

Fully Transient One-Dimensional Based Diesel Particulate Filter Modeling Including Catalytic Surface Reactions

Eighth DOE Crosscut Workshop
on Lean Emissions Reduction
Simulation

May 17th-19th, 2005

Presentation by:
Dr. Christopher Depcik
Research Fellow
The University of Michigan



MUST READ!!!



- If the reader wishes to use any of this work within any publications and/or presentations they must tell me (depcikc@umich.edu) and reference it as:
 - Personal communication with Christopher Depcik at the Eighth DOE Crosscut Workshop on Lean Emissions Reduction Simulation, May 17th, 2005
 - <http://www.cleers.org/workshop8/index.php>
- I am busy finishing a few additional runs and working on publishing a more complete description of the work
 - I will submit it to the CLEERS open citations
 - http://www.cleers.org/open_citations/index.php

Abstract



Classical one-dimensional based Diesel Particulate Filter (DPF) modeling has been predicting pressure drops, the oxidation of diesel particulate and the exothermic reactions that result with good accuracy for over the last 20 years. To advance the state of the art and to account for the possibility of catalyzed filters, this classical model was enhanced to include the propagation of chemical species and particulates into the formulation of the model. In addition, full transient capability was incorporated into the model to account for regulatory tests where the inlet conditions to the DPF can change instantly. This transient capability allows the model to capture surface intermediate chemistry effects where the timescales of the process are much smaller compared to surface temperature timescales. While a compressible formulation of the equations of motion for the model will yield the most accurate results, it is rather impractical for multiple simulation runs because of its long computational time. As a result, an incompressible formulation is described and compared to full variable-property reacting-gas dynamics to illustrate differences between the models. It was found that the source terms used in the formulation of the DPF model are large enough to offset most of the effects of compressibility. As with previous catalyst modeling efforts, all pertinent assumptions and numerical solvers are presented.

Outline of Talk



- Modeling Approach
- One-Dimensional Fluid Dynamics
 - Basic numerical algorithms and validation
 - Catalyst Modeling Application
 - Algorithms used within Diesel Particulate Filter modeling
 - Urea SCR, Lean NO_x Trap and Fuel Reforming
 - Diesel Particulate Filter Modeling Application
 - Flow profiles
 - Particulate oxidation
 - Pressure drops
 - Surface chemistry

Modeling Approach



- Approach Diesel Particulate Filter (DPF) From Slightly Different Perspective
- Applied Fluid Dynamics
 - Start with governing equations of motion in one-dimension
 - Find appropriate source terms and surface models (literature)
 - Previous DPF work is one-dimensional *based*
 - Determine what is missing and what can be advanced
 - Propagation of chemical species
 - Transient terms
 - Incompressible versus compressible
 - Surface chemistry
 - Create solvers and platform for solution



Fluid Dynamics

- Compressible Flow, Variable-Property Reacting-Gas Dynamics
 - Thermodynamic properties are a function of temperature and species composition
 - Euler and Navier-Stokes equations in one-dimension
 - Simplified models exist by using incompressibility and time-scale approximations
- Generality of Numerical Methods Applied to Specific Devices
 - Source terms and von Neumann analysis allows for fully transient simulations
 - Additional models incorporated for surface temperatures and reactions

One-Dimensional
Fluid Dynamics

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}$$

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y_j \end{bmatrix}$$

$$\mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p + \tau_{xx} \\ \rho u H + u \tau_{xx} + q_x \\ \rho u Y_j + \rho Y_j V_j \end{bmatrix}$$

$$\tau_{xx} = \frac{-4\mu}{3} \frac{du}{dx}$$

$$V_j = -\frac{D_j}{Y_j} \frac{dY_j}{dx}$$

$$q_x = -k \frac{dT}{dx} + \rho \sum_{j=1}^{NM} h_j Y_j V_j$$



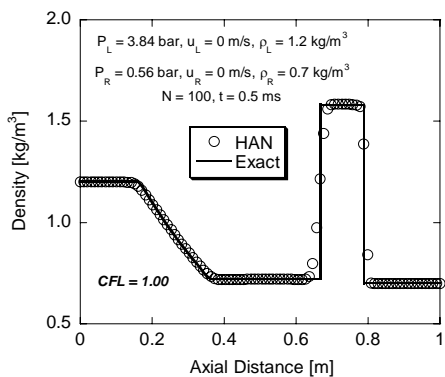
Validation of Gas Dynamics

- Hancock Predictor-Corrector Method
Incorporating Roe's Approximate Riemann Solver
 - MUSCL scheme with variable properties
 - Prevents oscillations from occurring instead of damping afterwards
 - Relatively fast in comparison to other numerical methods
 - Validation against all pertinent source terms

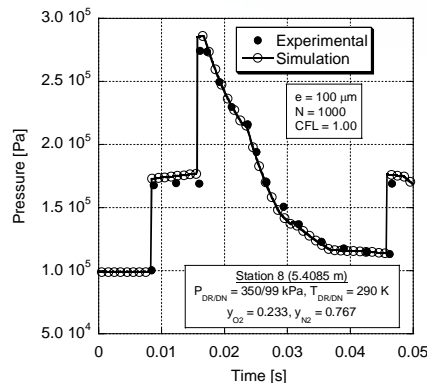
$$\mathbf{S} = \begin{bmatrix} -\frac{\rho u}{A} \frac{dA}{dx} \\ -\frac{\rho u^2}{A} \frac{dA}{dx} \\ -\frac{\rho u H}{A} \frac{dA}{dx} \\ -\frac{\rho u Y}{A} \frac{dA}{dx} \end{bmatrix} + \begin{bmatrix} 0 \\ -\rho G \\ \rho Q \\ \rho \dot{\omega} \end{bmatrix} \begin{matrix} \text{Friction} \\ \text{Heat Transfer} \\ \text{Kinetics} \end{matrix}$$

(Depcik Ph.D., 2003)

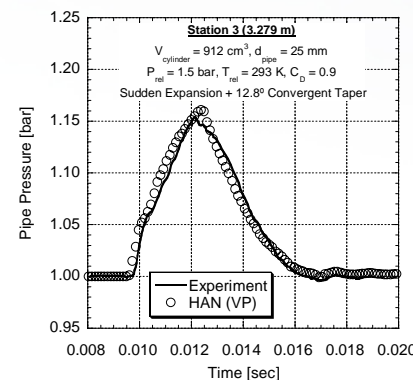
(Depcik & Assanis, 2005)



