Emissions Control Technologies, Part 2

Eulerian CFD Models to Predict Thermophoretic Deposition of Soot Particles in EGR Coolers

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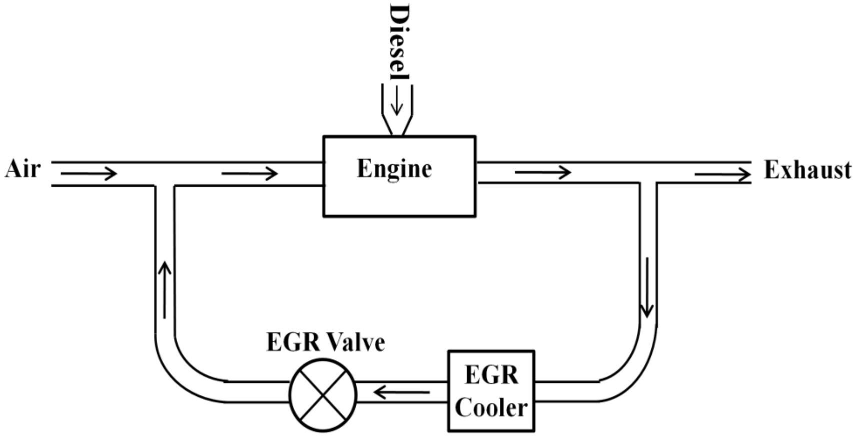
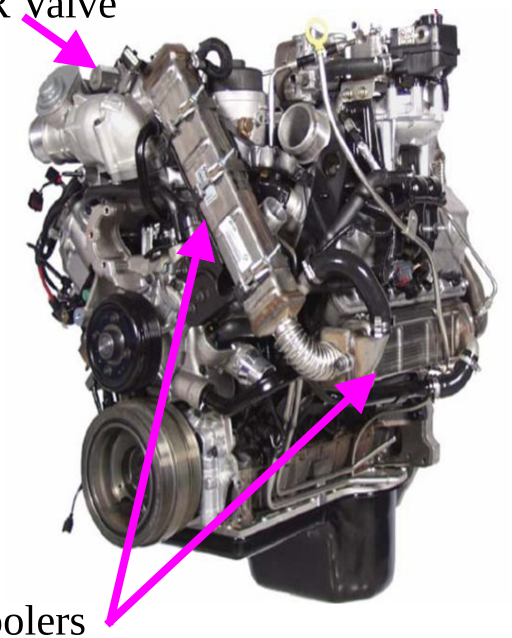
Exhaust Gas Recirculation (EGR)

The introduction of exhaust gas into the engine intake:



EGR Valve



EGR Coolers

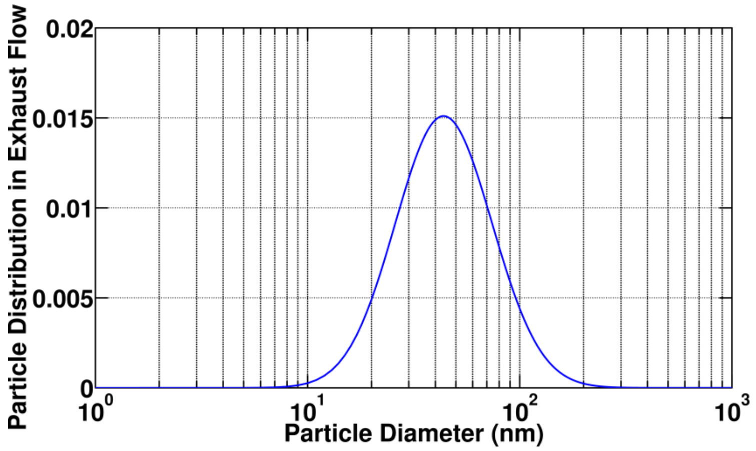
EGR:

- Inert combustion products
- Not participate in combustion
- Reduces flame temperature
- Effective way of reducing nitrogen oxides (NOx) formation

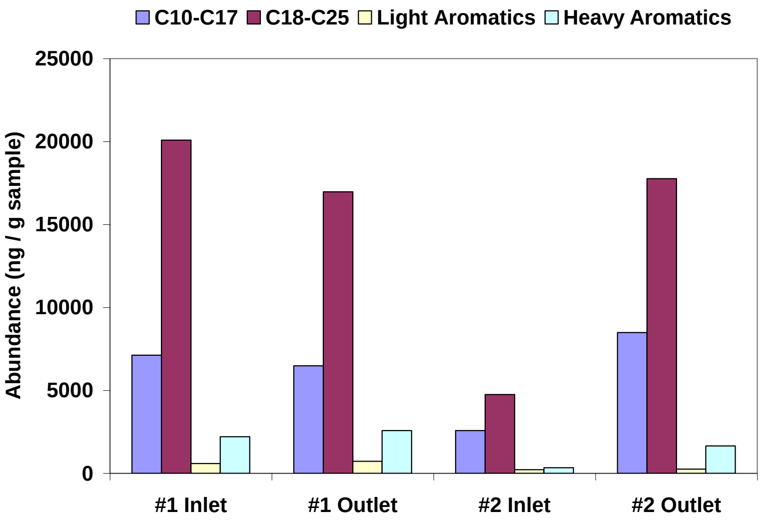
- Most current diesel engines have a single EGR cooler
- Engine coolant (80-90°C) to cool EGR
- Presence of cold surfaces causes soot deposition and HC condensation

What are deposits?

