DEVELOPMENT OF A CFD MODEL FOR PREDICTING FOULING PROCESS USING DYNAMIC MESH MODEL

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ABSTRACT

This paper presents a comprehensive computational model capable of simulating fouling layer thickness evolution using dynamic mesh methodology with the purpose of helping in the knowledge of formation and evolution of fouling deposits. The main objective of this study is to develop a new computational methodology that can reproduce the deposit generation during fouling process with an innovated work method. Dynamic Mesh model, from Ansys Fluent software, and external routines have been used to implement this advanced numerical model which improves computational capabilities in relation to others techniques.

Dynamic mesh model allows one to move the boundaries of a region relative to other boundaries of the zone. The displacement of the nodes of the mesh is the mechanism that use this model to adjust the geometry accordingly with the fouling layer evolution. During the simulation process, the geometry under investigation is modified to reproduce the emergence and gradual change of fouling layer. Different rules of deposition and removal of the fouling process can be implemented in the proposed algorithm. The direct interaction between fouling expressions and governing equations of the main flow is used to predict deposits formation and growth. This is about a versatile tool capable of recreating multiple fouling conditions and reproducing fouling processes from diverse physical natures.

In this paper, numerical simulations of soot fouling layer formation have been presented. Deposit development has been calculated inside different heat exchanger technologies used in exhaust gas recirculation (EGR) systems to analyse fouling process and to verify the advantages of this new computational strategy.

INTRODUCTION

Nowadays, fouling is involved in numerous industrial processes and it can occur on any fluid-solid surface producing adverse effects, such as heat transfer reduction or the increase in pressure drop across the apparatus (Awad, 2011). In the automotive industry, coolers of the exhaust gas recirculation system are used on engines to reduce the NOx emissions through the reduction of the intake temperature. The build-up of deposits inside these devices causes significant degradation in heat transfer performance, often on the order of 20-30% (Hoard, et.al, 2008). The requirements imposed on exhaust systems have rapidly increased in recent years and current regulations require the greatest emission reduction of any previous stage. The Real Driving Emissions (RDE) legislation and the World-harmonised Light-duty Vehicles Test Procedure (WLTP) require good performance and continued development of EGR technology (Sellers et.al, 2014) avoiding breakdowns caused by fouling deposits.

In exhaust gas systems, studies about fouling effects have been normally focused on experimental data, examining the formation and evolution of the fouling layer through in-situ measurements, similar to the researches carried out by Abd-Elhady et al. (2011), Sluder et al. (2013), Han et al. (2015) and Salvi et al. (2016). Recently, several numerical studies have appeared with the aim of clarifying the mechanism that causes the fouling layer growth and evolution. Abarham et al. (2009) have developed a one-dimensional model to simulate particle soot and hydrocarbon condensation inside an EGR cooler obtaining results about deposited soot mass, condensed hydrocarbon mass and pressure drops across the cooler with a reasonably good agreement with the experimental results. In the same way, Mehravaran et al. (2011) have studied fouling layer build-up and they have suggested a simple one-dimensional model to predict the deposition velocity and soot layer thickness inside EGR devices.

In recent years, Computational Fluid Dynamics (CFD) has played an important role in fouling researches. CFD, which uses numerical analysis to solve and analyse fluid flows, is used to carry out simulations of exhaust gas flow inside exhaust gas recirculation coolers. Making an example of this, Nagendra et al. (2011), making use of CFD tools, have presented in their study simulations of soot particles deposition in wavy-fin EGR coolers achieving results with various Reynolds numbers and wall temperature gradients. In like manner, Stauch et al. (2011) or Zhang et al. (2008) have carried out CFD simulations with the goal of evaluating the particle deposition rates and fouling layer growth inside EGR coolers and industrial ducts. To incorporate the fouling effect, most of this studies employ a virtual deposited mass that changes the properties of a constant thickness-wall and, thus, the reduction of the cross sectional area and the change in flow pattern cannot been modelled. The fact that they do not include local effects complicates the calculation of the deposit evolution and, thus, their applicability is limited to simple geometries where those parameters can be defined.

In a previous work, Paz et al. (2013) have developed a CFD fouling model capable of simulating the fouling deposits growth and progression keeping in mind local effects and the structural changes of the fouling layer. In the manner of other applications, like the one carried out by Brahim et al. (2003), the computational effort and cost in terms of CPU time and memory of the 3D simulations carried out with these models is very high and, in most of cases, they only can be used in two-dimensional simulations.

Taking as a starting point the previous studies, and with the aim of contributing to the study of fouling process inside heat exchanger devices, the main objective of this research is to develop a calculation strategy to simulate the fouling process using Dynamic Mesh model from Ansys Fluent. The external algorithm will be programmed in *C* and it will be coupled to the computational fluid dynamics software package Ansys Fluent via the user-defined functions feature. Using the Dynamic Mesh model, it is expected that this tool will reproduce the fouling layer evolution recreating the movement of the fouling-fluid interface caused by particle deposition and having in mind the local scale effects involved in the fouling process like the presence of entrance effects, thermal gradient variations along the device and strong cross-section changes inside the heat exchanger. Moreover, this model will help in the analysis of the adverse effects resulting from fouling build-up, like the increase in pressure drop, the heat transfer reduction or the diminution in the cross sectional area inside the heat transfer devices of the EGR technology and inside the heat exchanger equipment of other industrial applications.

