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Simulation of air pollution due to marine engines

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Abstract. This paperwork tried to simulate the combustion inside the marine engines using the newest computer methods and technologies with the result of a diverse and rich palette of solutions, extremely useful for the study and prediction of complex phenomena of the fuel combustion. The paperwork is contributing to the theoretical systematization of the area of interest bringing into attention a thoroughly inventory of the thermodynamic description of the phenomena which take place in the combustion process into the marine diesel engines; to the in depth multidimensional combustion models description along with the interdisciplinary phenomenology taking place in the combustion models; to the FEA (Finite Elements Method) modelling for the combustion chemistry in the nonpremixed mixtures approach considered too; the CFD (Computational Fluid Dynamics) model was issued for the combustion area and a rich palette of results interesting for any researcher of the process.

1. Introduction

Manufacturers of diesel engines were first involved in matters concerning the emission of exhaust gas in stationary applications. A study on exhaust emissions from diesel, is a challenge for both designers and manufacturers of equipment for gas treatment. It also means a deep understanding of the combustion process. Such an arrangement has resulted in treating more serious environmental problems in the water. Anticipating this development, engine manufacturers have initiated research on engine emissions. These studies have attempted to find techniques to reduce exhaust emissions, techniques that comply with the current rules and the future [1].

This paperwork presents some introductive aspects, emphasizing the fact that the simulation of the processes inside the marine engines was a permanent subject of study for the specialists. The complexity of all the associated phenomena and their strong correlation is making out of this a very difficult task. Once with the emerging of modern computer technologies, mainly the computers with high computer power, essentially contributed to the development of combustion models but not only [2].

Therefore, in the last decades, the computer simulations and models grow exponentially. Simultaneously, appeared and developed complex calculus algorithms which permitted solving complex differential equations systems of modelled phenomena, thus the central point of the research activity migrated from the purely experimental sphere to the one of theoretical and applicative activities [3].

The complexity of the resulting models and how they performed, permitted today the leap from the studies which merely estimated the behaviour of such system to the prediction of their behaviour, being a powerful tool for any research activity [4].

The numerical simulation is based on some theoretical hypothesis which allow obtain the numerical model closely simulating the real processes inside the engine [5]. This is involving two stages:

- physical modelling which identifies the system particular traits by considering a hierarchy in the importance of the phenomena which describes the equations system more or less complex depending on the nature of the study and the grade of detail;
- mathematical modelling is the next stage which, by meaning of certain modifications done over the equation system, permit to have finally, some calculus procedures which may be implemented for issuing solutions with the smallest amount of computer effort, and within a certain precision domain [6].

The paperwork, as it is stated in this introductive chapter, is:

- tridimensional modelling of the geometry of the combustion chamber and the CFD (Computational Fluid Dynamics) net/grid of the finite elements involved;
- tridimensional simulation of the thermo-chemical behaviour of the combustion process and calculating the interesting parameters and the distribution of the mass fraction for the burning by-products.

The main objectives of the study the reaction of combustion of a fuel mixture are: determining the final composition of substances, the amount of heat released, as the combustion temperature at the end of this development.

Stoichiometric combustion equations are:

$$\begin{cases} C + O_2 = CO_2 \\ H_2 + \frac{1}{2} O_2 = H_2O \\ S + O_2 = SO_2 \end{cases} \tag{1}$$

Chemical compounds within the chemical reactions in the combustion of diesel engine combustion chambers have different physical and chemical properties and therefore the mixture and the reactions that occur can be treated by FEA by the concept of chemical species [7].

FEA dedicated programs can calculate the mass fractions Yi of each species in the mixture by solving the convection-diffusion equation for a number i of chemical specialists.

Mathematical modelling of training pollutants at energy systems ship

Differential thermal models define each time at least three components of fluid heat engine: burnt gas, gas from the flame and the original mixture, characterized by three different temperatures. On the chemical is considered that the fluid motor comprises only two components gas mixture burned and initially-because it allowed the assumption that chemical reactions of combustion resulting instantly. In line with this representation are defined: m_{gaj} - burned gas mass in the new element j format in time $\Delta\alpha$ at the flame temperature: $m_{ai\alpha}$ - the initial mixture mass in the α moment, $m_{gaa-\Delta\alpha}$ - the mass of burned gas formed until $\alpha - \Delta\alpha$. Fluid mass conservation equation, defined independently of the number of components that make up the burnt gas is [8]:

$$m_{gaa-\Delta\alpha} + m_{gaj} + m_{ai\alpha} = m_{ai} \tag{2}$$

where m_{ai} is the mass of initial mixture, present in the engine cylinder when the trigger combustion. The burned gas model inhomogeneous thermal mass is the sum of the elements.