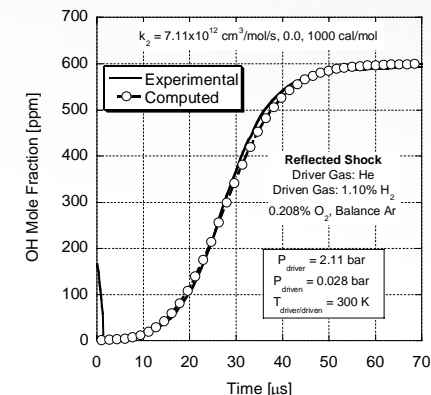
**Exact Riemann Solution
(Numerical Method)**



**Compressed Air
Shock Tube Study
(Friction)**



**Single-Cylinder
Experiments
(Heat Transfer & Area Change)**



**OH Production
Experiments
(Chemical Kinetics)**



One-Dimensional Catalyst Modeling



- Single Channel Based
 - Can be adapted for any device geometry
 - No gas storage and transient solvers
 - Constant Density and Velocity, Incompressible and Compressible

• Surface Species Equations

Surface Gas

Storage = Diffusion + Reactions

$$\frac{d\bar{C}_{s,j}}{dt} = \frac{k_{m,j}G_a}{1-\varepsilon} (\bar{C}_{g,j} - \bar{C}_{s,j}) - \frac{G_{ca}R_j}{1-\varepsilon}$$

Surface Gas
[Ex: NO₂]

Surface Intermediates

Storage = Reactions

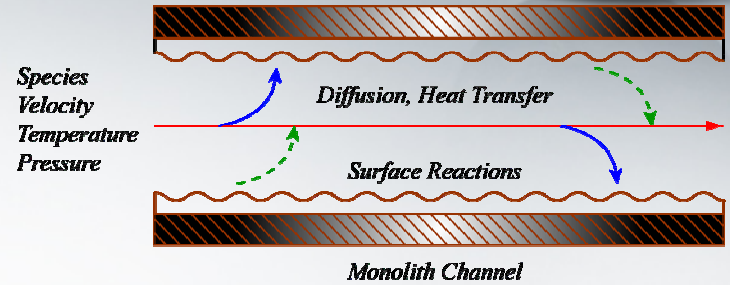
$$\frac{d\Theta_m}{dt} = \frac{\dot{s}_m}{\Gamma}$$

Fractional Coverage
[Ex: Ba(NO₃)₂]

• Surface Temperature Equation

Storage = Conduction + Heat Transfer + Reactions + Vol. Heating + Pseudo-2D HT

$$\rho_m c_m \frac{\partial T_m}{\partial t} = k_m \frac{\partial^2 T_m}{\partial x^2} + \frac{h_g G_a}{1-\varepsilon} (T_g - T_m) + \frac{G_{ca}}{1-\varepsilon} \sum_{j=1}^{NM} R_j H_j + \dot{q} + \frac{Q_{i \rightarrow m}}{(1-\varepsilon)V_{cat}}$$

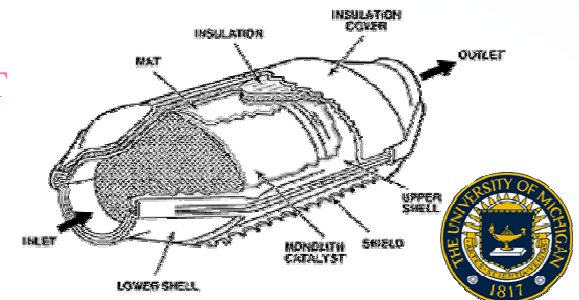


(Depcik Ph.D., 2003)

(Depcik & Assanis in review)

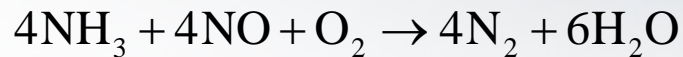
$$S = \begin{bmatrix} \sum_{j=1}^{NM} \frac{-k_{m,j}G_a}{\varepsilon} (C_{g,j} - W_j \bar{C}_{s,j}) \\ -\frac{\rho f_F u |u|}{2} \left(\frac{G_a}{\varepsilon} \right) \\ \frac{-h_g G_a}{\varepsilon} (T_g - T_m) \\ \frac{-k_{m,j}G_a}{\varepsilon} (C_{g,j} - W_j \bar{C}_{s,j}) \end{bmatrix}$$

Mass Diffusion
Friction
Heat Transfer
Species Diffusion





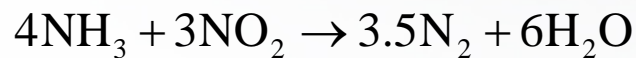
Urea SCR Catalyst Model



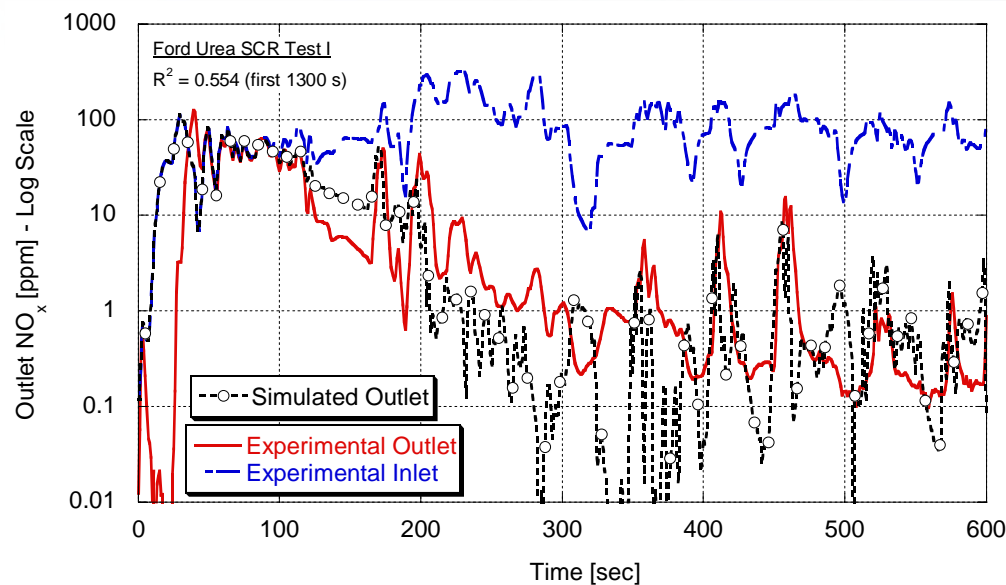
“standard SCR”



