# CFD STUDY OF THE FOULING LAYER EVOLUTION DUE TO SOOT DEPOSITION AND HYDROCARBON CONDENSATION INSIDE AN EXHAUST GAS RECIRCULATION COOLER

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## ABSTRACT

The fouling deposits that appear in the gas-side of the exhaust gas recirculation (EGR) coolers are commonly made up of soot particles and hydrocarbons condensate. The buildup of this less thermally conductive material causes the degradation of the performance of the cooler, even clogging the tubes after only few hours of work.

The present study examines the hydrocarbon condensation coupled with particle matter deposition on the heat exchanger surfaces of a test probe using computational fluid dynamics simulations. The proposed methodology considers the physicalchemical characteristics of hydrocarbon species and takes into account the deposition and removal mechanisms to compute the fouling accumulation and the condensate flux that appear on the upper surface of the deposit.

The fouling process has been simulated during five hours taking into account the hydrocarbon species dodecane  $(C_{12}H_{26})$ , pentadecane  $(C_{15}H_{32})$ , hexadecane  $(C_{16}H_{34})$  and eicosane  $(C_{20}H_{42})$ . The growth of the fouling deposit has been computed and the areas where hydrocarbon condensation takes places have been detected. The evolution of the condensation process has been monitored and the total amount of hydrocarbon has been estimated. Results show that, as fouling layer grows, hydrocarbon condensation is reduced due to the increase of the temperature of the deposit. For the selected boundary conditions, dodecane condensation does not take place at any moment of the test, while C15, C16 and C20 condenses mainly in the area located at the end of the test section, where the temperature of the deposit is lower. Eicosane has produced the highest amount of condensate and, at second hour of test, 68.7% of the area of the probe is exposed to eicosane condensation.

#### **INTRODUCTION**

In the automotive industry, the strict emissions regulation that have been implemented worldwide since the last decades, have extended the use of the exhaust gas recirculation (EGR) system to reduce the NOx emissions [1]. To minimize the NOx formation, the EGR system reduces the combustion temperature diminishing the amount of oxygen and its concentration in the combustion chamber, replacing a portion of the fresh air.

The new homologation test procedures require the reduction of the pollutant emissions in all areas of the engine map, demanding the use of the EGR system throughout the evaluation process. High EGR rates correspond to an increase of both the soluble organic fraction (SOF) and the concentration of soot particles in the exhaust gas [2, 3], leading to the creation of fouling deposits that may clog some tubes, making unusable some ducts of the heat exchanger [4].

On the heat exchanger walls of the EGR cooler —the compact heat exchanger in charge of reducing the temperature of the recirculated exhaust gas— fouling layer appears. These fouling deposits cause the cooler performance degradation inducing the increase of charge temperature and emissions. Moreover, fouling phenomenon increases the pressure drop along the heat exchanger that adversely affects the control of the EGR rate and results in decreased fuel efficiency due to increased pumping work [5].

The EGR cooler deposits are a combination of a solid fraction (elementary carbon and metallic ash) and SOF (condensed hydrocarbons) [6]. This fouling layer is caused by the deposition of particulate matter (PM) from the accumulation mode (mainly in the range from 0.1  $\mu$ m to 0.3  $\mu$ m) and the hydrocarbon (HC) condensation from the nucleation mode [7], as Figure 1 illustrates. Volatile mass is transferred to diesel exhaust particles by adsorption and condensation [8] and, together with the carbonaceous soot, form a wet soot deposit with a complex structure [6].



Fig. 1. Scheme of the deposition of aggregates and hydrocarbon condensation.

The study of deposit formation due to particulate matter accumulation and hydrocarbon condensation has been addressed in numerical and experimental studies [9-13]. The interaction between the different deposition and removal particle mechanisms and the influence of the engine parameters, such as the fuel type or the EGR ratio, have been examined in order to have a better understanding of this phenomenon.

With the aim of contributing to the study of the fouling formation in EGR systems, the main objective of this study is to recreate the hydrocarbon condensation process that occurs on the fouling deposit. Using computational fluid dynamics (CFD) software, the fouling layer evolution due to particulate matter deposition and hydrocarbon condensation has been simulated following the methodology developed by Paz et al. [14]. Four different hydrocarbon species in the range  $C_{12}$ - $C_{20}$  have been selected and the fouling process has been simulated inside a test probe during five hours. The changes in the fouling layer thickness and deposit temperature have been monitored during the test and the evolution of the condensate flux has been analyzed in a local manner in the entire area of the test section.