The variation ξ_α in degrees of crankshaft rotation or in seconds is called a feature of heat release or characteristic of combustion.

$$\xi_{\alpha} = \frac{\nu_{c\alpha}}{\theta_c} \tag{3}$$

where: ξ_{α} - fraction of fuel; ν_{α} - fuel quantity in moles, entering the moment of opening the combustion reaction to date α.

It accepts the following hypothesis: the amount of gas burned at one time is proportional to the amount of unreacted fuel. This assumption, widely accepted is rational because it follows the general hypothesis that chemical reactions resulting instantaneous [9].

In the model with elements of variable gas mass is made the fundamental hypothesis that air-fuel ratio of each new element of gas that form corresponding theoretical dosage. This assumption determines the mass of an element of the newly formed gas. Then the mass and chemical composition of newly formed elements change gradually by mixing with air. Mainly, you can imagine that the initial mixture has two components, one available for combustion and other gases burned available for dilution by mixing, the first of the components defined depending on combustion characteristic and last according to feature in the mass transfer of air burned gases. Accordingly, the current mass of burned gas element can be considered to consist of two components, one of which is the mass of the initial stage item new format and the other, the mass of air added by mixing [10].

To define the internal energy of gas burned is necessary to specify their state heat separately, since the model assumes that each element of gas is burned in an independent development time. Thermal state of each element changes in relation to the interaction energy between itself and the surrounding systems [11].

Air quality control. Partial pressure of reactive oxygen and nitrogen can be influenced by changing specific quantities of air that enters the engine, or by changing the ratio of oxygen and nitrogen. The report can be changed by the exhaust gas recirculation (EGR-exhaust gas recirculation) [12].

In principle, the exhaust gases can be recycled both before (case 1) and after the turbo (case 2), as shown in figure 1:

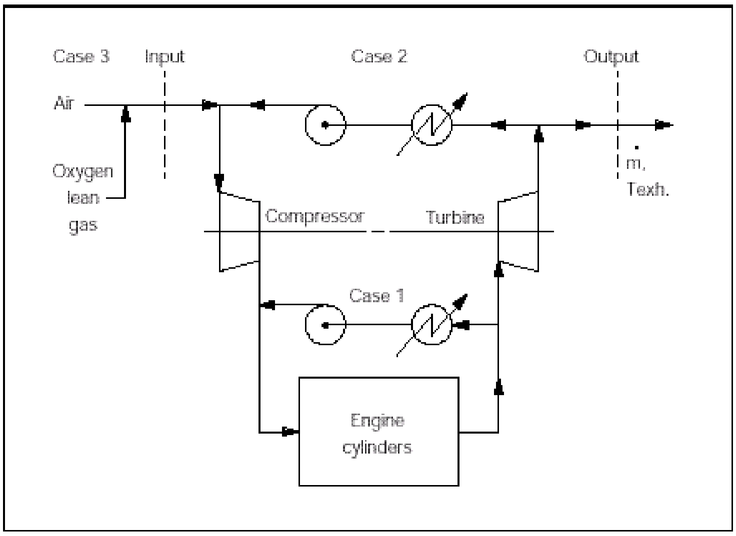

Figure 1. Burnt gas recirculation.

The influence of combustion pressure. The high combustion by increasing the injection advance, will lower the peak temperature and thus will reduce NOx emissions, but will inevitably lead to increased fuel consumption. Regimes characteristic of the three parameters (actual specific consumption of fuel-specific fuel oil consumption SFOC, Bosch Smoke Number, and NOx) are shown in figure 2. It is used but not an attractive method because of increased fuel consumption [12].

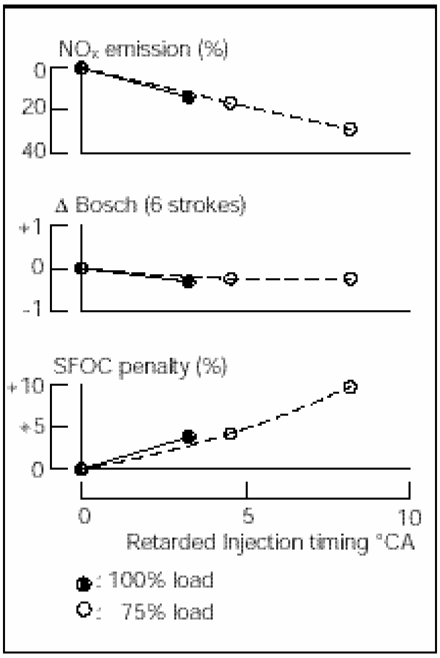

Figure 2. Regimes characteristic of the three parameters.