“fast SCR”

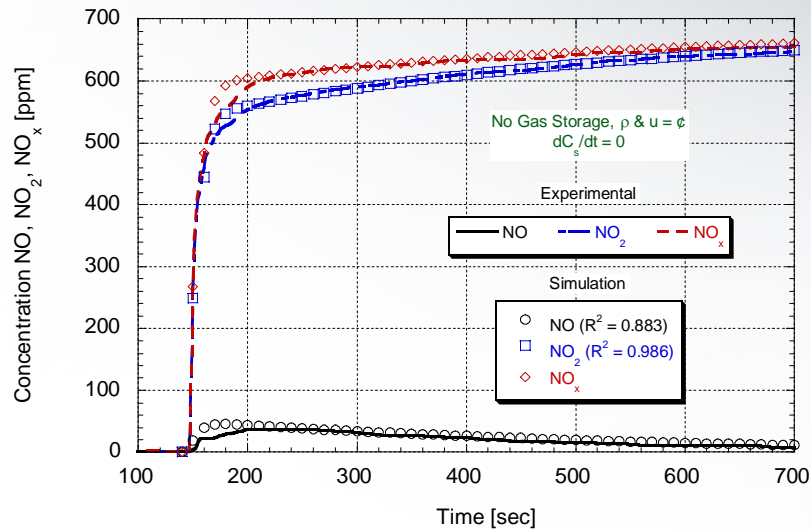


“slow NO₂”

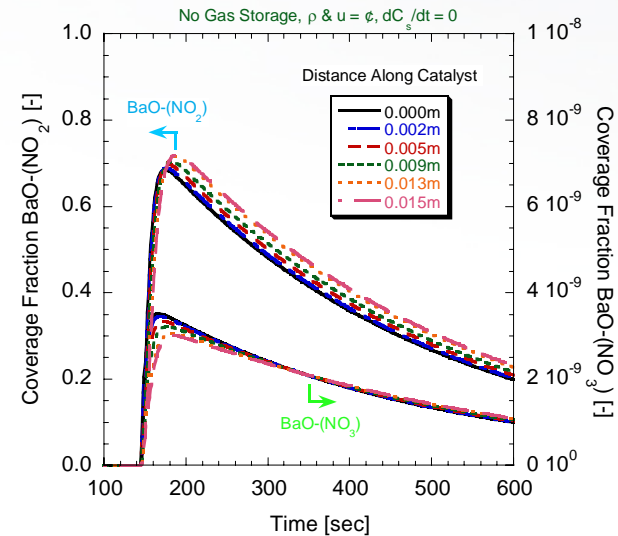
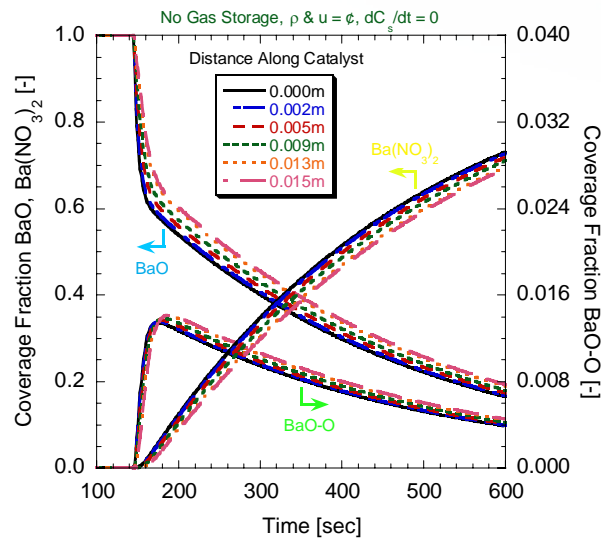
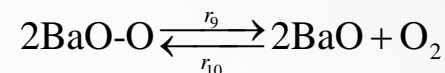
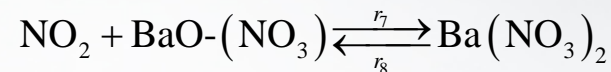
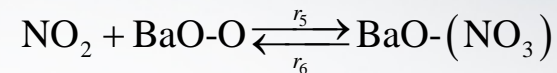
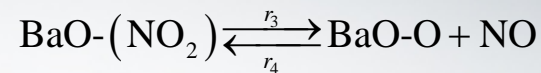
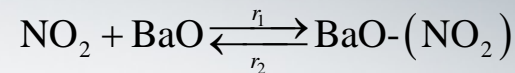




Lean NO_x Trap Model



Olsson, et al. 2001 – BaO/Al₂O₃

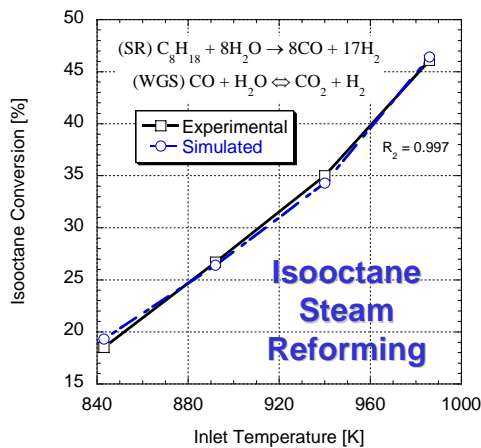


Example in upcoming catalyst paper



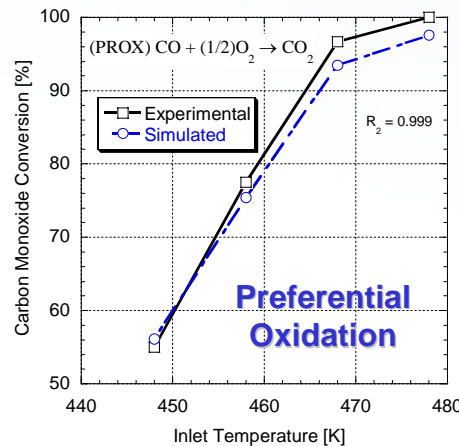
Fuel Processing Models

- Kinetic Validation Work at the University of Michigan
- Models Will Be Used in Optimization of H₂ Production for Complete Fuel Processor System

