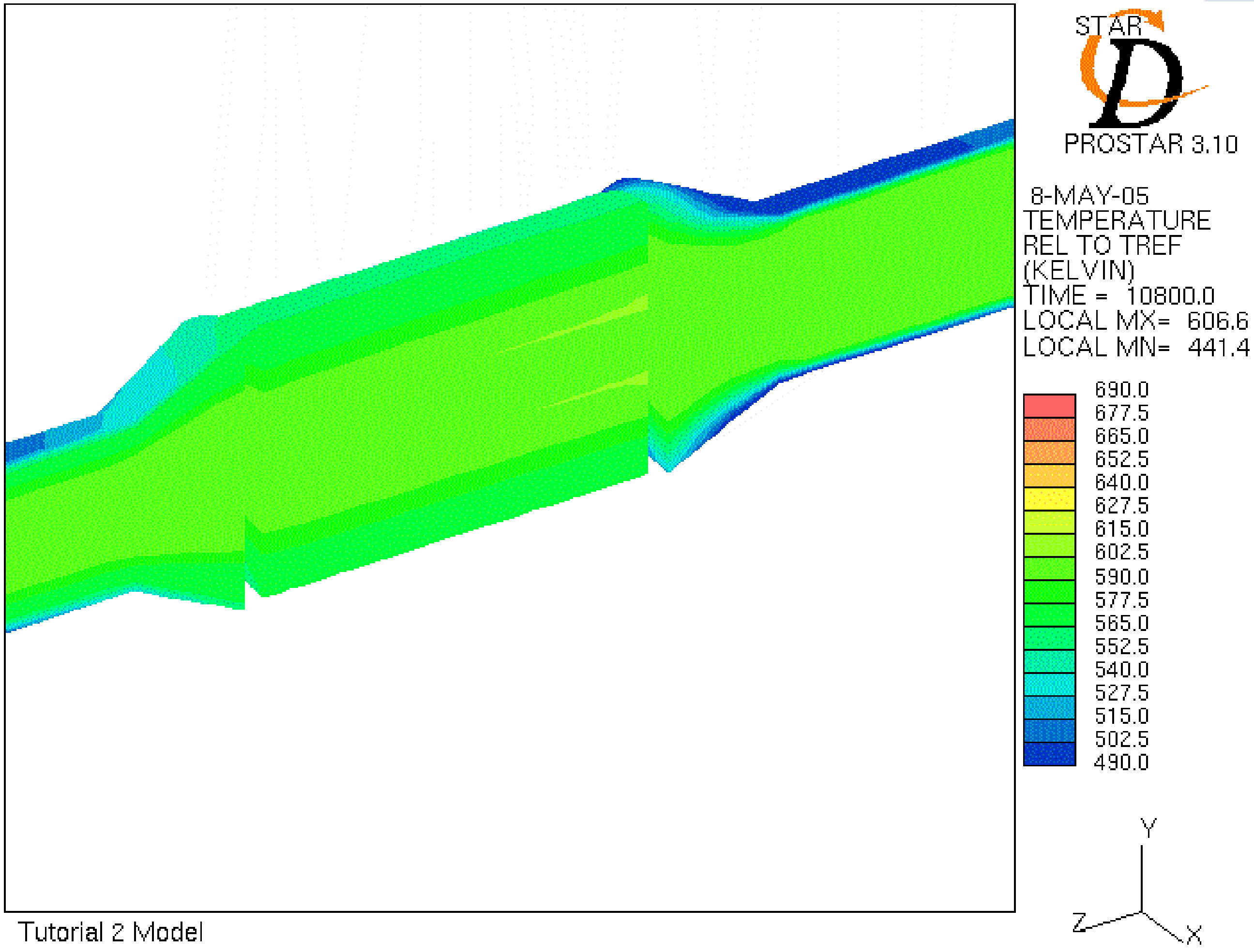
DPF Regeneration: Results

- Retained soot density



DPF Regeneration: Results

- Temperature (Solid, upstream and downstream gas)



Computer Resources

- Axisymmetric DPF-CRT loading simulations
  - 1.5 minute step sizes over 3 hr loading period
  - 5 representative channels
  - NOx assisted catalytic and thermal oxidation chemistry
  - 20 minutes CPU (single processor pentium IV)
- 3-D DPF loading with complex geometry
  - 1.5 minute step sizes over 3 hr loading period
  - 30 representative channels
  - 1.5 hr CPU (single processor xeon)
- 3-D DPF Regeneration
  - 0.2 step sizes over 1 min period
  - 25 representative channels
  - thermal oxidation
  - 4 hr CPU (single processor xeon)

Characterization of DPF Monoliths and Wash coats

- Agreement of a standard of “ideal” laboratory tests
  - loading only
  - loading and continuous regeneration
  - forced regeneration
- Agreement of a standard model to characterize DPF properties
  - under the “ideal” laboratory conditions
  - models are sufficiently concise so “fits” of laboratory data are practical
- Vendors characterize their products by publishing standard model properties fit to standard tests

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