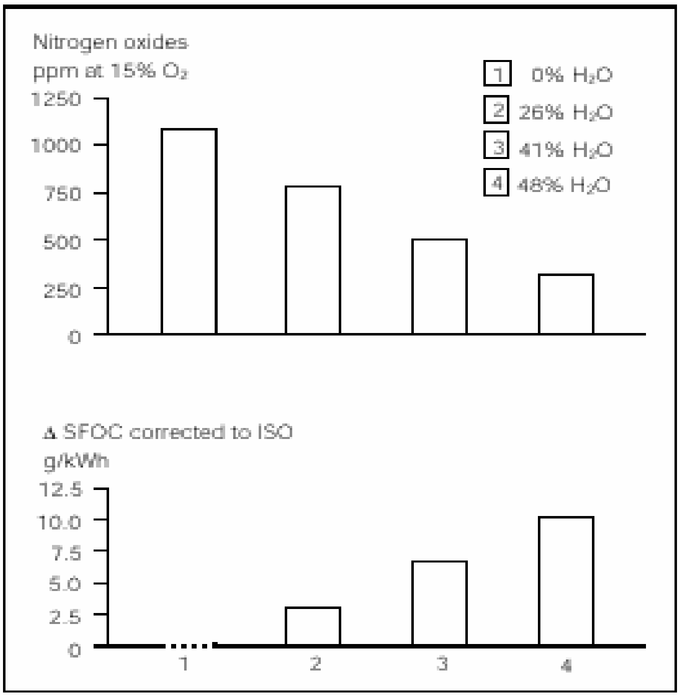

Figure 3. The impact on NOx emissions and fuel consumption.

Water emulsion fuel. It was found years ago, the emulsion fuel leads to a significant reduction of NOx, and today two power plants equipped with MAN B & W using this method for controlling NOx emissions, without any effect on costs maintenance. Figure 3 shows the impact on NOx emissions and fuel consumption.

Selective Catalytic Reduction (SCR). By this method, the exhaust gases are mixed with ammonia (NH3), before passing through the layer of special catalysts at a temperature between 300°C and 400°C, where NOx is decomposed into N2 and H2O. An outline of the system is shown in figure 4.

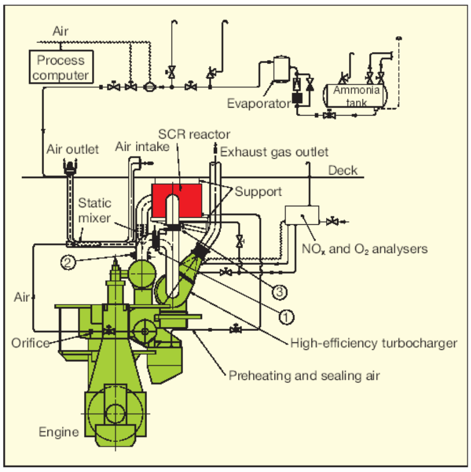

Figure 4. SCR system.

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2. Experimental

Computer simulation took as its starting point a diesel engine, manufactured by Wartsila, type 6L26 used in the propulsion of small ships, shown in figure 5.

Dimensional CAD model of the injection area was generated using SolidWorks software in 2004, resulting in a geometry as shown in figure 6:

Figure 5. Wartsila 6L26 diesel engine type considered.

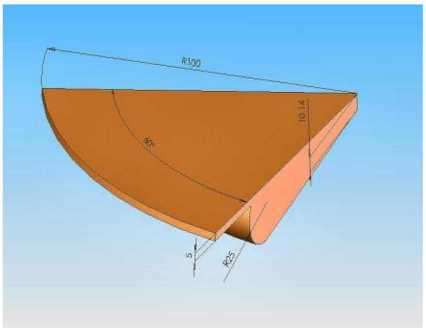

Figure 6. CAD model of the combustion chamber.

Diameter hole injection valve was found to be 0.22 mm and injection pressure 55 MPa. The analysis was done for the total development time of the flame, corresponding to a crankshaft angle of 10 ° ATDC.