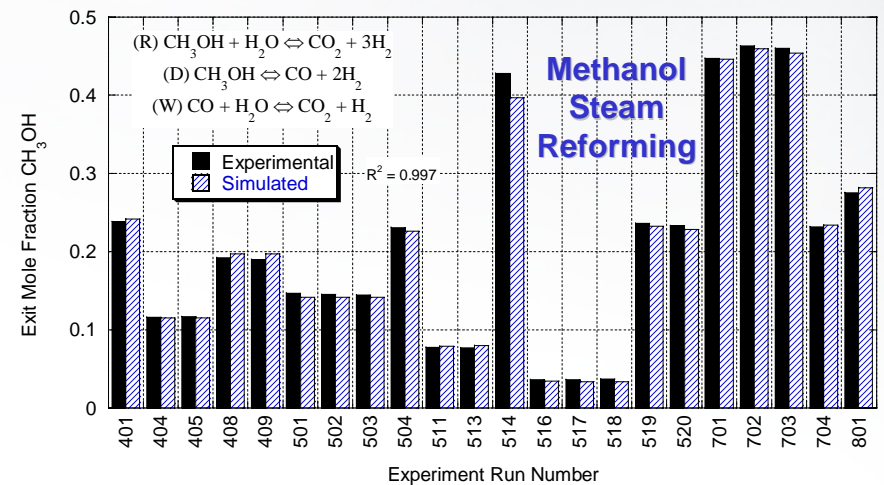


$$R_{SR} = k \exp\left[-E_a / (R_u T_m)\right] p_{C_8H_{18}}^m p_{H_2O}^n$$

$$R_{WGS} = k \exp\left[-E_a / (R_u T_m)\right] \left[p_{CO} p_{H_2O} - (p_{CO_2} p_{H_2}) / K_p \right]$$



$$R_{PROX} = k \exp\left[-E_a / (R_u T_m)\right] p_{CO}^m p_{O_2}^n$$



$$R_R = \frac{k_R K_{CH_3O}^* (p_{CH_3OH} / p_{H_2}^{1/2}) \left[1 - (p_{H_2}^3 p_{CO_2} / K_R p_{CH_3OH} p_{H_2O}) \right] C_{S_1}^T C_{S_{1a}}^T}{\left[1 + K_{CH_3O}^* (p_{CH_3OH} / p_{H_2}^{1/2}) + K_{HCOO}^* p_{CO_2} p_{H_2}^{1/2} + K_{OH}^* (p_{H_2O} / p_{H_2}^{1/2}) \right] \left(1 + K_{H^{(a)}}^{1/2} p_{H_2}^{1/2} \right)}$$



Sampara, Depcik & Assanis in progress



Very Brief Summary of Literature DPF Models



- Bulk Gas Mass¹

$$\frac{\partial(\rho_i u_i)}{\partial x} = (-1)^i \frac{4}{d_m} \rho_w u_w$$

- Bulk Gas Momentum¹

$$\frac{\partial p_i}{\partial x} + \frac{\partial(\rho_i u_i^2)}{\partial x} = -F \frac{\mu_i u_i}{d_m^2}$$

- Bulk Gas Energy^{1,2}

$$\rho_I u_I c_{p,g} \frac{\partial T_{gI}}{\partial x} = \frac{4}{d_m} h_{gI} (T_m - T_{gI})$$

$$\rho_{II} u_{II} c_{p,g} \frac{\partial T_{gII}}{\partial x} = \frac{4}{d_m} [h_{gII} + \rho_w u_w c_{p,g}] (T_m - T_{gII})$$

- Bulk Gas Species^{1,3}

$$Y_{g,O_2} = Y_{g,O_2}|_{i=1} \quad \text{or}$$

$$\phi \rho_g \left(\frac{\partial Y_{g,O_2}}{\partial t} + u \frac{\partial Y_{g,O_2}}{\partial x} \right) = -k \rho_g Y_{g,O_2}$$

$i = 1$ (inlet, I); $i = 2$ (outlet, II)

Pressure Drop¹

$$p_I - p_{II} = \left(\frac{\mu_w u_w}{K_{m/d}} + \beta_{m/d} \rho_w u_w^2 \right) [t_m + t_d]$$

Soot Thickness^{1,2}

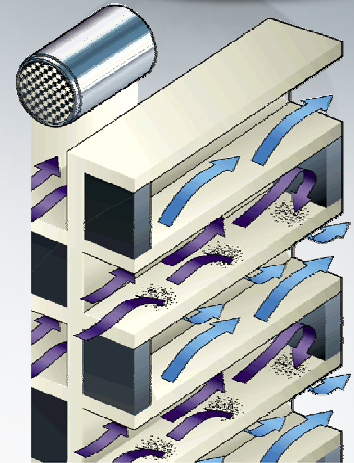
$$\rho_d \frac{\partial t_d}{\partial t} = - \sum_{k=1}^2 \left(\frac{W_{C(s)}}{W_k} \right) (\rho_w u_w) \frac{X_{s,O_2}}{\alpha_k} \left[1 - e^{-(k S_p t_d \alpha_k)/u_w} \right]$$

Surface Energy^{1,2}

$$\frac{\partial}{\partial t} [(\rho_m c_m t_m + \rho_d c_d t_d) T_m] = k_m t_m \frac{\partial^2 T_m}{\partial x^2} + k_d \frac{\partial}{\partial x} \left(t_d \frac{\partial T_m}{\partial x} \right) + h_{gI} (T_{gI} - T_m) + h_{gII} (T_{gII} - T_m) + \rho_w u_w c_{p,g} (T_{gI} - T_m) + \Delta H_{\text{reac}}$$

Ideal Gas Law¹

$$p_i = \rho_i R_i T_{gI}$$





DPF Bulk Gas Source Terms

- Bulk Gas Mass $S_{mass_I} = -\frac{4}{d_m} \rho_I u_w$ $S_{mass_{II}} = \frac{4}{d_m} \rho_w u_w$ $\rho_I = \sum_{j=1}^{NM} C_{gI,j}$ $\rho_w = \sum_{j=1}^{NM} C_{s,j}$

- Inlet channel mass loss should be a function of the properties in the inlet channel not the surface

- Bulk Gas Momentum $S_{mom_I} = -F \frac{\mu_I u_I}{d_m^2}$ $S_{mom_{II}} = -F \frac{\mu_{II} u_{II}}{d_m^2}$