- Soot:
  - Elemental carbon ranging from 10 nm to 300 nm with a 57 nm mean diameter
  - Majority of deposit is dry fluffy soot particles
- Hydrocarbons (HCs):
  - Unburned and partially burned fuel and lube oil
- Acids:
  - Sulfuric acid, nitric acid , organic acids such as formic and acetic acid
- Ash:
  - Oxidized or sulfated metals



EGR soot particles probability density function



Speciation of the extractable fraction of HC from EGR cooler deposit (Hoard et. al. DEER 2007)

Motivation

The buildup of deposits (fouling) in EGR coolers:

- Significant degradation in heat transfer (20-30%)
- Increases pressure drop (about twice)
- Current EGR coolers are not appropriate for future emission standards
- Future low-emission systems have more fouling issues (Lower cooler-out temperature, Higher EGR flow)
- Coolers are currently oversized to compensate deposition effects

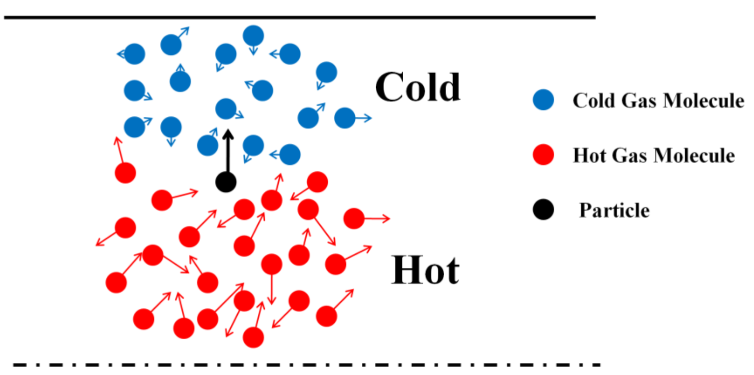
A fouled cooler in an engine test (200 hours)

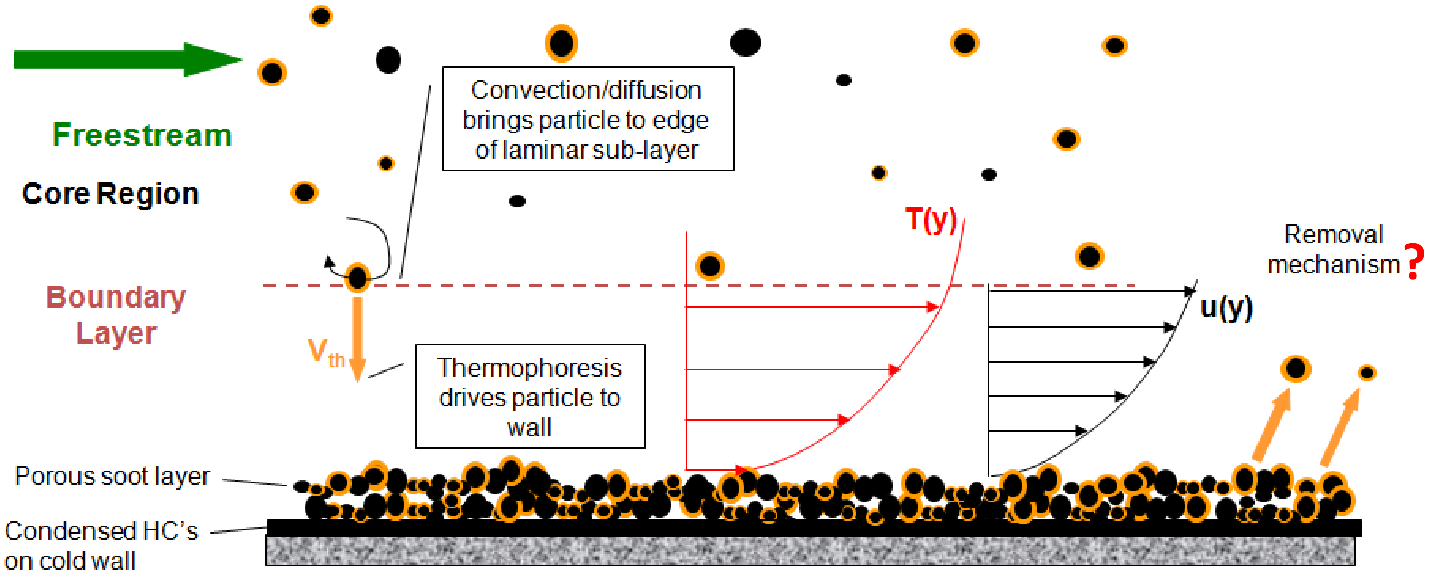
Thermophoresis – Talbot Formula

$$V_{th} = -K_{th} \frac{\nu}{T} \vec{\nabla} T$$

Velocity of particle toward surface is a function of:

- Kinematic viscosity
- Temperature gradient
- Thermophoresis coefficient





Convection/diffusion brings particle to edge of laminar sub-layer

Thermophoresis drives particle to wall

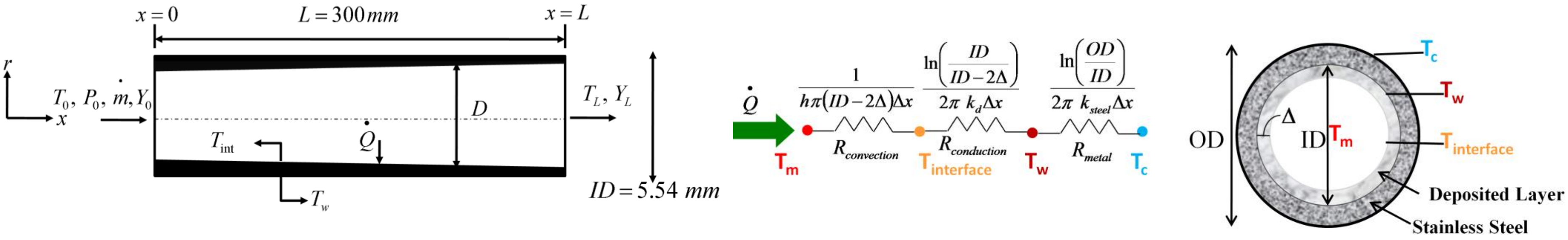
1D Model

Most EGR coolers are shell & tube heat exchangers, limited this study to tube flows

- The deposit layer properties function of gas-deposit interface temperature
- Gas properties vary along the length
- Diffusion in addition to thermophoresis

Potentials

- Variable sticking and removal coefficient can potentially be added
- Radiation heat transfer can be added



A schematic of the surrogate tube and the heat transfer model

Governing Equations – 1D Model

- A second order differencing method developed in MATLAB to solve governing equations

Bulk Gas Flow

Mass:

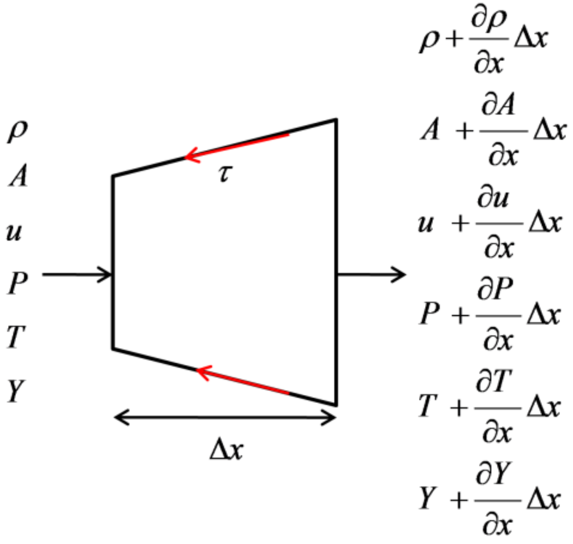
$$\frac{d(\rho_g uA)}{dx} = \frac{d(\dot{m})}{dx} = 0$$

Momentum:

$$\frac{dP}{dx} = -\frac{1}{2}\frac{\rho_g\, f\, u^2}{D} - \dot{m}\frac{du}{dx}$$

Energy:

$$\dot{m}\frac{d(c_p T)}{dx} = -\dot{m}\frac{d(u^2/2)}{dx} + \frac{(T-T_w)}{R_{Convection} + R_{conduction} + R_{metal}}$$



Particles

Mass:

$$\dot{m}\frac{dY}{dx} = \pi D\left(\rho_g D_B \frac{\partial Y}{\partial r} + \rho_g Y V_{th}\right)\Big|_{r=D/2}$$

Near wall Gradients:

$$\left.\frac{\partial T}{\partial r}\right|_{r=D/2} = \frac{Nu(T_{\text{int}} - T)}{D} \qquad \left.\frac{\partial Y}{\partial r}\right|_{r=D/2} = \frac{Sh(Y_{\text{int}} - Y)}{D} = -\frac{ShY}{D}$$

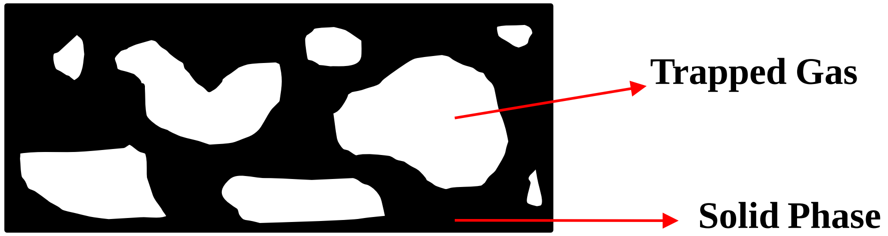
Deposit Thermal Conductivity

Deposit is treated as a cluster made of a fluid and a solid constituents.