Static and dynamic pressures in the combustion chamber resulting from fuel combustion are given in the figure 7. Figure 7 presents the situation of the pressure in the combustion chamber, a cross section through it at one-half the area of ignition in the cylinder head, perpendicular to the axis OY, and in addition, for the most important results is given graphically for each finite element pressure the plane of symmetry of the jet. Fields of speed of the combustion chamber are given in the figures attached. In distribution, the highest speeds are reached in the jet fuel (max. 438 m/ s) and lowest in the rest of the combustion chamber. As shown in the chart that the situation in a plane of symmetry passing through the center of the jet injection, the maximum speed is reached at a distance of 60 mm away from the hole injection (figure 8).

Temperatures resulting in the combustion chamber are given in figure 9. On very small portions, to end the enclosure reaches very high values up to 3870^0K, media room is between $2100\text{-}2400^0$K. Highest density of flue gas is achieved in the area of injection (max. 1.22 kg/m^3), the average of the rest of the combustion chamber volume of 0.2 kg/m^3.

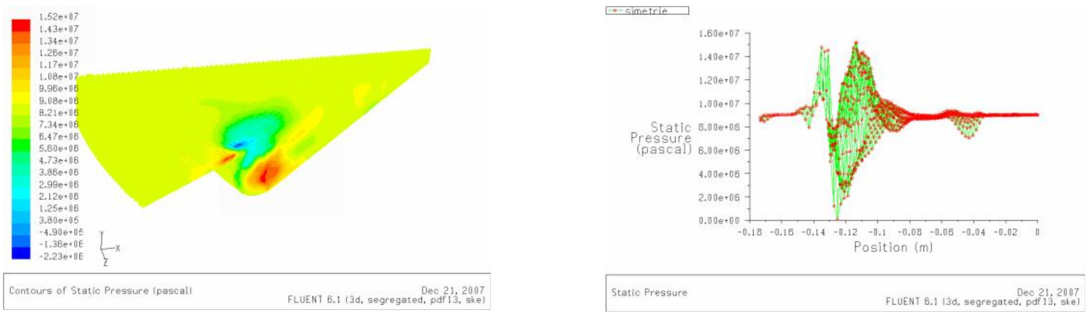

Figure 7. Static and dynamic pressures.

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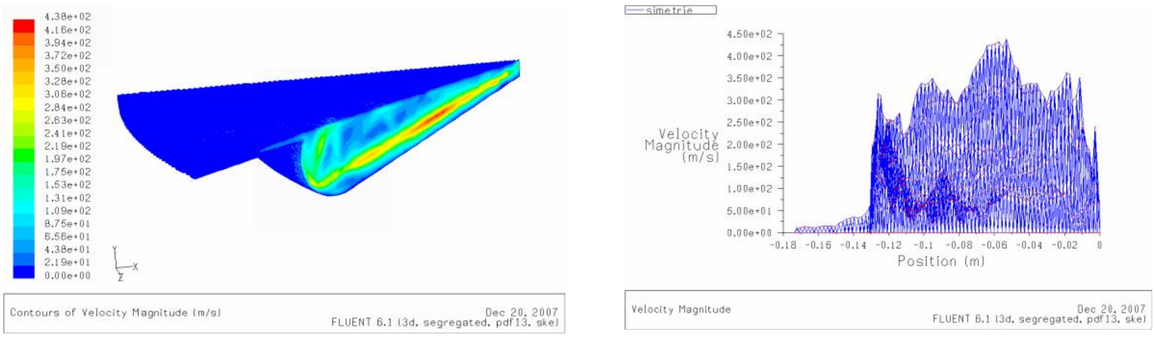

Figure 8. Fields of speed of the combustion chamber.

Effective thermal conductivity (figure 10) is maximum in the areas of injection and combustion chamber extreme, reaching maximum of 58.5 W/mK and minimum of 1.08 e^{-1} W / mK in the middle of the combustion chamber.