- Bulk Gas Energy

- Literature equations can be recovered when
 - No gas storage approximation is used
 - Specific enthalpy is used instead of total enthalpy

$$S_{eng_I} = -\frac{4}{d_m} \left[h_{gI} (T_{gI} - T_m) + \rho_I u_w H_{Im} \right] \quad S_{eng_{II}} = -\frac{4}{d_m} \left[h_{gII} (T_{gII} - T_m) - \rho_w u_w H_{mII} \right]$$

- Bulk Gas Species

- Species flow from inlet channel to wall, then from wall to outlet channel

$$\bar{S}_{spc_I} = -\frac{4}{d_m} u_w \bar{C}_{gI,j} \quad \bar{S}_{spc_{II}} = \frac{4}{d_m} u_w \bar{C}_{s,j}$$

Governing Equations of Motion

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}$$

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ \rho Y_j \end{bmatrix} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \\ C_j \end{bmatrix}$$

$$\mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \\ \rho u Y_j \end{bmatrix}$$

One-Dimensional Based DPF Model



- Two Channel Based
- Pressure Drop Across Wall

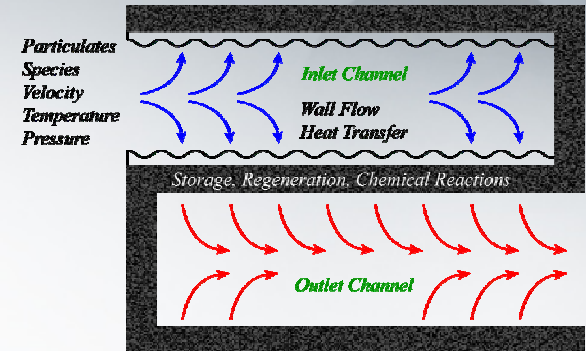
Pressure Drop = Wall Drop + Deposit Drop

$$P_I - P_{II} = \Delta p_{wall} + \Delta p_{deposit}$$

Darcy's Law

$$\Delta p_{wall} = \left(\frac{\mu_w u_w}{K_m} + \beta_m \rho_w u_w^2 \right) t_m$$

Forschheimer



- Surface Gas Species

Storage = Wall Flow + Deposit Reactions + Catalytic Reactions

$$(V_m + V_d) \frac{d\bar{C}_{s,j}}{dt} = u_w A_s (\bar{C}_{g1,j} - \bar{C}_{s,j}) - \frac{N_c}{2} \dot{n}_j - A_{cat} R_j$$

- Surface Deposit

Storage = Gas Flow + Deposit Reactions

$$\frac{dm_{ds}}{dt} = \dot{m}_{dg} - \dot{m}_{ds}$$

$$\dot{i}_d = k_{pre} T_m \exp(-E_a/R_u T_m) t_d X_{s,O_2}$$

$$\dot{m}_{ds} = \dot{i}_d \rho_d \Delta x [4d_m - 8t_d]$$

- Surface Energy

Storage = Cond. + Eng. Trn. + Ht Trn. + Dpst Rxns + Cat. Rxns + Vol. Ht + Pseudo-2D HT

$$\frac{\partial}{\partial t} [(\rho_m c_m V_m + \rho_d c_d V_d) T_m] = k_m V_m \frac{\partial^2 T_m}{\partial x^2} + k_d \frac{\partial}{\partial x} \left(V_d \frac{\partial T_m}{\partial x} \right) + \rho_w u_w A_s (H_{lm} - H_{mII})$$

$$+ h_{gI} A_s (T_{gI} - T_m) + h_{gII} A_s (T_{gII} - T_m) + \frac{N_c}{2} \sum_{j=1}^{NM} \dot{n}_j H_j + A_{cat} \sum_{j=1}^{NM} R_j H_j + \dot{q} V_m + Q_{i \rightarrow m}$$



Inlet Channel (I)

$$S_{inlet} = \begin{bmatrix} \text{Mass Flow} & -G \rho_I u_w \\ \text{Friction} & -\left(\frac{7.1135 \mu |u_I|}{d_m} \right) G \\ -G \left[h_{gI} (T_{gI} - T_m) + \rho_I u_w H_{Im} \right] & \\ \text{Species Flow} & -G u_w C_{gI,j} \end{bmatrix}$$

Outlet Channel (II)

$$S_{outlet} = \begin{bmatrix} & G \rho_w u_w \\ \text{Heat and Energy Transfer} & -\left(\frac{7.1135 \mu |u_{II}|}{d_m} \right) G \\ -G \left[h_{gII} (T_{gII} - T_m) - \rho_w u_w H_{mII} \right] & \\ & G u_w C_{s,j} \end{bmatrix}$$

$G = 4/d_m$

Numerical Solvers

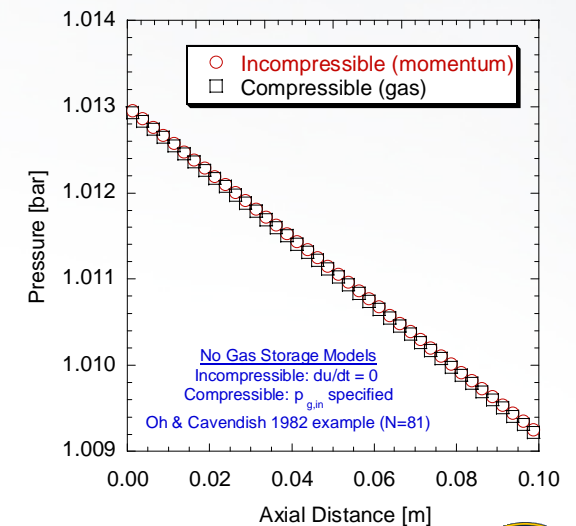


- Transient Solvers Described in Catalyst Modeling Paper
- Incompressible versus Compressible
 - Reduced stiffness
 - Interdependency of equations
 - $u \sim 10$ m/s vs $(u+a) \sim 350$ m/s
 - Momentum pressure
 - Can be used to approximate pressure drop
- No Gas Storage versus Transient
 - Can take larger time-steps
 - Transient solvers need von Neumann analysis