$$k_{cluster} = (1-\phi)^{1.5} k_{Solid} + \phi^{0.25} k_{Fluid}$$

Solid phase: Graphite

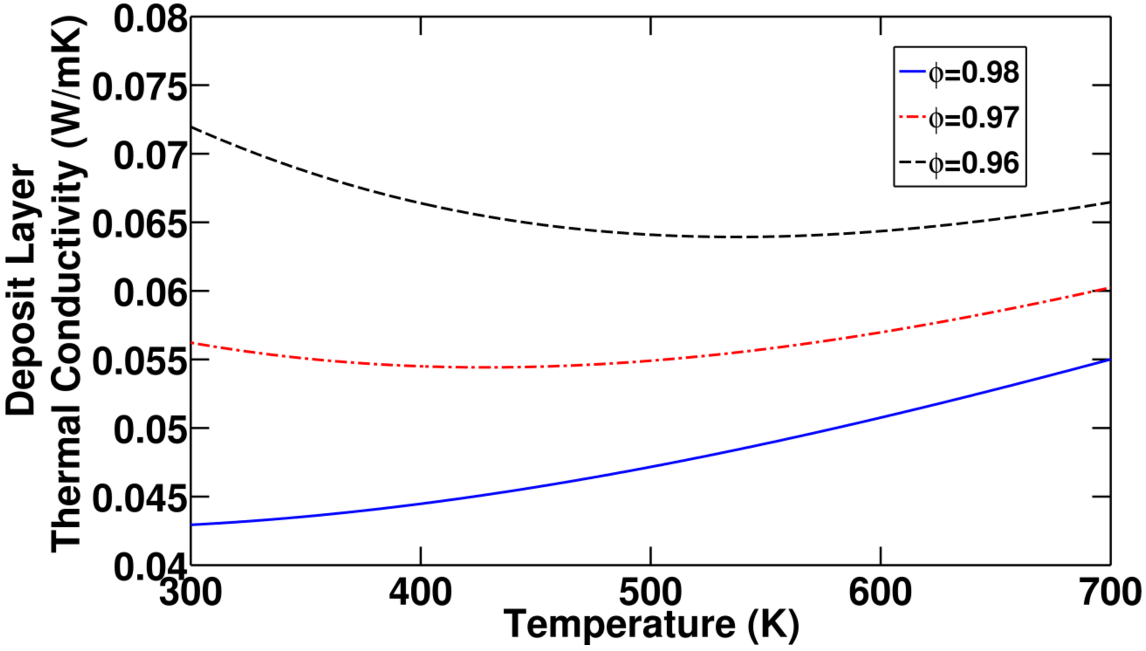
Fluid phase: Trapped EGR



98% porosity (ϕ)

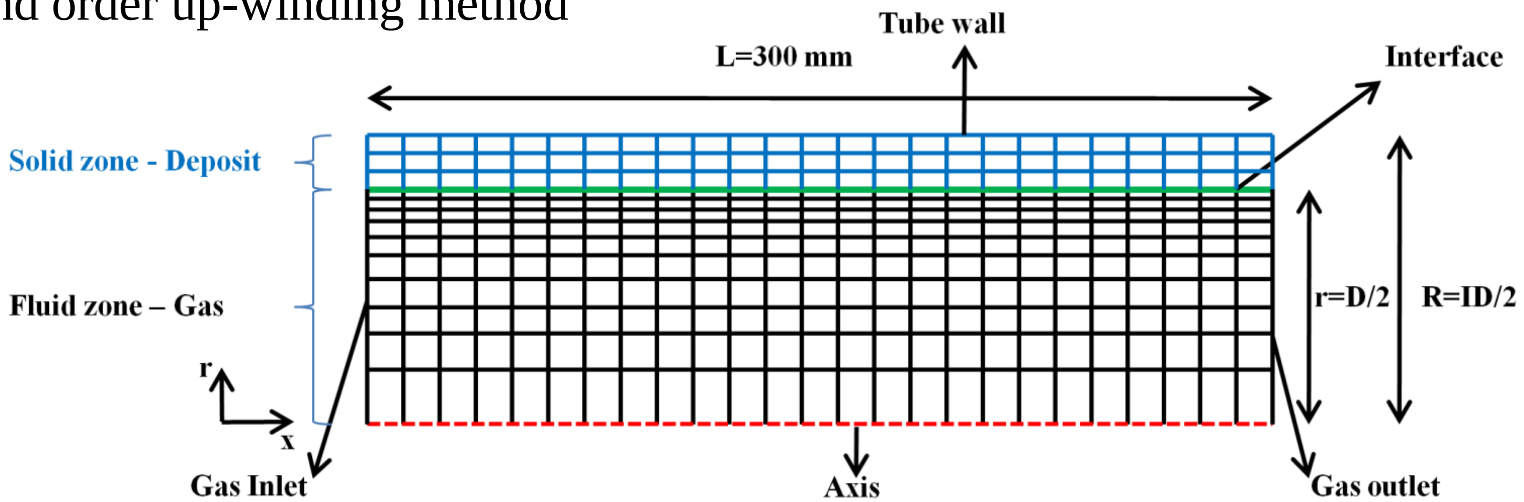
The equivalent density:

$$\rho_{deposit} = (1-\phi)\rho_{Soot}$$



Axi-Symmetric Model in FLUENT

- ANSYS-FLUENT commercial software
- A two zone model (Solid/Fluid) with subroutines for moving the mesh as layer grows
- RANS turbulence modeling
- RSM to model the Reynolds stress terms
- SIMPLE Algorithm for pressure correction
- Second order up-winding method



Governing Equations, Boundary Conditions

Bulk Gas Flow

Mass: $$\frac{\partial\left(\bar{\rho}_g\right)}{\partial t}+\nabla.\left(\bar{\rho}_g\mathbf{v}\right)=0$$

Momentum: $$\frac{\partial\left(\bar{\rho}_g\mathbf{v}\right)}{\partial t}+\nabla.\left(\bar{\rho}_g\mathbf{vv}\right)=-\nabla\bar{\mathrm{P}}+\nabla.\left(\bar{\boldsymbol{\tau}}\right)+\nabla.\left(-\bar{\rho}_g\overline{\mathbf{v}''\mathbf{v}''}\right)$$

Energy: $$\frac{\partial\left(\bar{\rho}_g\mathrm{c_p}\mathrm{T}\right)}{\partial t}+\nabla.\left(\bar{\rho}_g\mathrm{c_p}\mathbf{v}\mathrm{T}\right)=\nabla.\left(\mathrm{c_p}\frac{\mu}{\mathrm{pr}}\nabla\mathrm{T}\right)+\frac{\partial\bar{\mathrm{P}}}{\partial t}+\nabla.\left(-\overline{\mathbf{v}\boldsymbol{\tau}}\right)+\nabla.\left(-\bar{\rho}_g\overline{\mathbf{v}''\mathrm{T}''}\right)$$