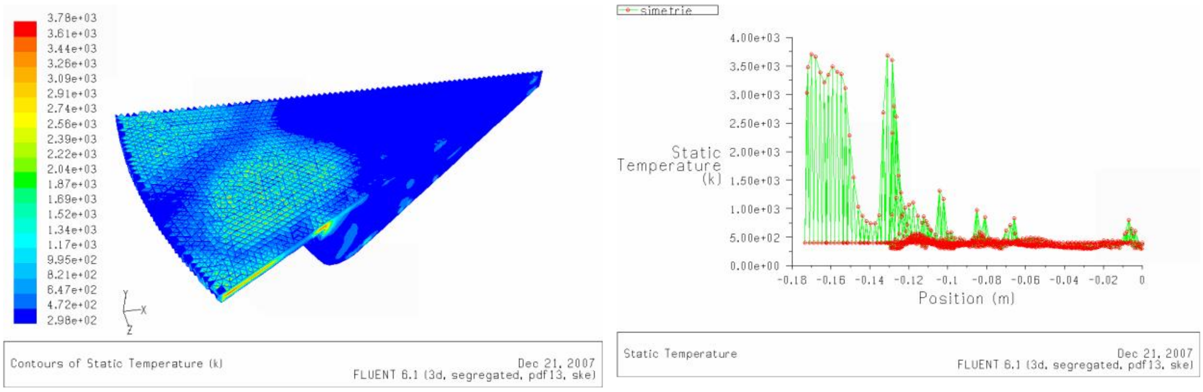

Figure 9. Temperatures in the combustion chamber.

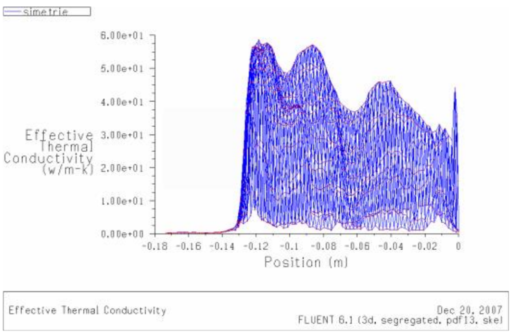

Figure 10. Effective thermal conductivity.

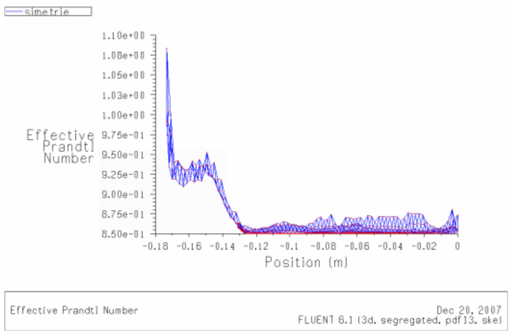

Figure 11. Prandtl number.

Maximum values of Prandtl number to reach the top and towards the end of the combustion chamber (max.1.1) and lowest in the area of injection (8.75 s-1) (figure 11). Entropy reaches maximum at the top of the combustion chamber with values up to 1.24 e4, the lowest values being in the area of injection (7e3). Turbulence kinetic energy, reaches maximum injection zone and along the jet fuel (figure 12).

The formation of compounds type NOx pollutants in the combustion process involve the existence of distinct mechanisms: the formation of thermal NOx, prompt NOx, NOx formed by fuel and post-combustion. Thermal NOx is formed by oxidation of atmospheric nitrogen present in air, NOx is formed due to prompt rapid reaction of the flame front, NOx formed in the fuel is produced by oxidation of fuel and the existing nitrogen from the reaction between NO and the involving fuel. NO formation is governed by two factors: the concentration of free oxygen and temperature size. NO formation is extremely sensitive to temperature value of activation energy due to the size that influence the reaction rate.

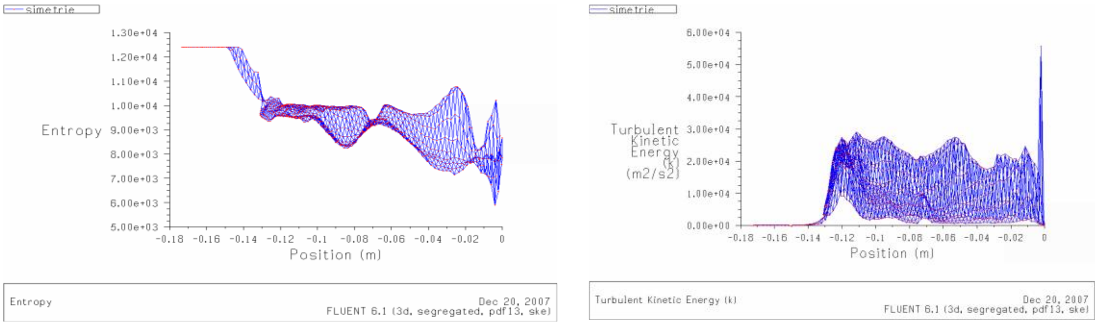

Figure 12. Entropy reaches maximum and turbulence kinetic energy.