$$\Delta t_{incompressible} \sim \frac{\Delta x}{u}$$

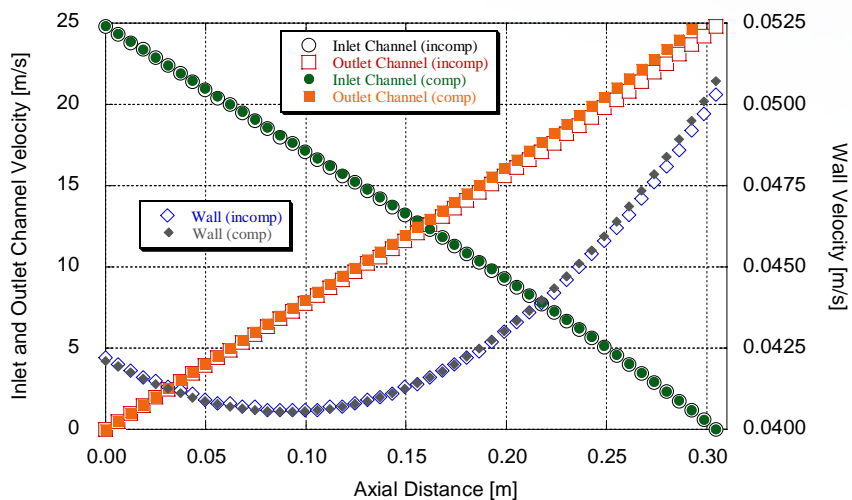
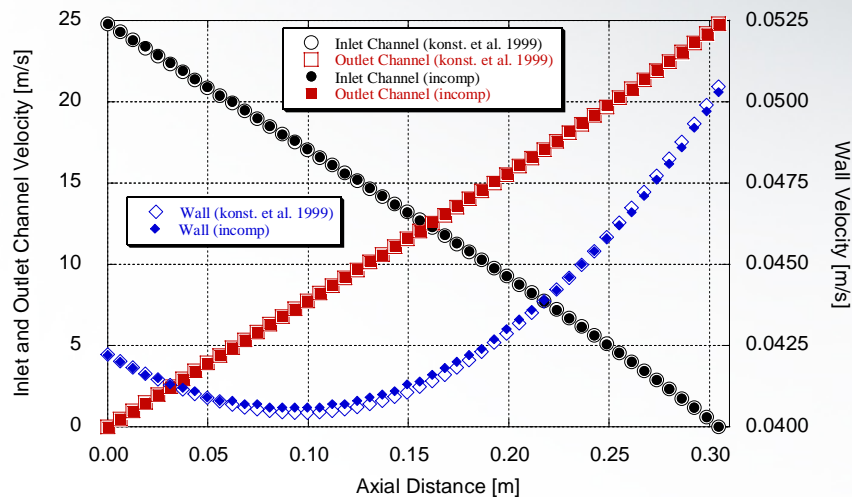
$$\Delta t_{compressible} \sim \frac{\Delta x}{u+a}$$

Isothermal Pressure Profile

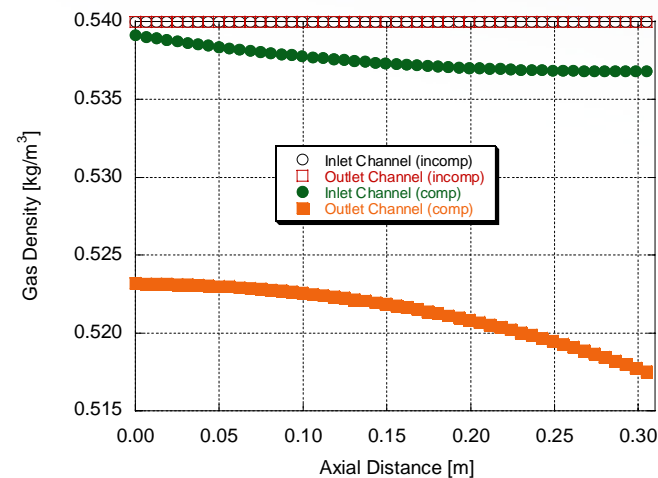




Validation of Flow Profile



- Compared to Konstandopoulos et al. 1999 Isothermal Diesel Particulate Filter Model
- Results Slightly Different due to Thermodynamic Properties and Algorithms
- Wall Temperature Held Constant
- Compressible Outlet Channel Density Lower because of Lower Pressure and Ideal Gas Law (Isothermal Run)

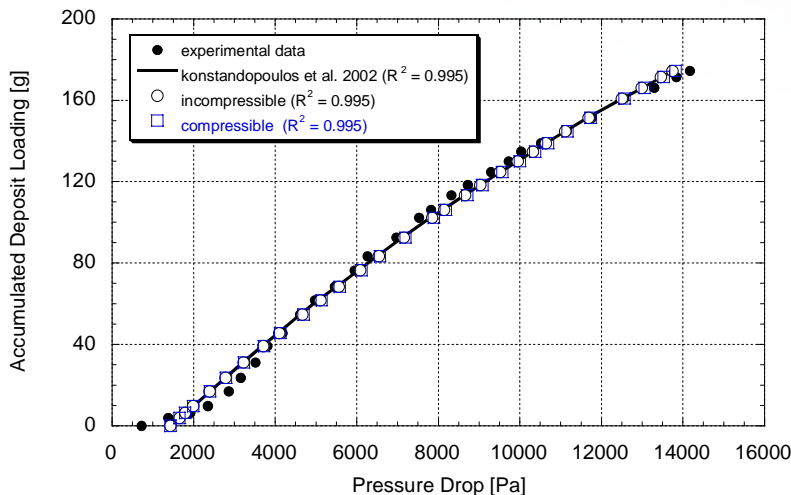




Validation of Particulate Loading

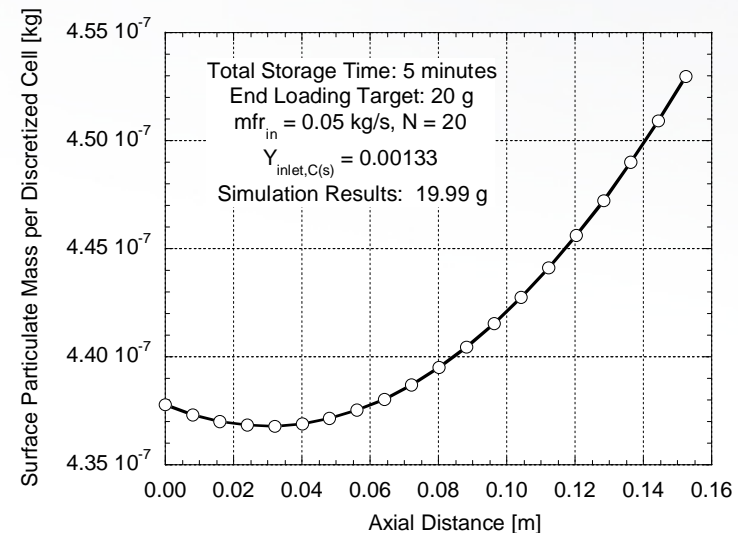
Pressure Drop vs. Deposit Loading

- Experimental Data from Gantawar et al. 1997
- Previous Literature Model Results from Konstandopolous et al. 2002