FOULING MODEL

Several authors, such as Epstein et al. (1988), Freeman et al. (1990), Kern et al. (1959) or Konak et al. (1974), have affirmed that the net growth of the fouling deposit depends on two opposing simultaneous processes: deposition and removal. They have proposed that the growth of the deposit is the net value of a deposition flux to the heat transfer surface and a removal flux from the heat transfer surface:

$$\frac{dm}{dt} = \dot{m}_d - \dot{m}_r \qquad (1)$$

These authors have explained that fouling deposit growth follows an asymptotic profile with a constant deposition rate, $\dot{m}_d$, and an increasing removal rate, $\dot{m}_r$, which is assumed to be directly proportional to the mass of the fouling deposit per unit area and wall shear stress.

Taking as reference these earlier studies and the previous CFD fouling strategy developed by us (Paz et.al, 2013), the presented model is in accordance with deposition-removal-type models. Different equations can be chosen to model the deposition and removal mechanisms that lead to deposit accumulation. The versatility of this computational model allows one to implement different mechanisms to reproduce the beginning and the evolution of the fouling process and, depending on the studied system, the expressions for the deposition and removal velocities must be selected and thoroughly adjusted.

In order to show the performance of this tool recreating the deposits formation inside a heat exchanger similar to the one used in the EGR technology, the equations have been taken from a previous study (Paz et.al, 2013). These expressions will be responsible for the estimation of the fouling layer thickness. The results obtained with these equations have been validated in earlier studies with heat exchangers exposed to fouling (Paz et.al, 2010, 2013, 2013-B). This research shows that the predicted results have been compared with the performance of real heat exchangers and they are in a good agreement with the experimental data. In this study these expressions will be used to exemplify the prediction of the fouling deposit evolution and they will still be good to show the performance of this proposed calculation strategy.

To show the operation mode of this simulation tool, the value of the fouling thickness evolution, which is required to adjust the local thickness of the fouling layer, will be obtained from the following expression:

$$\Delta x_f = \left(\frac{S_d(u_{di} + u_{th})C_b}{\rho_f} - \frac{\tau_w\, x_f}{\xi}\right)\Delta t \qquad (2)$$

where S_d represent the particle sticking probability, u_{di} is the deposition velocity, u_{th} is the thermophoretic velocity and C_b and ρ_f represent the particle concentration and the fouling layer density respectively. Moreover τ_w, x_f and ξ refer to the wall shear stress, the fouling layer thickness and the strength bond factor of the deposit.

NUMERICAL IMPLEMENTATION

The calculation strategy developed in this study has been implemented and coupling with the CFD software ANSYS Fluent. Dynamic Mesh model from this software package has been used to configure the motion of the fouling-fluid interface according to the fouling layer growth. The Dynamic Mesh Model has been used in previous studies where moving walls were needed and the validity of this tool has been verified in different industrial applications (Khayrullina et.al, 2015).