NOx calculated distribution is depicted in the plane of symmetry of jet fuel in figure 13.

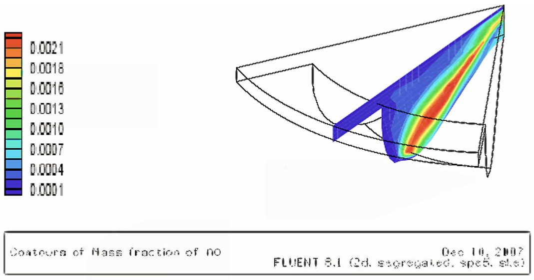

Figure 13. Distribution of mass fraction of NOx in combustion chamber.

3. Results and discussion

Combustion in diesel engine combustion chambers, was studied in detail over time, resulting in a rich literature, scientific articles and doctoral theses, given the importance of this process in performance and overall efficiency of the engine.

It can thus call this database to make a comparative validation, this kind of comparison is legitimate as long as the phenomena are common, with variations of course, taking the geometry of the combustion chamber, injection and compression parameters and assumptions basic models.

Author of [10] deals that phenomenology same area of interest as the present study, using simulation software Kiva III capable of simulating two-phase flow of diesel engines. Kiva as the program used for modelling discrete droplets of fuel model (Discrete droplet model) and contains submodels to simulate the collision, their disintegration and evaporation. For simulation, the author considers a Caterpillar engine type 3406 (in this paperwork we considered type Wartsila 6L26 engine).

It is noted that the maximum kinetic energy of turbulence was obtained for the end of the combustion chamber, with a maximum of 5.57 e4 = 55,700 K (cm2/s2) and the author obtained in the simulation 54,017 K (cm2/s2). The similarity is more than obvious (figure 14).

Flame front shape is identical in both simulations. Highest temperature is obtained in the middle of the jet of flame and has a maximum of 2380 0K in our simulation and 2300 0K in the comparative simulation of author (figure 15).

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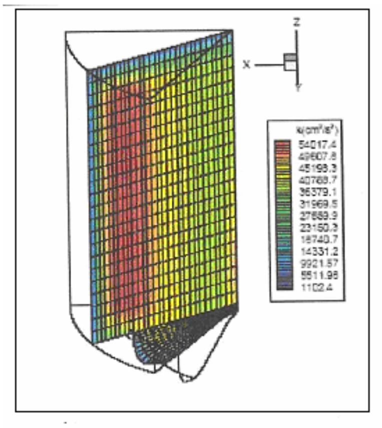

Figure 14. Kinetic energy of turbulence.

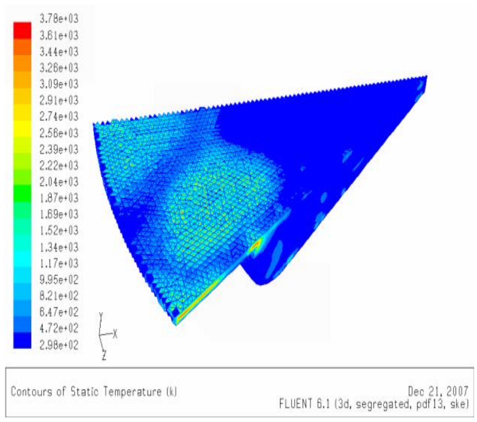

Figure 15. Temperatures.

4. Conclusions

The theoretical work is an extremely detailed inventory of thermodynamic models and gasdynamics phenomena occurring in combustion chambers of diesel engines, as follows:

-deepening multidimensional combustion models, accompanied by very close benchmarking of interdisciplinary phenomenology accompanying these complex processes.

-presentation precepts FEA modeling (Finite Element Analysis) of chemical combustion and fuel mixture model with non-premix used in the simulation.

-develop model CFD analysis (Computational Fluid Dynamics) of the combustion chamber with the deduction of all results of engineering analysis and pressures of the combustion chamber resulting from the combustion of fuel, speeds, temperatures, distribution density, viscosity, diffusion coefficients of different chemical species , thermal conductivity, specific heat, Prandl number distribution, entropy, internal energy, total energy, kinetic energy of turbulence, turbulence intensity, vorticity, response rate, molecular weight, the total enthalpy of each species, humidity, mass fractions of chemical species, molar concentration distribution of chemical species.

-interpretation of simulation results in terms of their comparison with reference works in the field, resulting in good correlation with experiments, thus proving the viability and accuracy of model created.

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