

Modeling of Thermophoretic Soot Deposition and Hydrocarbon Condensation in EGR Coolers

Mehdi Abarham, John Hoard and Dennis Assanis

University of Michigan, W.E. Lay Automotive Laboratory

Dan Styles, Eric W. Curtis and Nitia Ramesh

Ford Motor Company

C. Scott Sluder and John M. E. Storey

Oak Ridge National Laboratory

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ABSTRACT

EGR coolers are effective to reduce NO_x emissions from diesel engines due to lower intake charge temperature. EGR cooler fouling reduces heat transfer capacity of the cooler significantly and increases pressure drop across the cooler. Engine coolant provided at 40-90 °C is used to cool EGR coolers. The presence of a cold surface in the cooler causes particulate soot deposition and hydrocarbon condensation. The experimental data also indicates that the fouling is mainly caused by soot and hydrocarbons. In this study, a 1-D model is extended to simulate particulate soot and hydrocarbon deposition on a concentric tube EGR cooler with a constant wall temperature. The soot deposition caused by thermophoresis phenomena is taken into account the model. Condensation of a wide range of hydrocarbon molecules are also modeled but the results show condensation of only heavy molecules at coolant temperature. Thermal properties of fouled layer are calculated based on mass fraction of deposited soot and hydrocarbons. The experiments with the same conditions ran to validate the model. Hot EGR gases flow through the inner pipe and the coolant circulates around it in the outer pipe to keep a constant wall temperature. Effectiveness, deposited soot mass, condensed hydrocarbon mass, and pressure drop across the cooler are the parameters that have been compared. The results of the model are in a reasonably good agreement with the experimental results although

there are some fields that need to be studied in future to improve the model.

INTRODUCTION

The buildup of deposits in EGR coolers causes significant degradation in heat transfer performance, often on the order of 20-30%. Deposits also increase pressure drop across coolers and thus may degrade engine efficiency under some operating conditions. This makes fouling an important issue in diesel engines. Since there is not a firm theory for fouling layer formation in the EGR coolers and because of the complexity of the phenomena, findings on this subject is more towards experimental investigations rather than modeling. A few articles have paid attention to the physics of this problem with different theories and physical interpretation.

A comprehensive literature review on EGR fouling has been done by Hoard et. al. [1]. They gathered information available in literature on what are deposits and how they occur and what can be done to prevent them. A steady state model is developed by Housiadas and Drossinos to predict thermophoretic particle deposition in laminar and turbulent tube flow. The 1D and 2D models in their work provide the same level of accuracy until the gas to wall temperature difference is large. In that case, the 2D model shows significant improvements [2]. Thermophoretic particle deposition in tube flows is measured experimentally by Tsai et. al. by

using monodisperse NaCl particles under laminar and turbulent flow conditions. The previous empirical equations for thermophoretic deposition are in a good agreement with their experimental measurement. Also, they showed that Talbot's formula [3] for thermophoretic deposition is accurate compared to Waldmann's free molecular formula [4].

Another effort in this field is the work done by Lin and Tsai for investigation of thermophoretic deposition efficiency under developing flow at the entrance region. They found out that thermal entrance region of the tube makes the thermophoretic deposition efficiency slightly higher than the fully developed case for a long tube. They developed empirical equations to predict thermophoretic efficiency of a laminar flow in a circular tube in fully developed and developing flow under laminar flow conditions [5]. Chein and Liao studied diffusion and thermophoretic effects on nano-particle deposition in channel flow numerically. They examined two types of thermal conditions for different nano size particles and calculated particle deposition velocities for various wall temperature and different inlet temperature [6].

Lin developed an analytical procedure to predict the particle deposition efficiency by considering thermophoretic velocity in the conservation equations of particles. He investigated the effect of different important parameters like temperature difference of the inlet and wall, particle size, and Lewis number on thermophoretic efficiency [7]. Epstein studied particle deposition from a suspension flowing parallel to nonporous smooth and rough surfaces in terms of particle attachment, transport, and reentrainment. He also investigated sticking probability of particles to the wall for isothermal and nonisothermal conditions. Referring to the literature, he offered a sticking probability as a ratio of adhesive bond force between particles to average shear force on particles at surface [8].