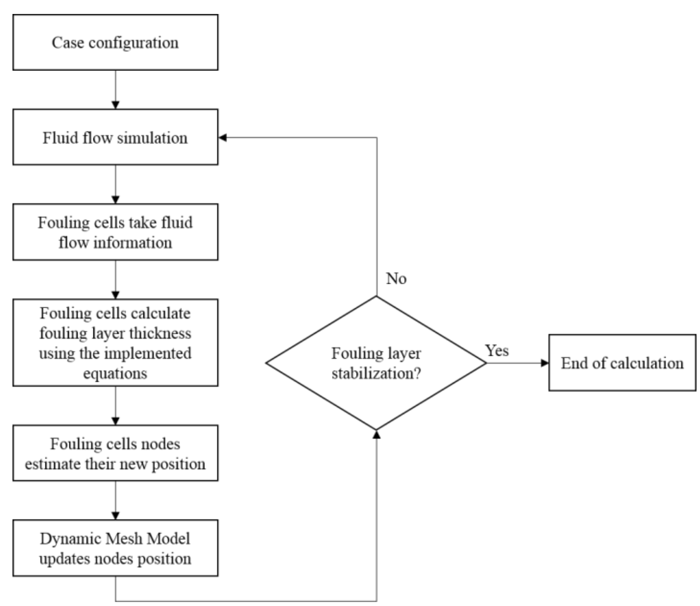

Figure 1: Schematic of the methodology of fouling layer movement

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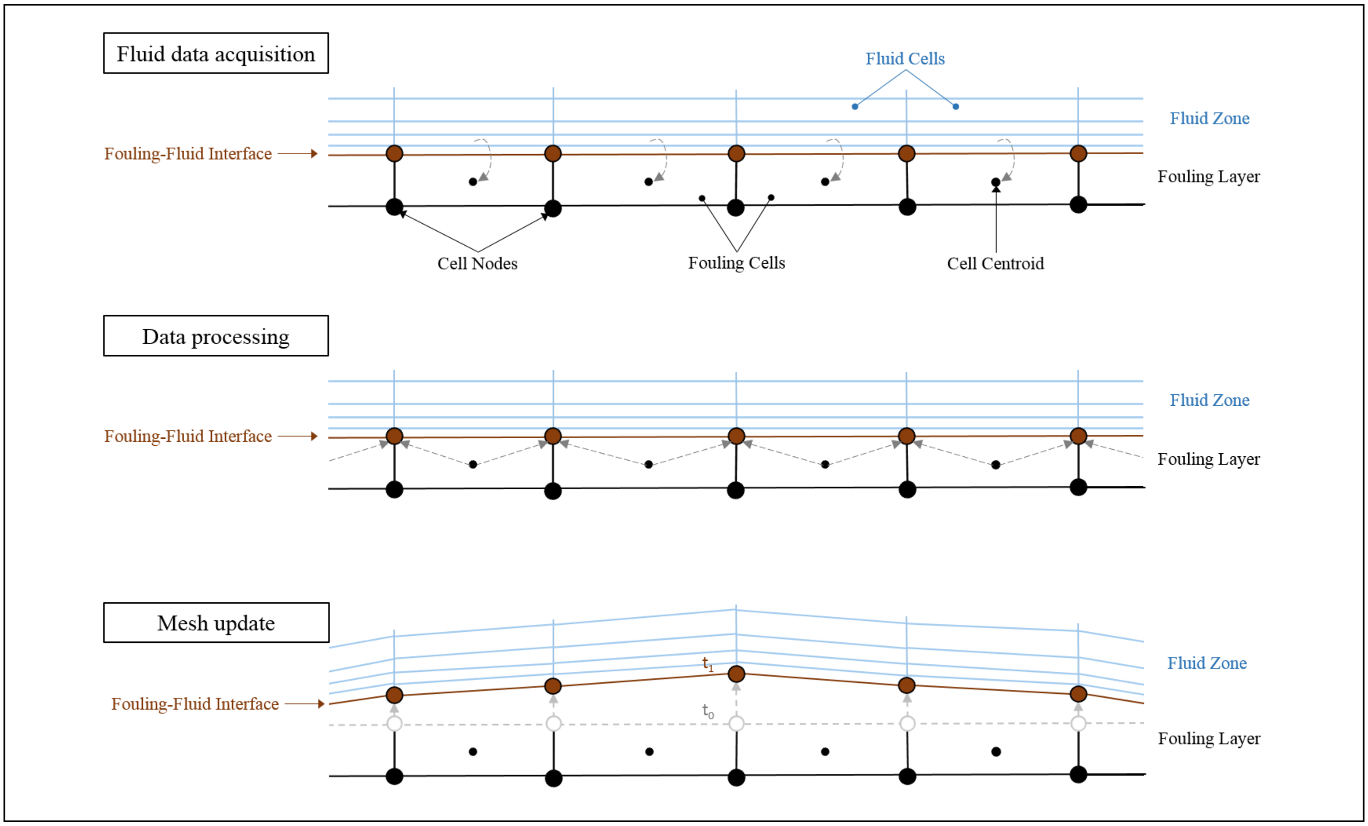

Figure 2: Schematic of data processing and mesh update

The Dynamic Mesh model allows one to move the boundaries of the cell zone relative to the other boundaries of the zone. This tool permits one to model flows where the shape of the domain is changing with time due to the motion on the domain boundaries (Ansys Inc., 2016). The movement of the mesh is carried out by the displacement of the nodes of the mesh to their new position. The cells of the mesh are deformed in order to adapt to the new mesh geometry and some re-meshing processes can take place to improve the mesh quality. The position of the boundaries of the cell zone and the volume mesh are updated by the CFD software at each time step of the simulation based on the solution at the current time. After that, a new time step is calculated and the process goes on.

Using external routines, the transient calculation and evolution of the fouling layer growth are carried out following a clearly defined methodology, which is repeated every time step of the simulation. Figure 1 shows the methodology of calculation of the fouling layer evolution which is made up of five steps: the gas flow simulation, sending information from fluid domain to the fouling cells, the calculation of the fouling layer thickness, the estimation of the new position of the nodes of the mesh and the update of the mesh. This process is repeated at every time step of the calculation until the stabilization of the fouling layer is achieved and, at that moment, the simulation is declared finished.

First of all, it is necessary to accomplish the gas-flow calculation in order to estimate the fluid properties. Ansys Fluent software provides comprehensive modelling capabilities to solve the fluid flow problem where the turbulent model and the boundary conditions must be selected to reproduce the flow. The fluid flow simulation provides the fluid domain solution at each time step and it serves as the basis of the calculation of the evolution of the fouling layer. Pressure, velocity and temperature fields are used to provide fluid information to the external routine and they are the starting point of the local fouling layer thickness estimation.