## METHODOLOGY

HC CONDENSATION MODEL

The hydrocarbon and hydrocarbon-derived species that are part of the exhaust gas flow can condense on the heat exchanger surfaces when the surface of the cooler is below the dew point of the compound at the local partial pressure. When condensation takes place, the phenomenon of interface mass transfer involves the molecules of the vapor phase that form droplets that become part of the fouling layer. The mass condensation flux from the exhaust gas stream to the deposit surface is function of the species mole fraction in the main flow and that of at the interface and it is defined by [5]:

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

where  $y_{g,i}$  is the mole fraction of the HC species in the gas-liquid interface,  $y_{g,o}$  is the mole fraction of the HC species in the exhaust gas stream,  $\rho_g$  represents the gas density and  $K_g$  is the mass transfer coefficient defined by analogy between heat and mass transfer as [13]:

$$K_g = \left(\frac{h_g}{\rho_g C_{p,g}}\right) \left(\frac{Pr}{Sc}\right)^{2/3} \tag{2}$$

where Pr represent the Prandtl number, Sc is the Schmidt number,  $C_{p,g}$  is the heat capacity of the gas,  $\rho_g$  is the gas density and  $h_g$  is the heat transfer coefficient which is related to the Nusselt number. Thus, the mass condensation flux can be rewritten as:

$$j_{g,i} = Nu \left(\frac{Pr}{Sc}\right)^{2/3} \frac{\alpha_g}{D} \rho_g \ln\left(\frac{1 - y_{g,i}}{1 - y_{g,o}}\right)$$
(3)

For each hydrocarbon specie, the mole fraction is calculated as the ratio of the partial pressure at the surface to the total pressure of the mean flow:

$$y_{g,i} = \frac{P_{g,i}}{P_{total}} \tag{4}$$

Partial pressure is computed utilizing the Antoine coefficients of the species as:

$$\log_{10} P_{g,i} = A - \frac{B}{T_{interface} + C}$$
(5)

where pressure is expressed in mmHg and temperature is expressed in °C.

#### NUMERICAL IMPLEMENTATION

As various authors have shown [15, 16], the particulate matter fouling deposits depends on two simultaneous phenomena: deposition and removal. Accordingly, in this study the calculation of the fouling layer evolution has been computed taking into account the deposition of the aggregates and the erosion of the particles. The fouling thickness evolution has been calculated following the expression:

$$\Delta x_f = \left(\frac{S_d(u_{di} + u_{th})C_b}{\rho_f} - \frac{\tau_w x_f}{\xi}\right) \Delta t \tag{6}$$

On the one side,  $S_d$  represents the particle sticking probability,  $u_{di}$  is the deposition velocity due to diffusion and inertial impaction,  $u_{th}$  is the deposition velocity due thermophoretic force,  $C_b$  represents the particle concentration and  $\rho_f$  is the fouling deposit density. On the other side, the removal process is computed taking into account the shear stress over the fouling layer ( $\tau_w$ ), the local thickness of the deposit ( $x_f$ ) and the bond-strength factor of the deposit ( $\xi$ ). The validity of the results achieved with this expression has been verified in earlier studies with heat exchangers exposed to particulate matter [17–19].

In order to compute the effect of the hydrocarbon condensation during the fouling process inside a compact heat exchanger, the equations presented in the previous section (equations 1-5) have been implemented and coupled with the particulate matter fouling model. As the schematic of the Figure 2 shows, the condensate mass will be added to the fouling layer, generating a deposit formed by the aggregates and the condensed hydrocarbon.



Fig. 2. Scheme of the fouling model.

Both the particulate fouling model and the hydrocarbon condensation model have been implemented in the CFD software ANSYS Fluent in order to reproduce the fouling layer evolution. Using a calculation methodology developed by Paz et al. [14], the growth of the fouling layer is recreated through the movement of the fouling-fluid interface, as Figure 3 shows. At each time-step of the calculation, the simulation of the fluid flow provides the fluid information and it serves as the basis of the calculation of the thickness of the fouling layer. The dynamic mesh model assumes the control of the displacement of the nodes of the mesh and updates their position reproducing the deposit evolution locally.



Fig. 3. Schematic of the mesh update

#### COMPUTATIONAL METHODOLOGY VALIDATION

The hydrocarbon condensation model and its computational implementation have been validated with the data of Warey et al. [11] and Abarham et al. [20].

The mass condensation fluxes of the alkanes dodecane  $(C_{12}H_{26})$ , hexadecane  $(C_{16}H_{34})$  and eicosane  $(C_{20}H_{42})$  have been measured under different coolant temperatures. The CFD boundary conditions are equivalent to those of the original paper and, as Figure 4 shows, the results achieved are similar.



from CFD simulations and from Warey et al. [11].