Florea et. al. simulated a transient fluid flow and heat transfer in the EGR cooler by using the CFD code FIRE (AVL) and presented temperature gradient and pressure field across the cooler. They then verified their 3D model with experimental measurements and showed the results are comparable in most cases but they did not take into account the effect of fouling in the model explicitly [9].

Another mass deposition in EGR cooler is hydrocarbons and sulfur condensation which can be significant on a mass basis in EGR coolers compared to soot deposition and they may play an important role in sticking the particles together after their attachment to the tube wall.

Although some authors such as Lepperhof [10] argue that a layer of HC on the surface is essential to act as a "glue" causing soot to stick to the surface, most authors agree that for particles as small as diesel soot, the soot sticks to the surface due to Van der Waals forces, whether or not there is HC present. Nonetheless, it is

clear that condensed HC will change the character of the deposit layer.

Hoard et.al. [11] analyzed the extractable fraction of the deposit HCs. They showed the relative amounts (nanograms of each component per gram of deposit sample) of C10-C17 alkane, C18-C24 alkane, and light and heavy aromatics extracted from EGR cooler deposits. These are generally in the range of the heaviest fraction of diesel fuel, or the typical range of lube oil.

The relatively low temperature cooler surfaces can cause condensation of acids and water from the exhaust. The condensation of sulfuric acid in EGR coolers is nicely described by McKinley. When the cooler surface is near the dew point of sulfuric acid, the acid condenses along with water of hydration. The result is a highly concentrated sulfuric acid condensate [12].

Sluder et al. studied the fundamentals of EGR cooler deposit formation by using surrogate tubes to represent the EGR cooler. They showed that the deposits initially contain a substantial fraction of HCs that are volatile at 350 °C and the fraction decreases over the time. This decrease is due to the fact that the deposit surface temperature reaches a temperature at which HC condensation is no longer occurring. They also investigated the effect of different biodiesel blends on surrogate tubes [13]. In another effort, they studied effects of gas flow rate, coolant temperature, and oxidation catalyst on cooler deposits [14].

In this study, the previous model for soot deposition in EGR cooler [15] is extended and coupled with the hydrocarbon condensation model. Experimental measurements are used for verification of the model. First, the extended soot deposition model is described and then hydrocarbon condensation model is discussed. The cooler efficiency, pressure drop, soot and hydrocarbon deposited mass are the parameters compared to the experimental data.

SOOT DEPOSITION: MODEL DESCRIPTION AND GOVERNING EQUATIONS

In this section the extended model for soot deposition prediction is described. To simplify the geometry and reduce the complexity of the fouling phenomenon, and to improve understanding of soot deposition, a simple concentric tube is used as the cooler with a constant wall temperature. Hot EGR gases flow through the inner pipe and the coolant circulates around it in the outer pipe to keep a constant wall temperature. The coolant temperature rise is negligible. This low rise in coolant temperature is due to large heat capacity of coolant compared to that of EGR flow. That is why wall temperature is assumed to be coolant temperature. The tubes are made of stainless steel. The soot deposition caused by thermophoresis phenomenon is taken into account the model. Thermophoresis is a phenomenon

that results in a net force that drives particles from a high temperature region to a lower one due to more vigorous collisions with gas molecules from the hotter region. This phenomenon will be discussed in detail later in this section. Soot properties, and other thermo-hydraulic conditions of real experiments are provided from the experimental data to the model. The schematic of the model is shown in Figure 1. The coolant side is not included in the figure. The tube length (L), diameter (D), inlet and mean temperature (T_{inlet} , T_m), and concentration of particles (C_{inlet} , C_m) are demonstrated.