Once the fluid flow problem is solved, the external routine acts and the fouling growth prediction is carried out, as the schematic of Figure 2 shows. In order to compute the displacement of the mesh, the cell centroids of the cells of the fouling layer take charge of the calculation of the fouling layer growth. To that end, the cell centroids of the cells of the fouling layer receive the fluid flow information required for the calculation of the fouling layer evolution. This part of the cell is responsible for managing the information and computing the fouling thickness results.

After fluid data acquisition, each cell of the fouling layer calculates the thickness of the fouling deposit. The calculation of the fouling thickness is based on the solution of the fluid flow and on the equations and the input parameters that the user has selected. This algorithm allows one to choose the expressions and parameters that are considered opportune to estimate the layer thickness. The versatility of the proposed methodology permits the user to select the mathematical

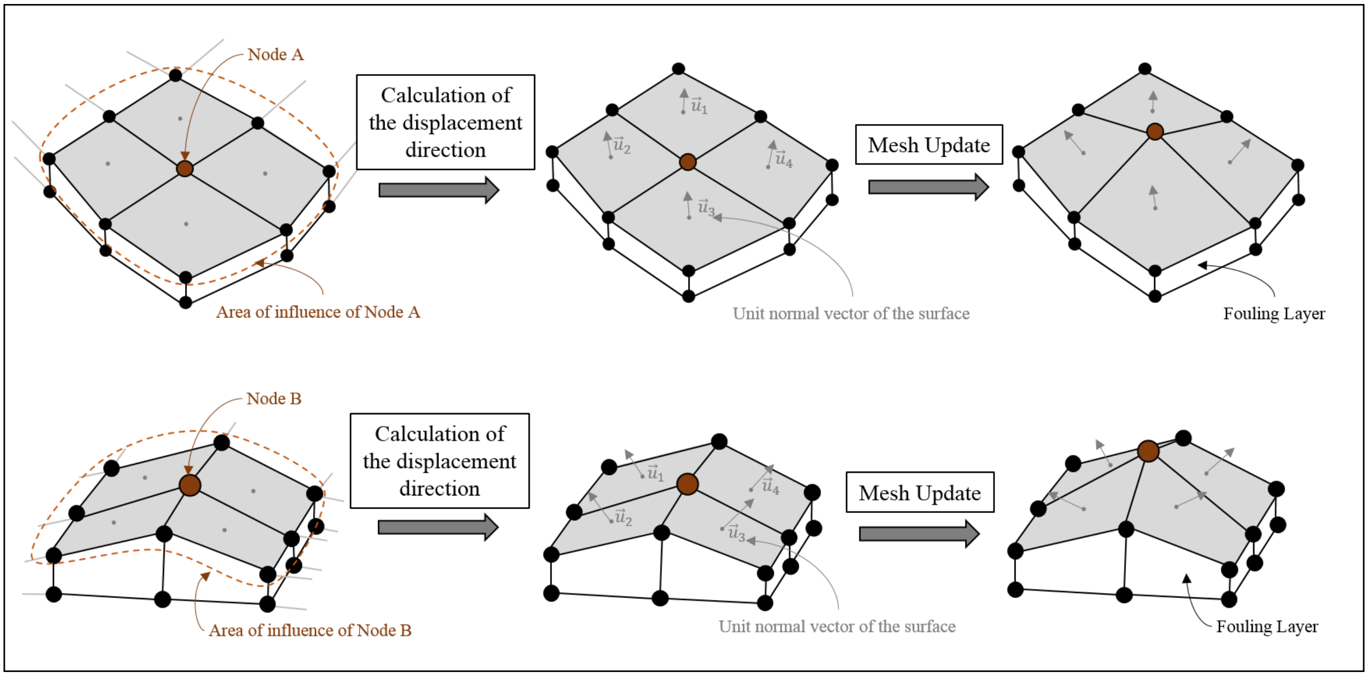

Figure 3: Example of the calculation of the displacement direction in two different nodes

statements with complete freedom and to add the necessary input parameters to obtain accurate results of the fouling layer evolution. Using these expressions, the fluid flow properties, such as the temperature, velocity, wall shear stress or thermal gradient, together with the input data parameters, are computed to reach the thickness of the fouling layer.

To reproduce the growth of the fouling deposit, and once the thickness of the deposit has been calculated, the new positions of the nodes of the fluid-fouling interface are determined. Keeping in mind the fouling results achieved by the surrounding cells, the nodes of the fluid-fouling interface estimate their new places inside the computational grid. The new location of each node is calculated through different data processing activities and taking
into account the fouling layer thickness estimated by all the cells that are in the proximity of the node. Depending on the distance between the node and the cell centroid of the adjacent cells, the nodes of the interface compute their locations weighting the fouling layer thickness of all surrounding cells following the next expression:

$$f = \frac{\left(\frac{1}{d_1} \cdot f_1\right) + \left(\frac{1}{d_2} \cdot f_2\right) + \cdots}{\frac{1}{d_1} + \frac{1}{d_2} + \ \ldots} = \frac{\sum\left(\frac{1}{d_n} \cdot f_n\right)}{\sum \frac{1}{d_n}} \qquad (3)$$