In the same way, the total mass of condensate has been computed, as Figure 5 shows, and the model results are quite close to those reported by Abarham et al. [20].



Abarham et al. — CFD □ Fig. 5. Hydrocarbon condensed mass from CFD simulations and from Abarham et al.[20].

## GEOMETRY AND MESH

The test probe selected in this study is made up of two ribbed plates symmetrically staggered, as Figure 6(a) shows. The ribs of this device have been designed to study the fouling phenomenon under a non-uniform flow pattern [14, 21].

The ribbed plates, the side walls of the heat exchanger and the flanges of the device are made of aluminum. The fouling layer is located on the gas side, above the heat transfer surface of the ribbed plates, as Figure 6(b) shows.

The mesh has been created using the ANSYS Meshing preprocessing module. As shown in Figure 6(c), the grid of the surfaces is made up of triangles of 0.5mm. To solve the viscous region with precision, the near wall region has been meshed with a layer of 10 linear-growth prismatic cells and the core volume has been filled with tetrahedral elements. The total 3D cell number of the full assembly is approximately  $7 \times 10^6$  cells.



Fig. 6. (a) Exploded view of the heat exchanger, (b) detailed image of the fouling layer domain and (c) detailed image of the cells of the mesh of the heat exchanger surface.

## **BOUNDARY CONDITIONS**

In this work the hydrocarbon species have been selected in accordance with the measurements of Sluder et al. [22] and Liang et al. [23], which determine that the major alkanes species in diesel fuel are in the range  $C_{11}$ - $C_{23}$ . Dodecane ( $C_{12}H_{26}$ ), pentadecane ( $C_{15}H_{32}$ ), hexadecane ( $C_{16}H_{34}$ ) and eicosane



Fig. 7. Deposit profiles and fouling thickness at different moments of the test.

 $(C_{20}H_{42})$  have been selected. In order to evaluate the condensation process under a very high concentration of hydrocarbon (1030-1100 ppmC), the value of the input flow for each specie has been set in 100  $\mu$ L/min, as Table 1 presents.

On the one hand, the exhaust gas flow rate has been fixed in 115 L/min (8.87 kg/h) and the gas temperature has been set at 200°C. On the other hand, to promote the HC condensation, the temperature of the walls in contact with coolant has been established at  $30^{\circ}$ C.

The aggregates have been identified as spherical particles with diameter in the range from 15 to 637 nm. The particle number distribution presents a lognormal form with a mean diameter of 91.9nm and the total number concentration is around  $2.01 \times 10^{-6}$  part/cm<sup>3</sup>.

It has been considered that the deposit has homogeneous properties. Due to the soot deposit shows a complex structure with high porosity, the thermal conductivity and the density of the fouling layer have been selected following the results reported by previous experimental studies. Thus, the thermal conductivity has been fixed at 0.041 W/mK [24] and fouling layer density has been fixed in 50 kg/m<sup>3</sup> [25].

Although previous studies show that ageing effects can have a substantial influence on the fouling deposit evolution [26], in this study it has been considered that the deposit is not subject to ageing and, thus the changes over time in deposit properties have not been considered.

Table 1. HC species included in the model.

Molecular formula	Name	Injection flow [µL/min]	Injection flow [mol/s]	Boiling point at 1atm pressure [°C]
$C_{12}H_{26}$	Dodecane	100	7.33×10 <sup>-6</sup>	216
$C_{15}H_{32}$	Pentadecane	100	6.03×10 <sup>-6</sup>	270
$C_{16}H_{34}$	Hexadecane	100	5.69×10-6	287
$C_{20}H_{42}$	Eicosane	100	4.65×10-6	343

#### **RESULTS AND DISCUSSION**

For the selected boundary conditions, the fouling process has been simulated separately for each HC specie during five hours.

In all of the cases studied, the evolution of the fouling thickness, temperature of the surface of the deposit, the regions where condensation occurs and the cumulative amount of condensate have been monitored during the test and subsequently analyzed.

For the sake of clarity, the results of the side walls of the heat exchanger have been omitted and the model results of the ribbed plates have been presented below.



Fig. 8. Temperature of the upper surface of the deposit.

In order to examine the fouling layer formation and evolution along the test probe, the Figure 7 illustrates the fouling layer growth caused by the particulate matter accumulation during the five hours of the test. The graphs show that the fouling thickness



Fig. 9. Species dew temperature and surface temperature at different moments of the test.