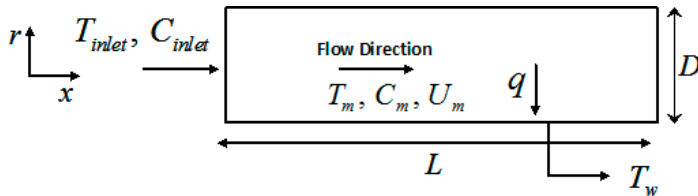


Fig 1 Schematic of the model

The mass conservation of particles and energy conservation equations of the flow inside the tube are simplified while the following assumptions are made:

- Coolant temperature is constant
- The particles do not interfere with the flow properties due to their low mass fraction within the bulk gas
- The radial variations of temperature and mean particle concentration are neglected compared to the axial changes
- Gas properties vary as a function of mean temperature
- Constant wall temperature equal to coolant temperature
- Soot properties do not vary with the temperature and layer thickness

The steady state equations are discussed in [2,16]; however, the current work being proposed also accounts for time varying parameters. After simplifying the energy equation in the aforementioned tube and using proper non-dimensional numbers in the equation, the following equation is obtained:

$$\frac{dT_m}{dx} = \frac{4Nu}{D Re Pr} (T_w - T_m) \quad (1)$$

Also, conservation of particles mass yields:

$$\frac{dC_m}{dx} = -\frac{4C_m}{DU_m} (V_t + V_d + V_{th}) \quad (2)$$

It is claimed that above equations are suitable for laminar and turbulent flow including entrance effect [2]. In the following sections, it will be described how to calculate thermophoretic velocity in the concentration equation and Nusselt number in energy conservation equation. Particle deposition is mainly because of

thermophoresis, diffusion, and turbulent impactions. V_d , V_t , V_{th} are Eddy diffusion, turbulent impaction, and thermophoresis velocities respectively. Particles with the size of $0.1 \mu m$ and less could be easily moved by the eddy motion toward the walls but larger particles (greater than $0.1 \mu m$) are under the effect of turbulent impaction and more than eddy diffusion [2]. Diffusion is important for transport of gaseous species, but not as important for particles in the range of EGR soot compared to thermophoresis effect. It was noticed that diffusion velocity is three to four orders of magnitude smaller than thermophoretic velocity and that is why it can be neglected in the model. For many heat exchangers operating in dusty flows, particles can be inertially deposited. This occurs when the particle is large enough that it cannot easily follow rapid changes in gas flow direction. However, small particles like diesel soot have very short relaxation times and thus follow the flow. So, turbulent impaction is not significant for small particles of EGR soot and it is not taken into account in the model [2]. So, thermophoretic velocity is the only velocity being considered in equation 2. Thermophoresis is the phenomenon that when a temperature gradient exists, particles move toward the cooler direction. Particles reaching the boundary layer are driven to the wall by thermophoresis. This force arises from the fact that hotter gas molecules have higher velocity. Thus, in a thermal gradient the gas on the hot side of the particle hits with higher force than the gas from the cooler side, and a net force is created toward the cooler region – i.e., wall [10]. The thermophoretic drift velocity of a small particle (in the range of nanometer or micrometer) is defined as:

$$V_{th} = -K_{th} \frac{V}{T} \vec{\nabla} T \quad (3)$$

$$K_{th} = \frac{2C_s C'}{(1 + 3C_m K_n)} \times \frac{k_g/k_p + C_t K_n}{1 + 2k_g/k_p + 2C_t K_n} \quad (4)$$

$$C' = 1 + K_n (A + B e^{-C/K_n})$$

where:

A, B, C, C_s, C_m, C_t : Thermophoretic constants which are 1.2, 0.41, 0.88, 1.14, 1.17, and 2.18 respectively [3].