where f represents the thickness of the fouling layer of each cell, d is the distance between the node and the cell centroid and n is the number of neighbour cells. In turn, the displacement direction of each node is also balanced according to the distance between the node and the centroid of the cell. Each node inspects the distance between it and the centroids of the surrounding cells and estimates its displacement direction following the next expression:

$$\vec{k} = \frac{\left(\frac{1}{d_1} \cdot \vec{u}_1\right) + \left(\frac{1}{d_2} \cdot \vec{u}_2\right) + \cdots}{\frac{1}{d_1} + \frac{1}{d_2} + \ \ldots} = \frac{\sum\left(\frac{1}{d_n} \cdot \vec{u}_n\right)}{\sum \frac{1}{d_n}} \qquad (4)$$

where n is the number of adjacent cells to the node, d represents the distance between de node and the cell centroid and $\vec{u}$ is the unit vectors of the normal direction to the surface of the fouling cells. With this expression, the closest cell centroids, i.e. those cells more affected by the movement of the node, influence the displacement of this node to a greater extent, while those that are away from the node hardly modify the movement direction. In this way, the node is displaced considering the position and the orientation of its neighbouring cells and avoiding priority movement directions, as Figure 3 shows. This interpolation allows one to simulate the fouling process inside complex geometries and contributes to obtaining smoothed profiles while eluding discontinuities on the fluid-fouling interface.

When the new position of the node is known, the Dynamic Mesh model carries out the update of the mesh. Dynamic Mesh model assumes control of the displacement of the nodes of the mesh and it moves them to their new situation causing the displacement of the fluid-fouling interface. With that, the fouling layer growth is reproduced and the deposit evolution will have influence in the next time step of the simulation.

This methodology is repeated at every time step of the calculation until the fouling layer stabilization is reached. When the thickness of the fouling deposit is constant, the simulation process is declared finished.

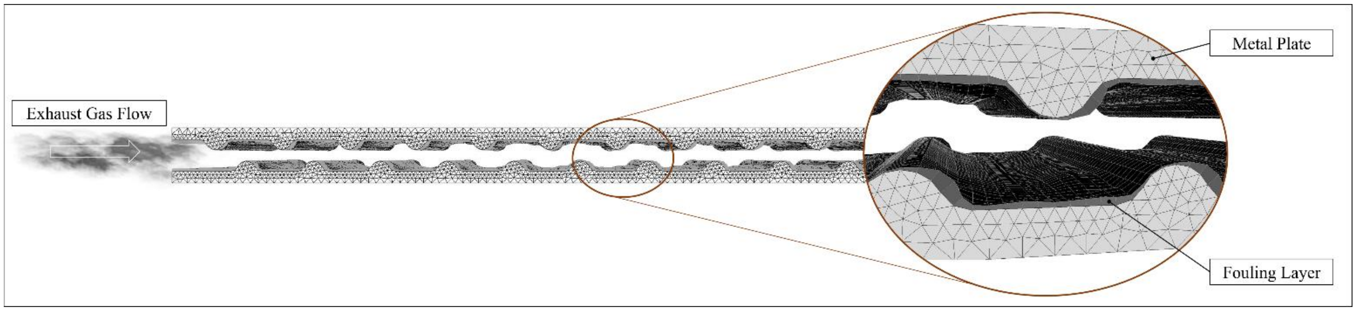

Figure 4: Heat exchanger made up two staggered ribbed plates

Due to the existence of different grid types (tetrahedral, hexahedral, polyhedral …), the numerical implementation of this computational strategy has been planned to be used with all of the grid types. The versatility of this calculation technique takes into account the numerous types of mesh and whatever the grid type may be, this methodology can be used to calculate the fouling thickness evolution under different boundary conditions.

In order to reduce the time of calculation of the fouling process, this external routine can be used in parallel processing. Parallel processing of Ansys Fluent software allows one to compute a solution by using multiple processes that may be executing on the same computer (ANSYS, Inc., 2016). Fragmenting the mesh into different partitions, this computational system accelerates the simulation process and considerably reduces the time of simulation. Taking advantage of the parallel processing system of Ansys Fluent software, the numerical implementation of this technique has been arranged to run under parallel processing conditions. The data processing between the mesh partitions has been optimised to ensure accurate calculations and to avoid the miscalculation of the position of the nodes, diminishing the simulation time.

In addition, to reduce the user intervention that was required in earlier simulation strategies, the simulation process has been automated. The external algorithm has been planned to minimize the user work in each step of the calculation process. In this way, this methodology makes easier the interaction between the user and the simulation getting a reduction in the time of the calculation.

All these improvements have been done with the purpose of reducing the computational cost of this calculation technique. With this, we have achieved a versatile tool which can be used to simulate the fouling process inside complex geometries in a relatively short period of time.

RESULTS AND DISCUSSION

To exemplify the operation of the presented methodology, we have reproduced the fouling process inside a heat exchanger device similar to the one use in the EGR technology. This apparatus is made up of two staggered ribbed plates symmetrically arranged and constituting a forced convection heat exchanger through which exhaust gases flow. Inside this single-pass channel particulate matter is deposited over the ribs making a soot fouling layer, as Figure 4 shows.