Particles

New Advective term

Diffusion term

Mass: $$\frac{\partial\left(\bar{\rho}_g\mathrm{Y}\right)}{\partial t}+\nabla.\left(\bar{\rho}_g\left(\mathbf{v}+\boldsymbol{V}_{th}\right)\mathrm{Y}\right)=\nabla.\left(\bar{\rho}_g\mathrm{D}_B\nabla\mathrm{Y}\right)+\nabla.\left(-\bar{\rho}_g\left(\overline{\mathbf{v}''\mathrm{Y}''}+\overline{\mathbf{V}''_{\mathbf{th}}\mathrm{Y}''}\right)\right)$$

Fluid Zone

$$\dot{m}\left(x=0,\ 0\le r\le D/2\ ,t\right)=\dot{m}$$

$$\vec{U}\left(0\le x\le L,\ r=D/2\ ,t\right)=0\quad(no\ \ slip)$$

$$P\left(x=0,\ 0\le r\le D/2\ ,t\right)=P_0$$

$$T\left(x=0,\ 0\le r\le D/2\ ,t\right)=T_0$$

$$\frac{\partial T}{\partial x}\left(\ x=L,\ 0\le r\le D/2\ ,t\right)=0\ (outflow)$$

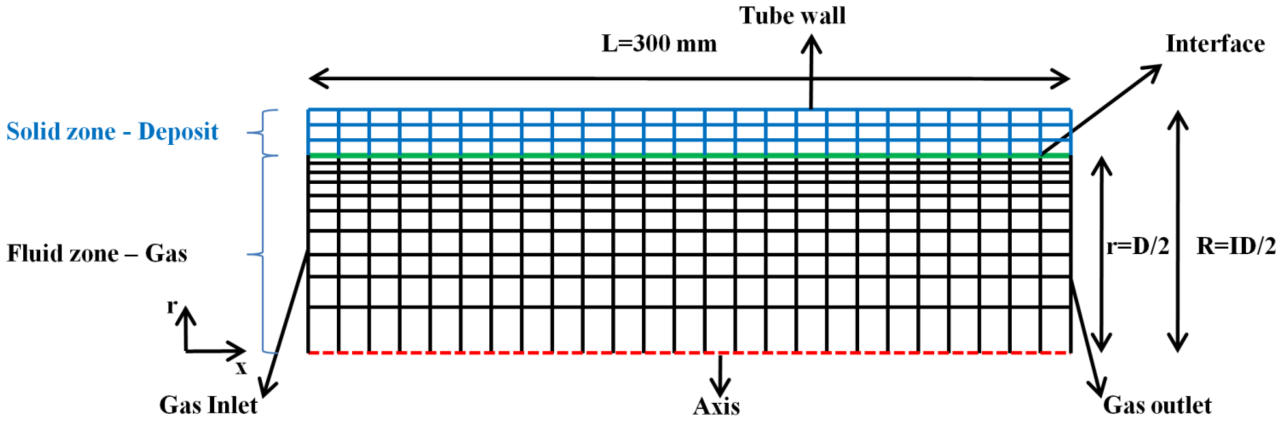
Solid Zone

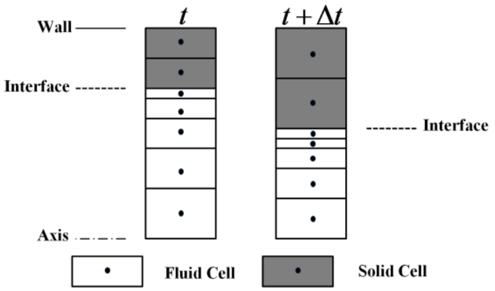
$$-k_g\frac{\partial T_g}{\partial r}\left(0\le x\le L,\ r=D/2\ ,t\right)=-k_d\frac{\partial T_d}{\partial r}\left(0\le x\le L,\ r=D/2\ ,t\right)$$

$$T\left(x=0,\ D/2\le r\le ID/2\ ,t\right)=T_0$$

$$T\left(0\le x\le L,\ r=ID/2\ ,t\right)=T_w$$

$$T\left(\ x=L,\ D/2\le r\le ID/2\ ,t\right)=T_w$$





Profiles Comparison

- Velocity, temperature, and particle mass fraction profiles are normalized and compared at x=L/2 (Exp. 8)

$$\dot{m} = 9\times10^{-4}\,kg/s, T_0 = 653\,K, T_w = 363\,K, P_0 = 196\,kPa, Y_0 = 28.9\times10^{-6}$$

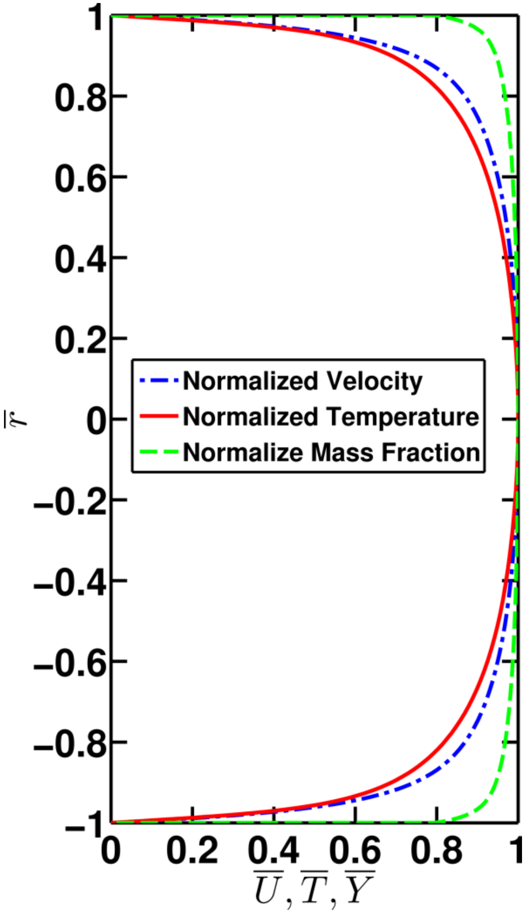
- Turbulence makes the velocity and temperature profiles flat
- Particle mass fraction profile is almost flat except at a large gradient region near the wall

$$\overline{U} = \frac{U}{U|_{r=0}}$$

$$\overline{T} = \frac{T - T_w}{T|_{r=0} - T_w}$$

$$\overline{Y} = \frac{Y}{Y|_{r=0}}$$

$$\overline{r} = \frac{r}{ID/2}$$



Deposition Flux

- Particle mass fraction and gas temperature gradient near the wall are calculated in UDFs. They are used to estimate the deposited mass.

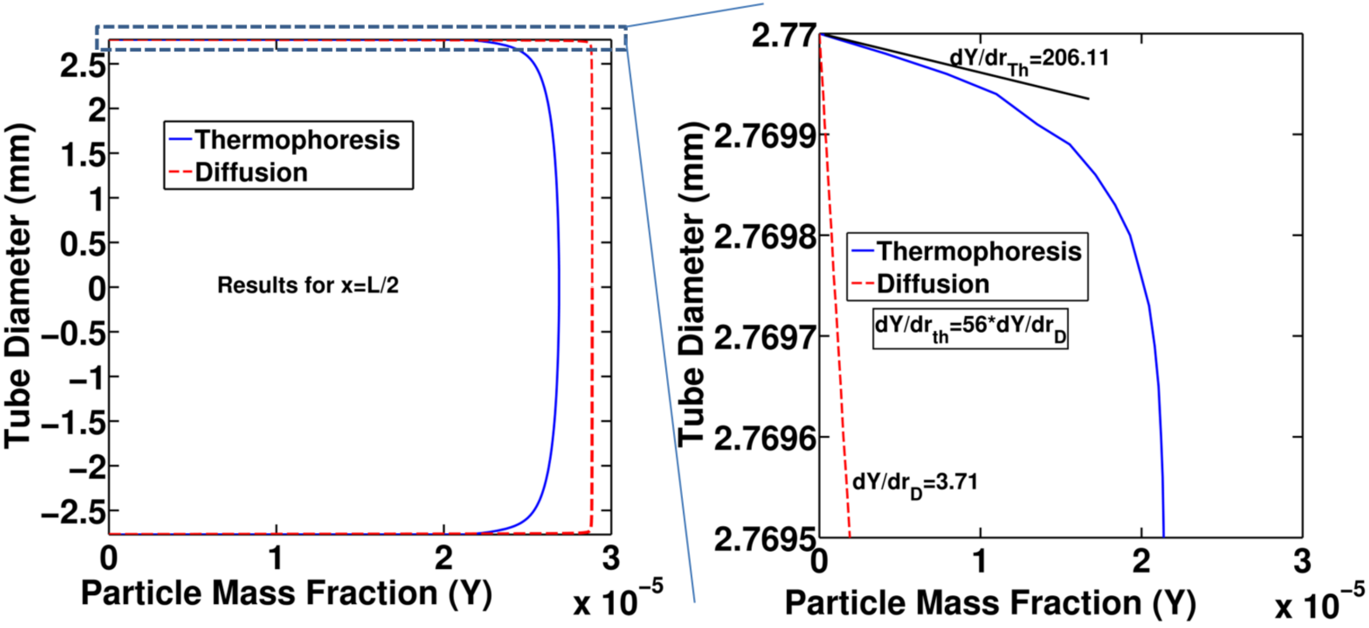
Brownian Diffusion Coefficient:

$$D_B = \frac{k_b T C_c}{3\pi\,\mu\,d_p} \propto \frac{T^{1.5}}{P}$$

Deposition Flux:

$$\vec{J}_{total} = \rho_g D_B \left.\frac{\partial Y}{\partial r}\right|_{wall}$$

Scale change



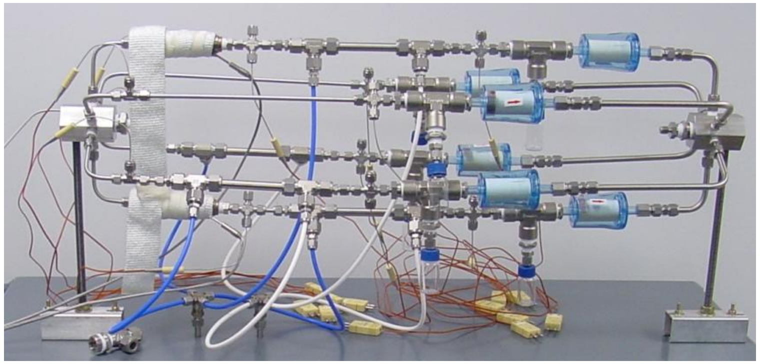
1D Model prediction

$$\frac{J_{th}}{J_D} = \left.\frac{\rho_g Y V_{th}}{\rho_g D_B \left.\frac{\partial Y}{\partial r}\right|_{r=\frac{D}{2}}}\right|_{x=\frac{L}{2}} = 34.1$$

$$\dot{m} = 9\times10^{-4}\,kg/s, T_0 = 653\,K, T_w = 363\,K, P_0 = 196\,kPa, Y_0 = 28.9\times10^{-6}$$

ORNL Experiments

- Orthogonal experiments to vary boundary conditions
- In selected experiments, inlet pressure :196 kPa, coolant temperature: 90°C (avoid water condensation) , low HC level
- Surrogate tubes were employed instead of EGR coolers



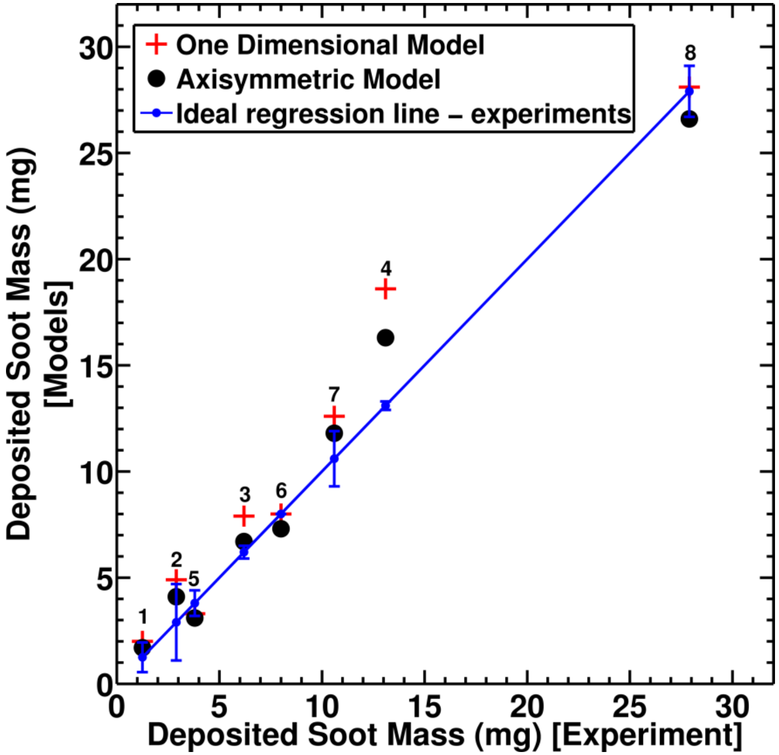
A snapshot of the experimental set up (ORNL)

$$Y = \frac{C}{\rho|_{P,T_{inlet}}}$$

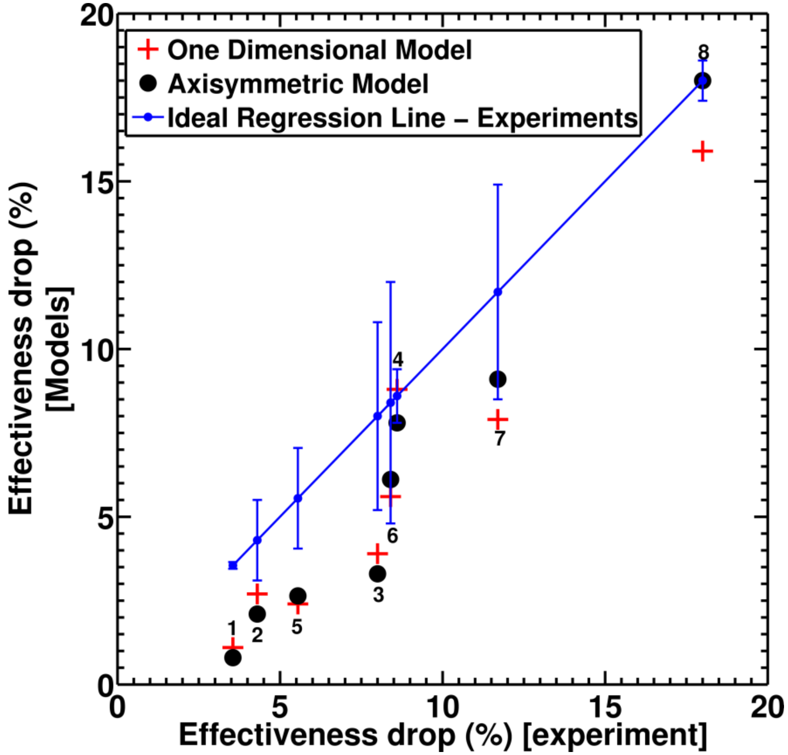
C : Particle Concentration
Y : Particle Mass Fraction
ρ : Gas Density

Experiment No.		Initial Reynolds Number (Re @ t=0)	Inlet Particle Concentration (mg/m³)	Inlet Temperature (K)
1	Low Flow	4500	7.5	493
2		4000	7.5	653
3		4500	30	493
4		4000	30	653
5	High Flow	9000	7.5	493
6		8000	7.5	653
7		9000	30	493
8		8000	30	653

CFD Models-Experiments Comparisons



Deposited soot mass gain (3 hours exposure)