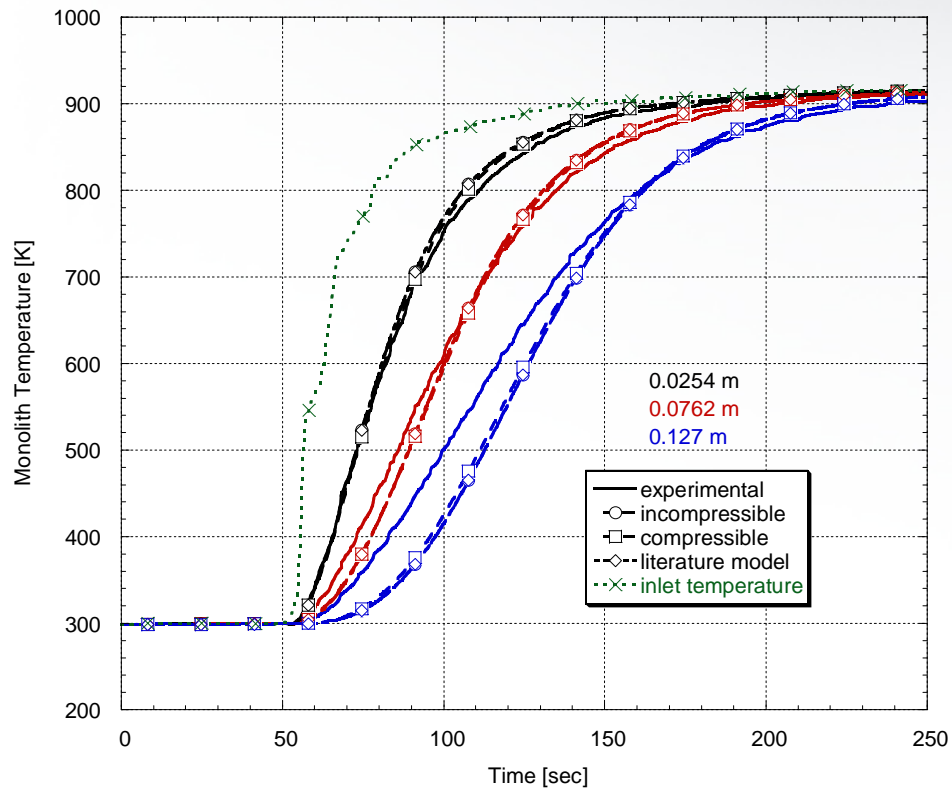
Example of Soot Propagation

- Numerical Test
- 5 Minute Isothermal Loading Event
- Mass Flow Rate of Soot Target Loading of 20 grams
- Test Results = 19.99 g

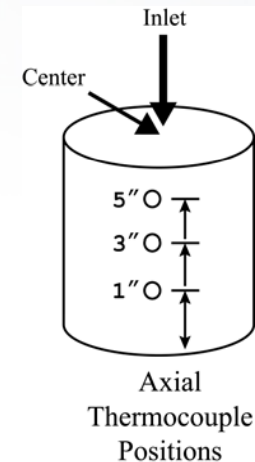




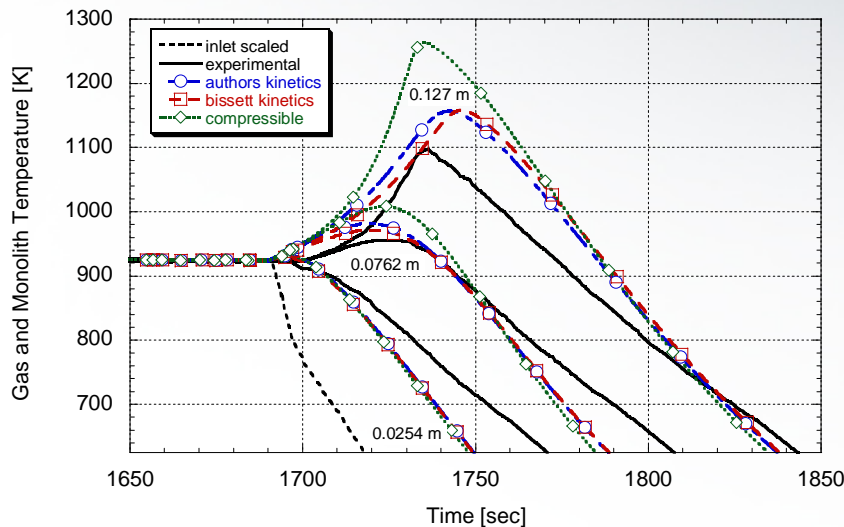
Validation of Energy Equations



- Young et al. 2002 SiC DPF Experiments
- Warmup of DPF by N₂ only
- Thermocouples placed 9 mm from center of DPF



Validation of Deposit Oxidation, Chemical Species and Exothermic Reactions¹



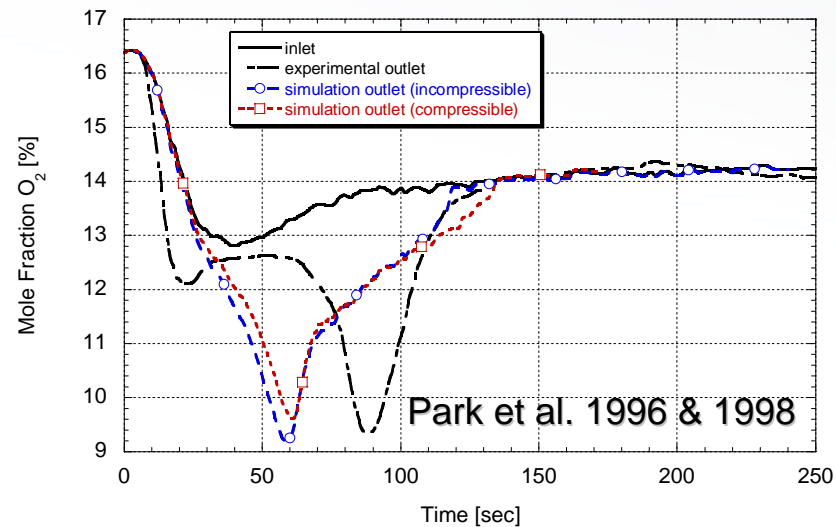
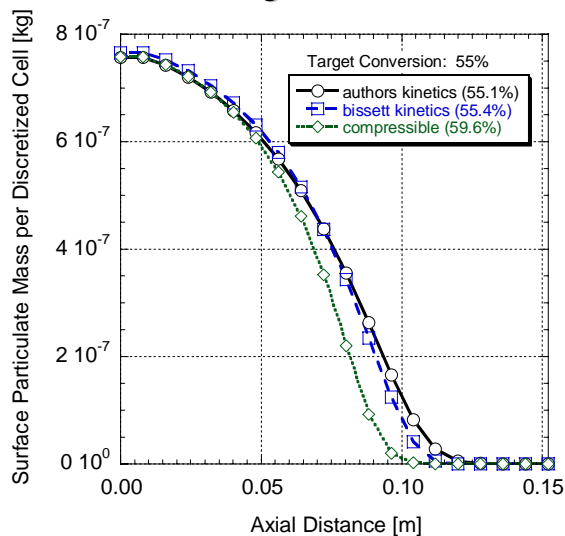
- Calibrated Incompressible Model to Young et al. 2002 O₂ Oxidation Experiment (Target Conversion = 55%)