To carry out the simulation, the mesh of the calculation is composed of four domains clearly separated. The gas domain, the fouling layer domain, the metal domain and the coolant domain are the four parts of the computational grid, as the schematic of Figure 5 shows.

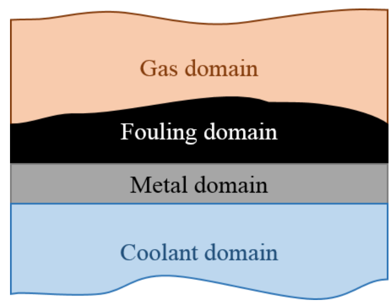

Figure 5: Schematic of the four domains of the mesh

In order to reproduce the fouling process inside this heat exchanger device, the particle number distribution that has been used is similar to the particle distribution generated by diesel engines. Figure 6 depicts the number weighted distribution of the particles used in the simulation.

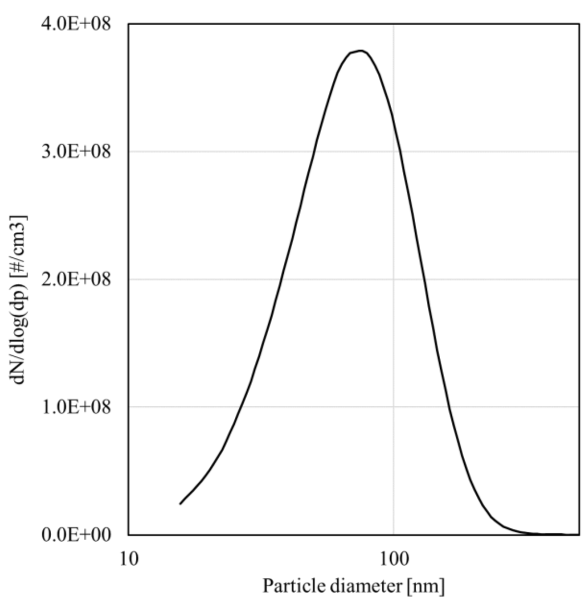

Figure 6: Particle diameter distribution

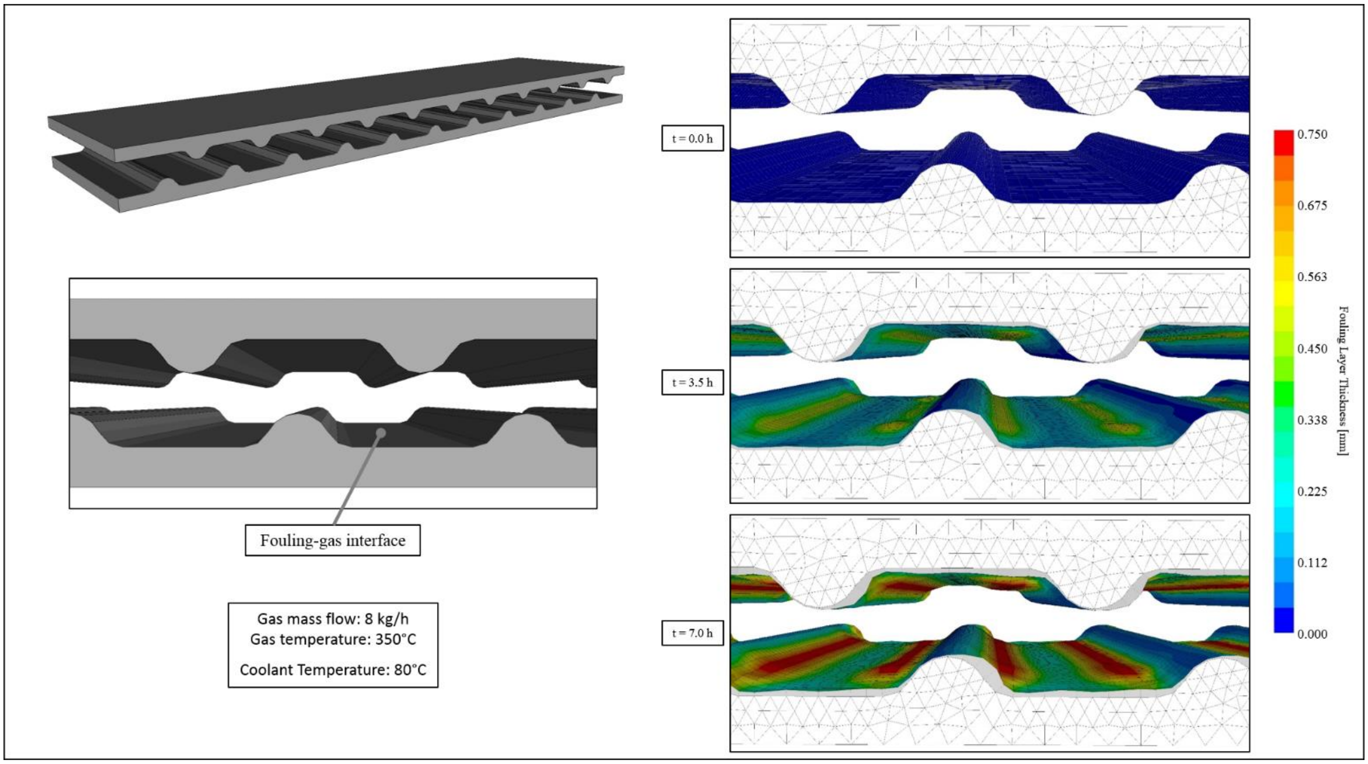

Figure 7: Results of the fouling process inside an EGR heat exchanger. Fouling-gas interface colored by fouling thickness [mm]

The coolant inlet and exhaust gas inlet have been simulated as mass flow inlets and exits have been configured as pressure-outlets. Walls have no-slip momentum condition and thermal conditions have been coupled for all the tube walls. As in previous studies (Paz et.al, 2013-B), the k-ε turbulent model has been used and a pressure-based solver has been selected with the SIMPLE pressure-velocity coupling scheme. Turbulence and momentum equations have been solved with high-order QUICK scheme.

Figure 7 exhibits the results that have been obtained. The images of the figure detail the fouling layer situation at three different time steps of the simulation. These pictures show the growth of the fouling layer as time passes and different thickness have been detected across the ribbed plate. These results allow one to analyse the behaviour of the fouling deposit in the face of soot particle deposition and removal locally. It can be observed that, in some areas, fouling thickness achieves values around 0.75mm, while on the summit of the ribs the deposit thickness hardly reaches some micrometres.

In addition, in order to evaluate the versatility of this computational methodology, the fouling layer growth has been modelled inside a corrugated tube and a wavy fin tube, two technologies widely used in EGR heat exchangers. Figure 8 and Figure 9 show the fouling layer evolution inside a corrugated tube and a wavy fin tube respectively. These images depict the fouling-gas interface at three different moments of the fouling process.

In both simulations it can be detected that, as time passes, the fouling layer grows due to the interaction of deposition and removal mechanisms and different fouling thickness can be observed across the test section. From clean conditions, fouling deposits start to build up on the heat exchanger walls causing a non-uniform layer. The influence of the features of the flow determines the deposition and removal processes and, as a result, the regions with low wall shear stress and high thermal gradient show the highest fouling thickness.

This calculation technique reproduces the fouling layer evolution recreating the movement of the fouling-gas interface having in mind the local scale effects along the device and taking into account the properties of the fouling layer as the layer builds up. In addition, the displacement of the gas-fouling interface leads the CFD software to evaluate the reduction of the cross sectional area, the increase in pressure drop along the device and the reduction of the heat transfer inside the heat exchanger. The growth of the fouling domain and, thus, the reduction of the gas domain allows the CFD software to reproduce the gas flow at every time step of the simulation.

CONCLUSIONS

In this study a calculation methodology has been developed to simulate the fouling process using Dynamic Mesh model from Ansys Fluent. Using the *C* programming language, an external algorithm has been programmed and coupled to the computational fluid dynamics software.

This calculation technique can reproduce the fouling layer evolution recreating the movement of the fouling-fluid interface having in mind the local scale effects involved in the fouling process. Making use of the Dynamic Mesh model, the nodes of the mesh of the interface between fouling deposit and fluid are moved to simulate the fouling layer growth. The low