Fig. 10. Areas where condensation occurs at each hour of the test.

of the deposit at the end of the test is slightly higher in the inlet region of the probe and it becomes thinner as it moves in X position. The strong thermal gradient that appears in the inlet region causes that particulate matter deposition due to thermophoresis mechanism to have a greater emphasis in this region.

In addition, it has been detected that, on the windward side of the ribs, the deposit shows local minimum due to the greater effect of the erosion and the low particle sticking probability in these areas. For this reason, the balance between the deposition and removal mechanisms causes that the deposit evolution on the windward side of the ribs to reach a stable value after three hours of test. On the contrary, the highest fouling thickness is located in the regions between ribs, where deposition occurs and removal mechanisms are unable to detach the particles of the deposit. In these areas deposition prevails over the removal mechanisms and the fouling layer grows throughout the test.

In order to compute the regions where HC condensation appears, the temperature of the upper surface of the deposit has been monitored, as shown in Figure 8. The growth of the fouling layer —which acts as an isolator— increases the temperature of the surface exposed to the gas flow. At the beginning of the test, due to the lack of deposit, the wall temperature is similar to the coolant temperature  $(30^{\circ}C)$  but, as test progresses and the fouling deposit grows, the surface temperature increases, reaching peaks at 150°C after 5 hours. The increase of the surface temperature is directly proportional to the fouling layer growth: the inlet region —where the fouling thickness is higher— shows the sharpest increase, especially the areas between ribs where the deposit is thicker. At the end of the test, the temperature of almost the entire surface of the plate is above 90°C.

As Figure 9 shows, the dew temperature of eicosane  $(96.5^{\circ}C)$  is high enough to ensure condensation throughout the test in the outlet region, which is in line with the study of Warey et al. [11] that indicates that heavier hydrocarbons are more likely to condense at the deposit temperatures typically encountered in EGR coolers (30-90°C). At the end of the analysis, the surface

temperature in the inlet region exceeds the dew point and condensation only occurs in the outlet region of the plate.

On the other hand, the dew point of dodecane is below the surface temperature during the entire test, thus, no condensation of dodecane has been detected. This shows that, to this hydrocarbon concentration, the condensation of dodecane does not take place under this boundary conditions at any instant of the test. In this manner, this HC specie does not contribute to the growth of the fouling layer. This has to be taken into account when assessing the design of the EGR cooler in the knowledge that, when it is exposed to dodecane under low coolant temperatures, no condensation occurs.

The evolution of the condensation process of each specie has been summarized in the Figure 10, which illustrates the areas where condensation takes place at each hour of the test. For the given hydrocarbon species, the area exposed to condensate is correlated to the species boiling point. The condensation of eicosane —the heaviest hydrocarbon specie— is more persistent and the region affected by eicosane condensation is more relevant during the entire test. At the second hour of the simulation the eicosane condensation occurs in 68.7% of the area of the plate and, at the fifth hour, 31.5% of the analyzed area still shows hydrocarbon condensation, as Figure 11 illustrates.

Since pentadecane and hexadecane have a close dew point, the behavior of these two species is similar and, in both cases, after the first hour of the test the area where condensation occurs is abruptly reduced and, at the second hour of the test, only the 12.6% and 23.3% of the area of the probe shows hydrocarbon condensation of pentadecane and hexadecane respectively.



Fig. 11. Percentage of area where condensation occurs.

Considering the deposit temperature and the molar fraction of the hydrocarbon species, the condensate flow has been computed. As Figure 12 shows, at the first hour of the test, the higher eicosane condensate mass flow is on the windward side of the ribs located in the outlet region of the plate and it is around  $2.5 \times 10^{-7}$  kg/s. To a lesser extent, the condensate mass flow of eicosane is also noticeable on the leeward side of the ribs and in the area between ribs, especially in the outlet region. Due to the increase of the deposit temperature, the hydrocarbon condensation is reduced, as Sluder et al. [22] have reported, and by the end of the test, the mass flow of eicosane condensate is reduced to a small zones located near the outlet of the test section and it value is reduced to  $6.0 \times 10^{-8}$  kg/s. In the same way, the condensate mass flow of pentadecane and hexadecane is most marked in the outlet area and its value is gradually reduced as test progresses. It should be noted that from the third hour of test



Fig. 12. Condensate flow at different moments of the test.



Fig. 13. Percentage of fouling thickness caused by eicosane condensate at different moments of the test.

the condensate flows of pentadecane and hexadecane drop to zero.