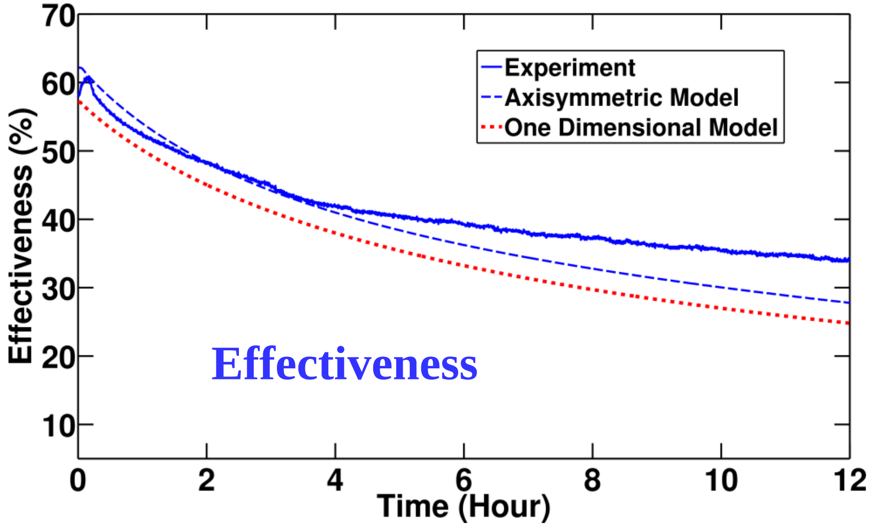


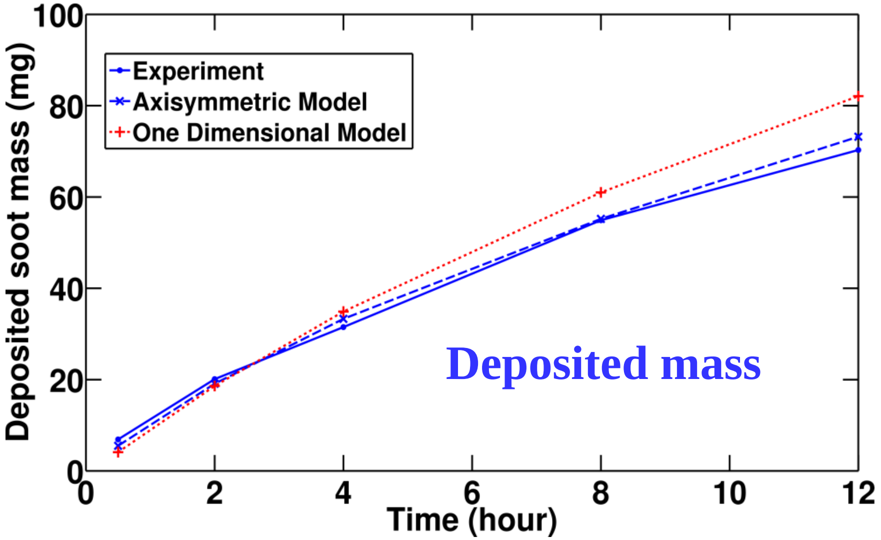
Effectiveness drop (3 hours exposure)

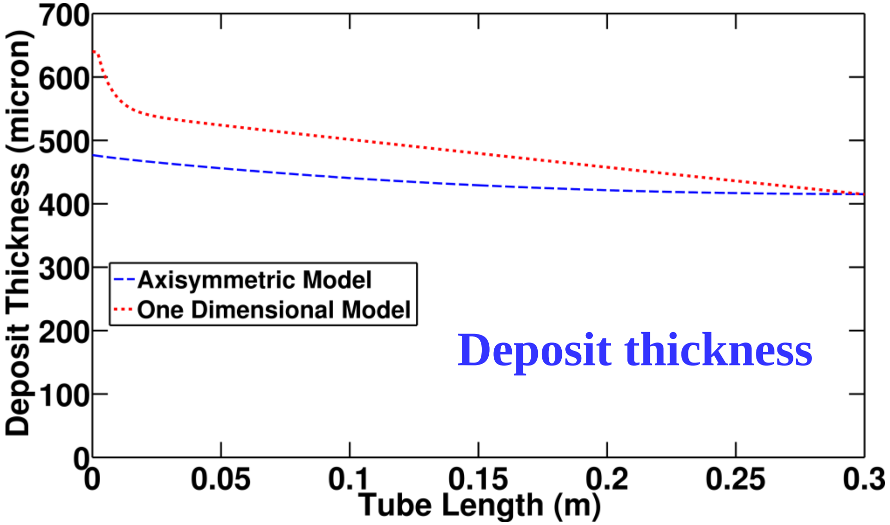
- Better estimation of mass deposited by the axi-symmetric model (14% compared to 1D)
- Overall, closer estimation of heat transfer reduction by the axi-symmetric model (2% compared to 1D)

Longer Exposure Comparison

- Significantly better estimation of mass gain by the axi-symmetric model
- 1D model deviates from experiment sooner
- Estimated thickness by axi-symmetric model is closer to experimental images – more uniform







$$\dot{m} = 9\times10^{-4}\,kg/s, T_0 = 653\,K, T_w = 363\,K, P_0 = 196\,kPa, Y_0 = 28.9\times10^{-6}$$

Conclusions

- Eulerian approaches to predict thermophoretic deposition on cooled surfaces in tube flows
- Taking into account the effect of the layer growth on heat and mass transfer
- More accurate compared to our previous analytical work (gas and deposit properties variation)
- 1D model
  - ✓ Fast and cheap for new investigations
- Axi-symmetric model:
  - ✓ Better prediction of deposited mass gain especially at longer exposure tests
  - ✓ More realistic deposit thickness prediction – consistent with experiments
  - ✓ Only way to simulate real EGR coolers with wavy channels and winglets (possible extension to 3D modeling)