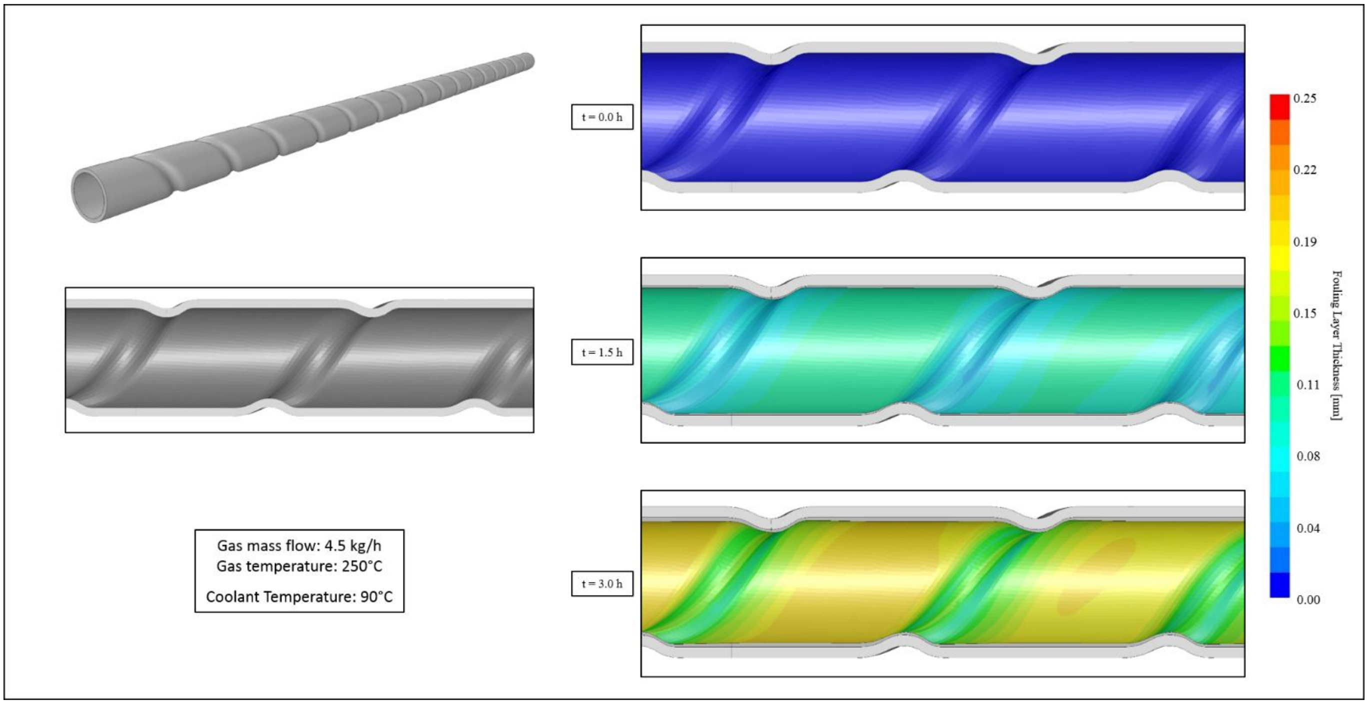

Figure 8: Results of the fouling process inside a corrugated tube. Fouling-gas interface colored by fouling thickness [mm]

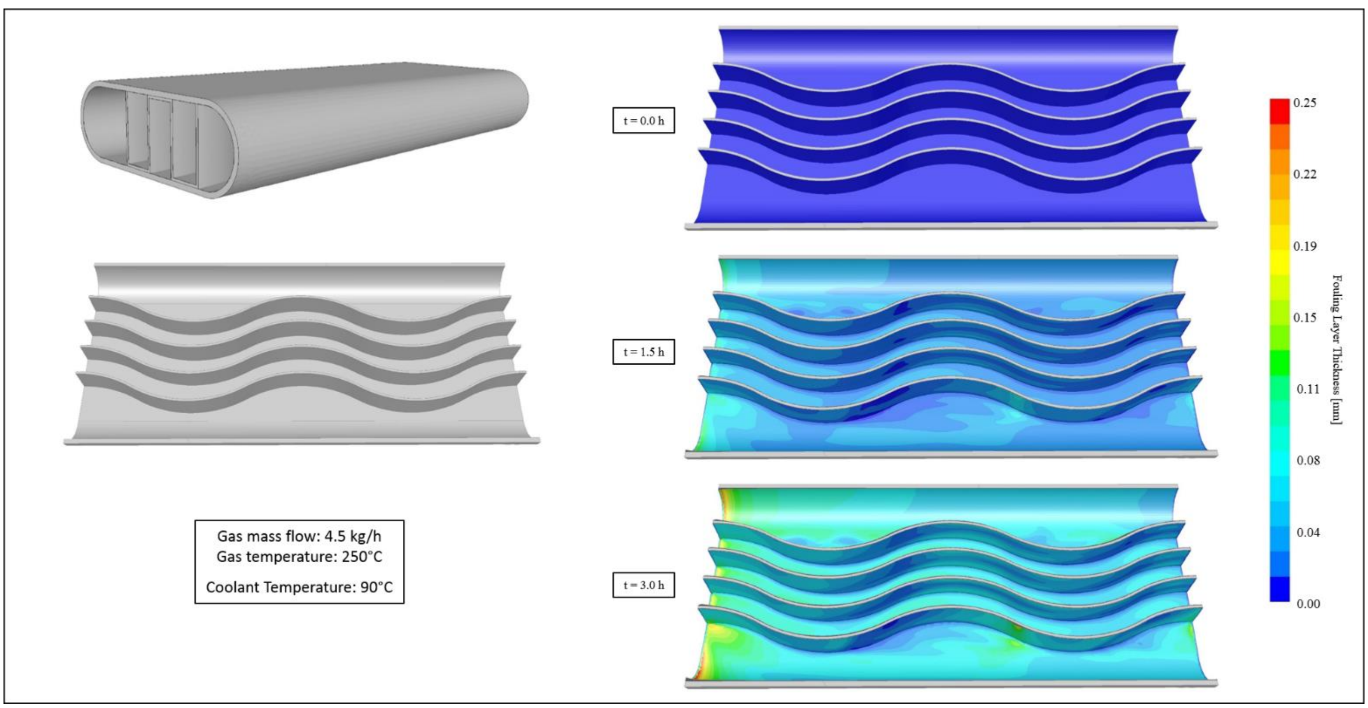

Figure 9: Results of the fouling process inside a wavy fin tube. Fouling-gas interface colored by fouling thickness [mm]

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computational cost of this tool allows the user to simulate complex geometries achieving results in a short period of time.

This methodology has been used to reproduce the fouling process inside three different technologies widely used in EGR systems. We have obtained the results of the fouling process inside these heat exchangers, which show the fouling layer evolution at different time steps of the calculation.

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