- Conditions unknown after 1720 s

- Used Same Kinetic Parameters with Park et al. 1996 & 1998 Experimental Work

- Some questions about experiment

Young et al. 2002

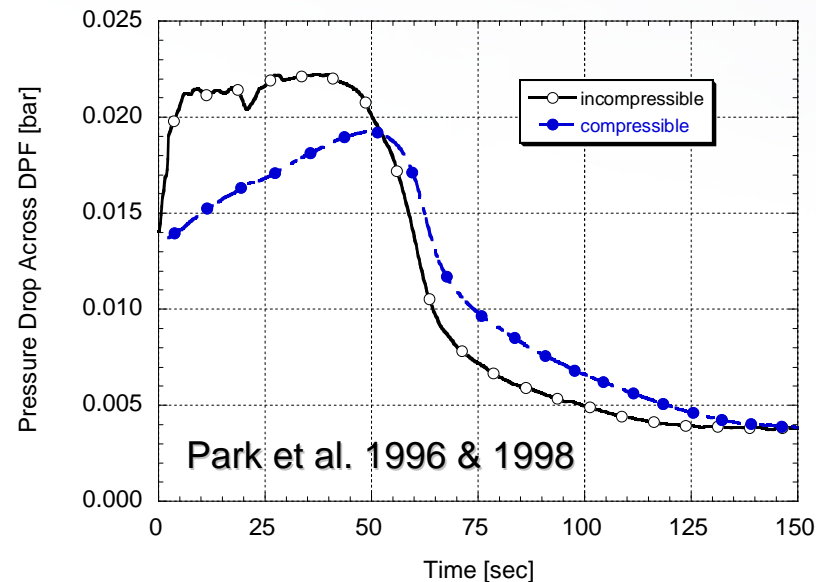


Park et al. 1996 & 1998

Validation of Deposit Oxidation, Chemical Species and Exothermic Reactions²



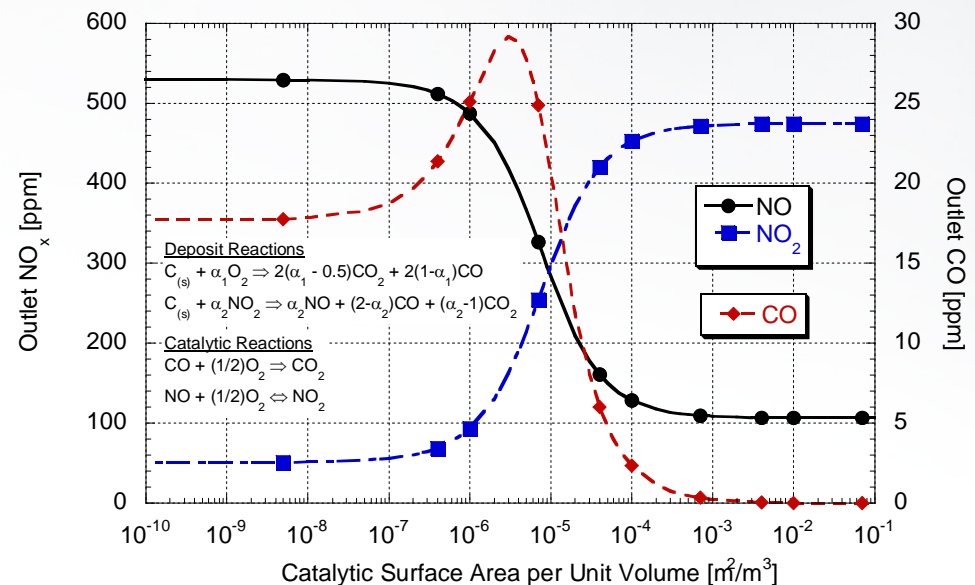
- Incompressible vs. Compressible Pressure Drop
 - Incompressible – momentum pressure
 - Compressible – ideal gas law
 - Not the same, yet not too different





Incorporation of Catalyzed Surface

- NO and CO Oxidation Reactions of a DOC (Kandylas and Koltsakis, 2002) Incorporated with O₂ and NO₂ Deposit Reactions
- Increasing Catalytic Surface Area
 - More NO conversion to NO₂
 - NO₂ subsequently converts more deposit to CO and CO₂
 - Trend of CO increases
 - Eventually catalyst reactions dominate
 - CO converted to CO₂
 - NO converted to NO₂



Comments



- Increasing Accuracy of Axial Derivative Solvers
 - Results presented here might change slightly
- Other Surface Models Available
 - Example: Konstandopolous et al. 2005
 - Possible collaboration through dynamically-linked libraries
- Graphical User Interface, DOS and Matlab Simulink Versions
- All Solvers, Algorithms and Run Time Conditions Discussed in Upcoming Papers
 - Catalyst modeling paper hopefully in print late 2005
 - CDPF modeling paper will be submitted soon



Conclusion

- Added Bulk Gas Species Equations to Diesel Particulate Filter 1-D Based Model
- Adjusted a Few of the Model Source Terms
- Created Fully Transient Solvers
 - All d/dt terms incorporated
- Compared Incompressible and Compressible Results
- Added Surface Gas Species Equation
- Incorporated Catalyzed Reactions