Neglecting the effects of hydrocarbon in the exhaust flow, such as the agglomeration of the particulate matter and the formation of bigger aggregates, the total contribution of hydrocarbon condensate to the deposit growth has been evaluated. As Figure 13 shows, the percentage of fouling layer thickness caused by eicosane condensate has been quantified and it has been detected that the most of hydrocarbon condensate is formed during the first hour of the test, during the earlier stages of the deposit formation. Moreover, it has been detected that the evolution of the percentage of fouling thickness caused by eicosane remains largely unchanged after the first three hours of the test.

Analyzing the percentage of fouling thickness caused by hydrocarbon condensate for the four species (Figure 14), it has been noted that, in accordance with a previous studies [5, 22], in comparison with the fouling thickness caused by the deposition of aggregates, the percentage of fouling thickness caused by hydrocarbons condensate is low. Moving forward along the plate, the percentage of condensate is increased and eicosane shows a more marked effect. The amount of condensate produced by the heaviest hydrocarbon is significantly higher and, thus, the percentage of the fouling layer thickness produced by eicosane is higher than the percentage caused by the condensation of pentadecane and hexadecane, particularly in the outlet region of the plate.



Fig. 14. Percentage of fouling thickness caused by hydrocarbon condensate at the end of the test.

The Figure 15 shows that, from inlet region to outlet region, the percentage of the fouling layer thickness caused by eicosane grows from 0.15% to 1.53% while that caused by pentadecane grows from 0.02% to 0.22%. The highest percentage of fouling layer thickness produced by condensate is located in the windward side of the ribs located in the outlet region of the plate —point G— where the fouling thickness is the lowest. This

effect is in line with Teng and Barnad [6] results that indicate that the deposit becomes "wet" near the outlet of the EGR cooler.



Fig. 15. Percentage of fouling thickness caused by hydrocarbon condensate on different points of the plate at the end of the test.

#### CONCLUSIONS

In this study, a hydrocarbon condensation model has been implemented in CFD software and, using a previous developed methodology, numerical simulations have been conducted in order to examine the hydrocarbon condensation inside a test probe. The evolution of the fouling layer has been computed and the condensation of dodecane ( $C_{12}H_{26}$ ), pentadecane ( $C_{15}H_{32}$ ), hexadecane ( $C_{16}H_{34}$ ) and eicosane ( $C_{20}H_{42}$ ) have been simulated during five hours.

CFD results show that species condensation is strongly influenced by the temperature of the upper surface of the fouling deposit and it has been noted that, as test progresses and the fouling layer grows, the temperature of the surface increases, reducing the species condensation.

For the selected boundary conditions, during the entire test, condensation of dodecane has not been detected in any area of the probe.

Condensation of pentadecane and hexadecane shows a similar behavior and the condensation of these two species is persistent during the first hours of the test, especially in the outlet region of the probe. At the second hour of the test, only 12.6% and 23.3% of the area of the probe shows hydrocarbon condensation of pentadecane and hexadecane respectively and, beyond three hours, the condensate flow of these two species is abruptly reduced.

The condensation of eicosane —the heaviest hydrocarbon specie— has been registered during the entire test. At the fifth hour, 31.5% of the analyzed area exhibits hydrocarbon condensation and the percentage of fouling thickness caused by condensate is as high as 1.5% in the areas more prone to condensation.

The achieved results illustrate the formation of fouling deposits considering a high concentration of hydrocarbon, however, further research is needed in order to study the condensation process under different species concentrations and various coolant and gas temperatures.

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## NOMENCLATURE

- $C_b$  Particle concentration, kg m<sup>-3</sup>
- $C_p$  Heat capacity, J kg<sup>-1</sup> K<sup>-1</sup>
- $\vec{D}$  Tube diameter, m
- *h* Heat transfer coefficient, W  $m^{-2} K^{-1}$
- *j* Mass condensation flux, kg m<sup>-2</sup> s<sup>-1</sup>
- *K* Mass transfer coefficient, m s<sup>-1</sup>
- *Nu* Nusselt number
- Pr Prandtl number
- Sc Schmidt number
- *S<sub>d</sub>* Particle sticking probability
- *T* Temperature, K
- $u_{di}$  Deposition velocity due to diffusion and inertial impaction, m s<sup>-1</sup>
- $u_{th}$  Deposition velocity due to thermophoresis, m s<sup>-1</sup>
- *x* Local thickness of fouling deposit, m
- y Species mole fraction
- $\alpha$  Thermal diffusivity, m<sup>2</sup> s<sup>-1</sup>
- $\rho$  Density, kg m<sup>-3</sup>
- $\tau_w$  Wall shear stress, Pa
- $\xi$  Strength bond factor of the deposit, kg m<sup>-1</sup> s<sup>-1</sup>

## Subscript

- f Fouling
- g Gas
- *i* Interface
- *o* Bulk flow

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