An approximation for radial temperature gradient for thermophoretic velocity is needed. The approximated gradient is defined as [2]:

$$\vec{\nabla} T = \frac{T_m - T_w}{\delta} \quad (5)$$

where δ is the boundary layer thickness. This thickness in our model is calculated based on the fluid mechanics

formulation of the viscous sub-layer thickness in a turbulent boundary layer [17].

$$\delta = \frac{5\nu}{u^*} \quad (6)$$

$$u^* = \sqrt{\frac{\tau}{\rho}} \quad (7)$$

$$\tau = \frac{1}{8} f \rho U_m^2 \quad (8)$$

Darcy friction factor is defined as [18]

$$f = (0.79 \ln \text{Re} - 1.64)^{-2} \quad (9)$$

$$3000 < \text{Re} < 5 \times 10^6$$

It is noted that there is always a constant mass flow rate at the inlet of the tube at a constant temperature. Also, no pulsation has been considered in the flow. It implies that the interface temperature can never exceed the mean temperature in the model and thermophoretic velocity can never be zero or a negative number. Thermophoretic velocity approaches to a significantly small number after a long exposure time in the model but it never reaches to zero numerically.

To calculate Nusselt number, it should be found out if the flow is fully developed or developing. Thermal entrance length can be calculated as [19]:

$$\left(\frac{x_{\text{thermal}}}{D}\right)_{\text{entry}} = 0.623 \text{Re}^{0.25} \text{Pr} \quad (10)$$

which is quite small compared to the tube length in our model (3%). So, the fully developed Nusselt number can be employed in the model as below [19]:

$$\text{Nu} = 0.021 \text{Re}^{0.8} \text{Pr}^{1/3} \quad (11)$$

Where the Reynolds number in tube is defined as

$$\text{Re} = \frac{U_m D}{\nu} \quad (12)$$

Also, pressure drop across the cooler is given by:

$$\Delta P = \frac{1}{2} \frac{f \rho L U_m^2}{D} \quad (13)$$

It should be noted that the effectiveness of the cooler is defined as [20]:

$$\varepsilon = \frac{T_{\text{inlet}} - T_{\text{outlet}}}{T_{\text{inlet}} - T_{\text{coolant}}} \quad (14)$$

HYDROCARBON CONDENSATION: MODEL DESCRIPTION AND GOVERNING EQUATIONS

Diesel exhaust contains a wide range of hydrocarbon and hydrocarbon-derived species. These include unburned and partially burned fuel and lube oil. Some of these compounds can condense on cooler surfaces. Condensation occurs when the surface of the cooler is below the dew point for the partial pressure of the compound. Thus, heavier species and higher concentration species will condense most.

In a free stream of a gas at (P,T) containing some different species and flowing over a surface (below the dew point of the species), a condensate film forms on the surface as shown in Fig 2.

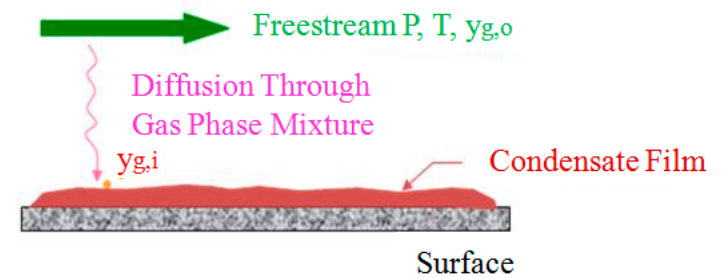


Fig 2 Condensation film forms on a surface

The phenomenon of interface mass transfer can be seen from the point of kinetic theory as a difference between two quantities: a rate of arrival of molecules from the vapor phase to the interface and a rate of departure of molecules from the liquid surface towards the vapor phase. When condensation occurs, the arrival rate is larger than departure rate. During evaporation, the departure rate is larger than arrival rate. It is obvious that during equilibrium the two rates are the same [21]. In case of condensation, mass condensation flux from the gas stream to the surface is defined by [21]:

$$j_{g,i} = K_g \rho \ln \left(\frac{1 - y_{g,i}}{1 - y_{g,o}} \right) \quad (15)$$

Where K_g is a mass transfer coefficient defined by analogy between heat and mass transfer as: