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COMPUTER MODELLING OF HIGH TEMPERATURE AIR COMBUSTION

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ABSTRACT

High Temperature Air Combustion, HiTAC, is an innovative combustion technology which offers improved heat transfer and a reduction in fuel consumption and NOx emissions.

This paper describes a project in which a computational fluid dynamic model of a furnace working on high temperature air combustion technology was developed using FLUENT® CFD software. The model was validated against experimental data obtained from KTH in Sweden. The predicted results compared very well with this experimental data, and were also closer than the predictions from the model built by KTH.

The model was applied to a steam boiler of Malta's Delimara Power Station. Two scenarios were considered: the boiler with conventional combustion and the boiler converted to HITAC. To reduce computational time, a 400:1 scaled down version of the boiler was modelled based on NOx scaling. Further reductions were made by taking advantage of the symmetry of the boiler and by obtaining the solution for a single burner, and then prescribing the parameter profiles for the single burner to the full boiler model as boundary conditions.

The computer model results showed much lower NOx emission levels when firing the boiler with methane compared to heavy fuel oil. Further reductions in NOx emissions were obtained with HITAC technology and using methane as a fuel.

INTRODUCTION

High Temperature Air Combustion, HITAC, also known as Flameless Combustion, Flameless Oxidation, Diluted or Mild Combustion, is an innovative combustion technology which offers three main advantages: reduction of the NOx emissions, improved heat transfer characteristics and a reduction in fuel consumption.

When highly preheated air (1100 to 1600 K) is used, combustion by autoignition takes place immediately after the mixing of fuel and air; thus stabilizing the flame by a pilot flame or a flame holder is not required. Combustion occurs with any type of conventional burner using highly preheated air, but in a HiTAC furnace combustion takes place as a lifted flame relatively free in space. The incoming preheated air is first diluted with the burned gas recirculating inside the furnace, and then it makes contact with the fuel. Flames formed in such a flow field have totally different features from those of conventional burner flames. The flame has low luminosity, and almost transparent reaction zones resembling a spreading mist in the furnace rather than a flame. In this situation NO_x emission and flame temperature are extremely low despite the high-temperature preheated air.

The relatively flat temperature profile of a HITAC furnace leads to a higher mean temperature level in the furnace and thus improved heat transfer characteristics, which will result in an increase in product quality and productivity, and hence a reduction in the physical size of the facilities as compared to traditional furnaces.

The preheating of the combustion air leads to a remarkable reduction in fuel consumption; reductions as high as 60% can be achieved. This reduction in fuel consumption results in lower CO_2 emissions. Furthermore, HiTAC technology has shown extremely low levels of emissions of NOx, which are far below the present regulatory standards [1,2,3,4].

Nomenclature

A	[gmol/cm^3]	Pre-exponential factor
$E_{\%}$	[kcal/gmol]	Activation energy
k	[m^3/kmol-s]	Rate coefficient
R	[kJ/kmol-K]	Universal gas constant
T	[K]	Temperature

THE MODEL

In this project, details of which can be found in reference [5], a computational fluid dynamic (CFD) model of a "hypothetical" furnace working on high temperature air combustion technology was developed using a CFD software package, FLUENT®, and using its inbuilt turbulence, combustion and radiation models. The inbuilt NOx production models needed some adjustments in order to correctly predict the low NOx emission levels. The main production route in HiTAC was found to be the N_2O intermediate route.

The model was based on a HiTAC furnace (500kW maximum firing rate), which was equipped with one-burner High-Cycle Regenerative System (HRS) at the Division of Energy and Furnace Technology of the Royal Institute of Technology (KTH) of Sweden, and whose dimensions and performance data were kindly provided by KTH.

To achieve good computational accuracy and computational speed, a higher cell concentration had to be ensured near the burner furnace front and in the flame reaction zone. In order to achieve these mesh properties, the furnace front wall, on which the burner is situated, was created first and then meshed according to the desired cell concentrations. An important step that was taken was that the front wall mesh also included the projected mesh of the back wall. This was done in order to make hexahedral volume meshing possible. Once this front wall was created (Figure 1) and meshed, it was extruded along the length of the furnace. In addition, the mesh close to the burner and close to back wall was made finer since in these regions higher turbulence was expected. The furnace was descretised in 590542 hexahedral cells. The maximum hexahedral cell skewness in the furnace was 0.65 (given from GAMBIT as equiangle skew). This value is within the recommended range proposed by FLUENT® for reacting flow problems.

The main models which were used in this work were the following:
Turbulence model: standard κ-ε model with standard wall functions;
Radiation model: Discrete Transfer Radiation Model
Combustion model: Finite rate/Eddy-dissipation model with a two-step reaction mechanism;
NO model: thermal, prompt and NO reburn mechanism,

The actual fuel composition used in the model was 0.02% Methane, 0.947% Ethane, 98.354% n-Propane and 0.679 iso-Butane, which was almost the same as the actual fuel used in the KTH tests except that very small amounts of other hydrocarbons were incorporated in the value for iso-Butane.

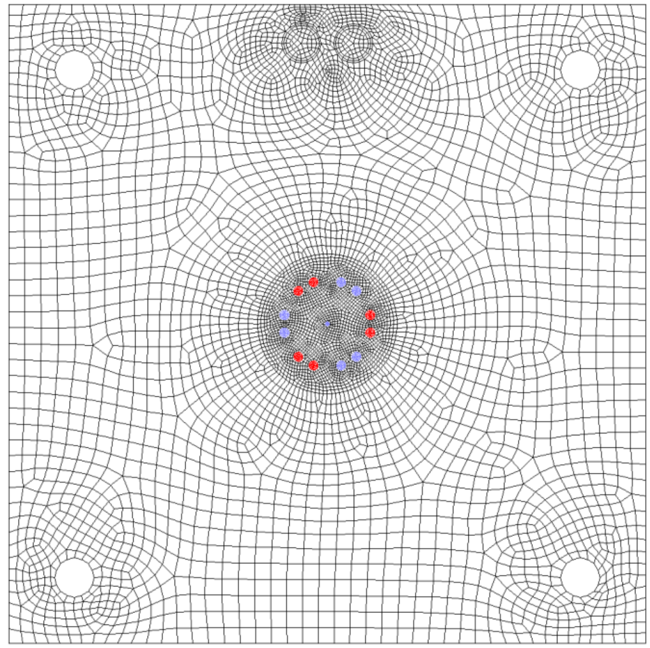

Figure 1 Meshed furnace front view

The reaction mechanism considered in this study was the multi-step mechanism as proposed by Westbrook and Dryer [6]:

$$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O \quad (1)$$
$$C_2H_6 + 2.5O_2 \rightarrow 2CO + 3H_2O \quad (2)$$
$$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O \quad (3)$$
$$C_4H_{10} + 4.5O_2 \rightarrow 4CO + 5H_2O \quad (4)$$
$$CO + 0.5O_2 \rightarrow CO_2 \quad (5)$$

The reaction rate for a single reaction can be written as

$$k = AT^n\,[\text{fuel}]^a\,[\text{oxidiser}]^b\,\exp(-E_a/RT)$$

The reaction rate coefficients were as proposed by Westbrook and Dryer [6], namely:

Reaction	A	n	a	b	E_a J/kmol
(1)	$1.50x10^7$	0	-0.30	1.30	$1.255x10^8$
(2)	$1.30x10^{12}$	0	0.10	1.65	$1.255x10^8$
(3)	$1.00x10^{12}$	0	0.10	1.65	$1.255x10^8$
(4)	$8.80x10^{11}$	0	0.15	1.60	$1.255x10^8$
(5)	$3.98x10^{14}$	0	1.00	0.50	$1.674x10^8$

Table 1 Kinetic coefficients for two-step reaction mechanism

VALIDATION OF THE MODEL

The model was validated against experimental data obtained from KTH in Sweden. Comparing the numerical simulation with the experimental results, the following conclusions were drawn.

Concentrations Validation

- The predicted O_2 and CO_2 contents were in good agreement with the measured values. Both of them showed the same locations and magnitudes of their maximum and minimum values.

- The measured CO agreed with the predicted level. The predicted CO concentrations on or close to the burner centreline are lower than the measured values, however the relative differences decrease with increasing distance from the burner. Meanwhile, the model underestimates the fuel consumption in the frontal part of the furnace. This implies that the chemical reaction rate of the fuel converting to CO in the model is slower than the actual reaction rate. Therefore, this model needs a further improvement for the region located near the burner domain.
- The agreement of the predicted and measured concentration of N_2 is good within the range of error of 3.16% except for the points on the burner centreline at 0.3m from the burner.
- The developed HiTAC model is superior to KTH's model as regards NO emission prediction. It was also noted that the N_2O-intermediate route is an important route for NO formation in HiTAC systems.

Furnace and In-Furnace Temperature Validation

- The predicted furnace temperature had the same trend as that measured but the predicted value was slightly higher than that measured. The results from KTH showed better results in the near-burner region, but the results from this model gave a better prediction of a HiTAC flame.
- The predicted temperature in the upper part of the furnace was slightly lower than that in the lower part.
- The temperature increases slightly with increasing distance from the burner face.
- The temperature gradually increases with increasing distance from the centreline as far as the reaction zone is considered.
- The difference between the predicted and measured in-furnace temperatures is relatively large close to the burner zone. However, the discrepancy is minimized to a reasonable agreement away from the burner zone, considering an error range of 3%.

CFD Modelling and Experiment for Validation

- The concept of the Gas Temperature Uniformity Ratio was a suitable parameter to classify the physical changes of a flame in a furnace.
- The numerical results are in good agreement with measurement with the exception of the small region located near the burner domain. This indicates that the Eddy-Dissipate-Concept with multi-steps reactions is a suitable combustion model to simulate HiTAC. This also indicates that HiTAC firing is controlled by both chemical kinetics and mixing.
- The transient behaviour characteristic was not considered in this work. However, this is important for HRS and thus it was the main reason for the discrepancies in the burner domain.
- The simulation failed to predict accurately the species concentration and temperature field in the burner domain.
- More measurement points were needed in the chemical reaction zone to represent better the in-flame parameters.

Figure 2 shows the concentrations of O_2 and CO_2 for two locations in the furnace. Similar graphs were obtained for other locations.

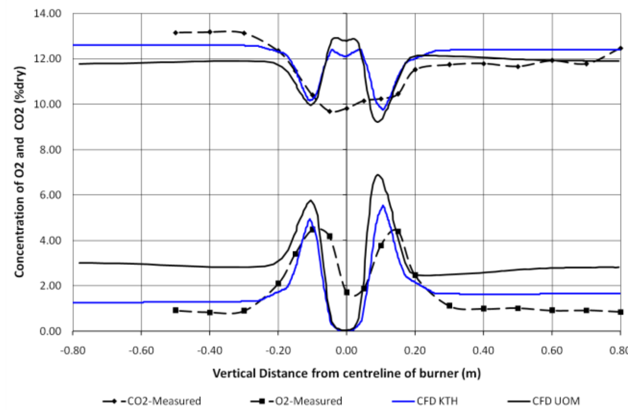

Figure 2 Concentrations of O_2 and CO_2 at x = 0 and x = 600mm

APPLYING THE MODEL TO A POWER STATION BOILER

The model was applied to one of the conventional steam boilers of Malta's Delimara Power Station (DPS). A CFD analysis was performed on the DPS boiler. Two scenarios were considered. In the first case, the performance of the boiler fired with methane was considered; in reality, the boiler uses heavy fuel oil. The air inlet temperature and equivalence ratio were the same in the model as that in current use at the Power Station. The second case was performed in order to analyse the performance of the boiler if converted to HITAC technology as compared to ordinary combustion technology.

Scaling

Due to the size of the boiler and the limitation in computational resources, a full size model of the boiler was not viable. Hence a scaled down version of the boiler was modelled based on NOx scaling, since this was found to be the most appropriate. This model is called SCALING 400 and was developed Hsieh et al [7]. Nearly all other scaling models were only capable to be applied to a single burner furnace and to scaling ratios of 3:1 and 4:1. On the other hand, the chosen model can easily be applied to different configurations and to an outstanding scaling ratio of 400:1. The only limitation was that the burner chosen for the model should be dimensionally similar to the one used. The detailed in-flame data from the SCALING 400 test series were used together with a fundamental examination of NOx formation mechanisms, and the possible NOx emission sources. Physically based scaling laws for the contribution of each of these sources were then developed. Together these laws comprise a general burner scaling model.

To further decrease the computational time by half, advantage was taken of the plane of symmetry of the boiler. Further reduction was obtained by obtaining the solution for a single burner firing in a *rig-type* furnace, including the complete detailed burner geometry; Figure 3. Once the solution for a single burner was obtained, the velocity, species, pressure, temperature and turbulence profiles at a chosen plane were extracted and prescribed on the full boiler model as boundary conditions. This method made it possible to reduce the number of elements used in order to account for the complex burner geometry. A coarser model could then be used for the full boiler model; Figure 4.

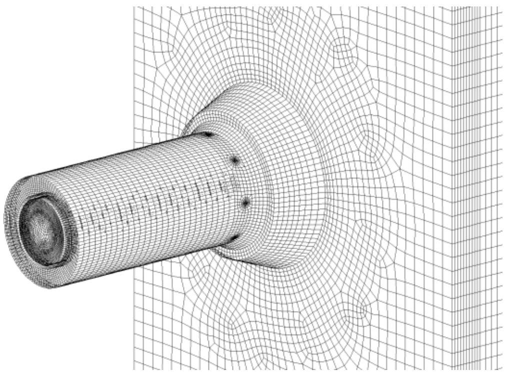

Figure 3 Meshed single burner model

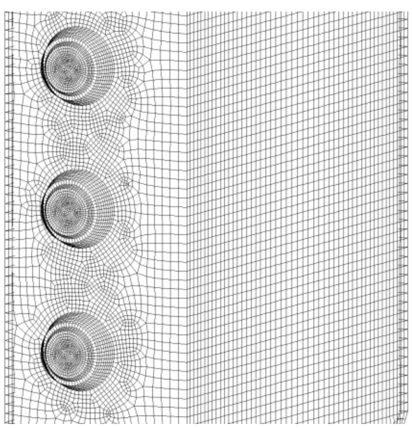

Figure 4 Meshed full boiler model

RESULTS FOR SINGLE-BURNER SIMULATION

To show the swirling flow, an iso-surface (surface of constant property) of velocity was created. Figures 5 and 6 show the contours of O_2 concentration on the 30m/s velocity surface. In these figures, one can easily see the swirling motion of the combustion air. Another important observation is the variation of the O_2 concentration on this iso-surface. In the combustion air inlet duct the O_2 concentration is equal to the value of O_2 in atmospheric air (21%). However, in the flame region, the O_2 in combustion air becomes depleted due to mixing with the combustion products and because it is consumed by reacting with methane.

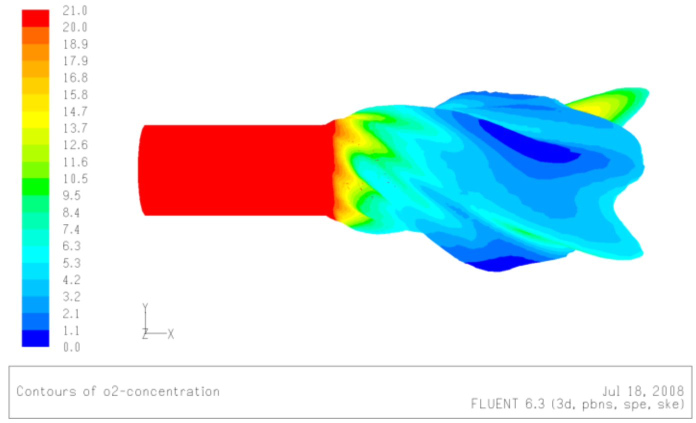

Figure 5 Contours of O_2 concentration on 30 m/s velocity surface –xy view

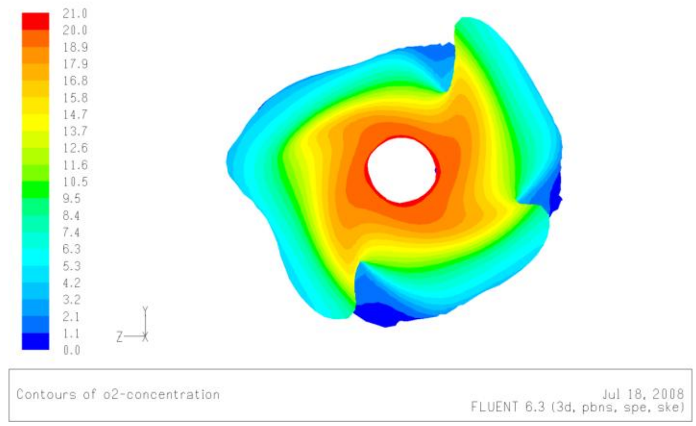

Figure 6 Contours of O_2 concentration on 30 m/s velocity surface –yz view

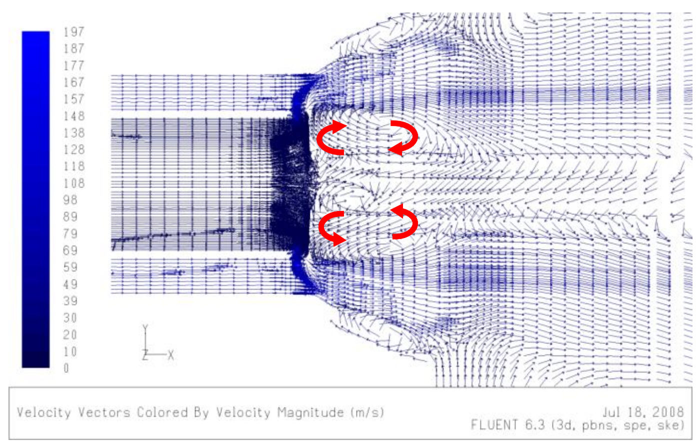

Figure 7 velocity vector plot of the flow in the near-burner region

Figure 7 is a vector plot showing the flow direction in the near burner region in the vertical (xy-plane) passing through the burner axis. The most important observation here is that the central recirculation zone has a similar shape to that described by Weber et al. [8]. It consists of two opposing recirculation regions in the form of a tulip (flower) as depicted by the red arrows. Another recirculation zone is formed exactly in front of the flue gas recirculation port.

RESULTS FOR THE FULL BOILER SIMULATION

In the following figures, some results of the full boiler simulation are presented. The planes of interest in this model are the vertical and horizontal planes cutting the burners' axes and therefore the data will be presented on these planes. The two cases analysed, i.e. conventional combustion technology and HiTAC combustion technology are shown one after the other. In both cases, the fuel was methane.

It is important to note that the colour coding is not the same in all the figures presented, and that all the data shown in contour plots is based on the 1MW burners and it is not the scaled data. The only scaled results possible according to the used scaling model are the NO_x emission at the boiler's exhaust.

Wall heat flux contours

One of the most important parameters in boilers is the wall heat flux since this value determines how much of the heat is transferred to the process water and therefore how much steam is produced. Figure 8 shows the total surface (wall) heat flux in W/m^2 on the boiler walls. The total surface heat wall includes both radiation and convection heat fluxes. As it may be noticed, the heat flux has a negative sign which means that heat is going out through the wall. In actual practice, this heat will be transferred to the process water in order to produce steam.

The highest heat flux is observed in the flame zone. The maximum wall heat flux in this zone was predicted to be equal to $298kW/m^2$. The minimum value occurred away from the flame zone and was predicted to be equal to $31.7kW/m^2$. Figure 9 shows the total surface (wall) heat flux in W/m^2 on the boiler walls when the boiler is working on HiTAC technology.

Comparing these results for HiTAC combustion (Figure 9) with those predicted for the boiler working on ordinary combustion (Figure 8), it can be noticed that the heat flux on the boiler's walls for the HiTAC case has a superior distribution. Also, the zone with the highest heat flux is relatively larger in the HiTAC case compared to ordinary combustion.

Gas temperature contours

Figures 10 to 13 present the gas temperature distribution inside the boiler for the conventional case and the HiTAC case. Static temperature (K) contours on the symmetry plane and the vertical plane through the burner axes are shown in Figures 10 and 11, while Figures 12 and 13 show static temperature (K) contours on the horizontal plane through the burners' axes and an arbitrary plane above the flame zone.

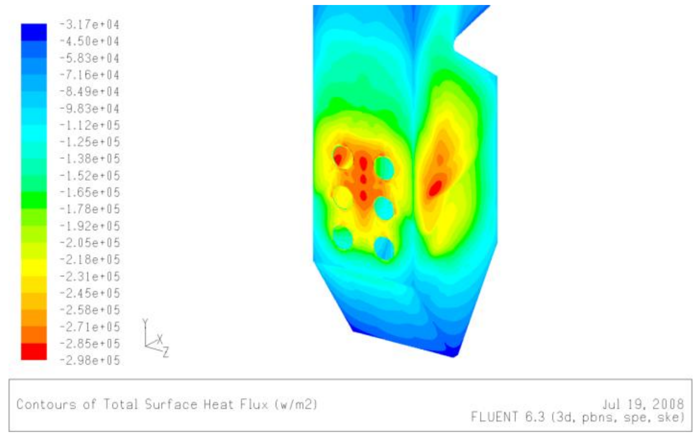

Figure 8 Conventional case - Contours of total wall flux in W/m^2

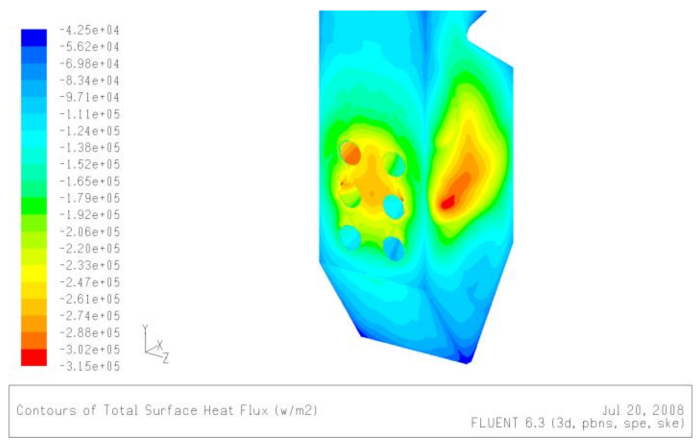

Figure 9 HiTAC case – Contours of total wall flux in W/m^2

It can be easily noticed that although the combustion air temperature for the HiTAC (700˚C) case is 425˚C higher than that for ordinary combustion (285˚C), the maximum predicted temperature in the boiler for the HiTAC case (3099K) is 1192K lower than that in the ordinary combustion case (4291K).

NO volume fraction distribution

Figures 14 and 15 show the NO volume fraction distribution on the vertical plane passing though the burner axes for the conventional case and the HiTAC case respectively.

The figures show that the NO emission level for the HiTAC case is almost half that for the conventional case. It should be noted that the colour scales for the two figures are not the same, with the scale for the conventional case being almost double that for the HiTAC case.

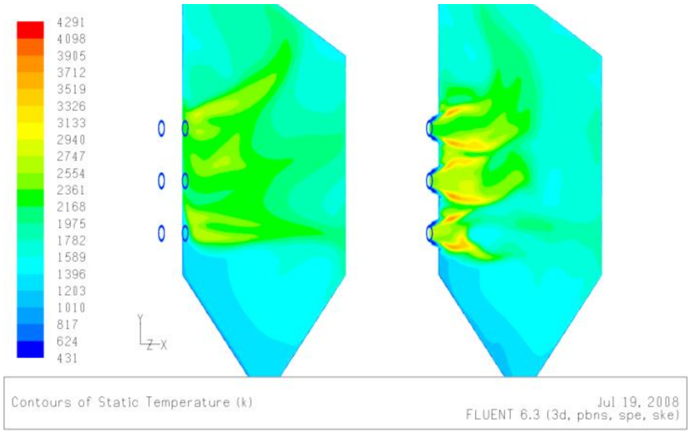

Figure 10 Conventional case - Static temperature (K) contours on symmetry plane and vertical plane through the burner axes

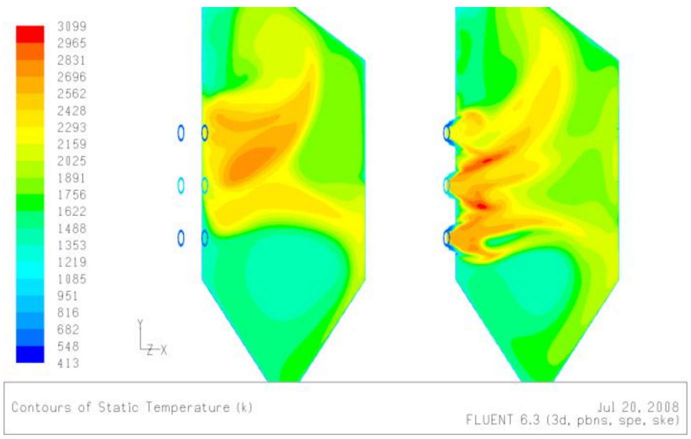

Figure 11 HiTAC case - Static temperature (K) contours on the symmetry plane and the vertical plane through the burner axes

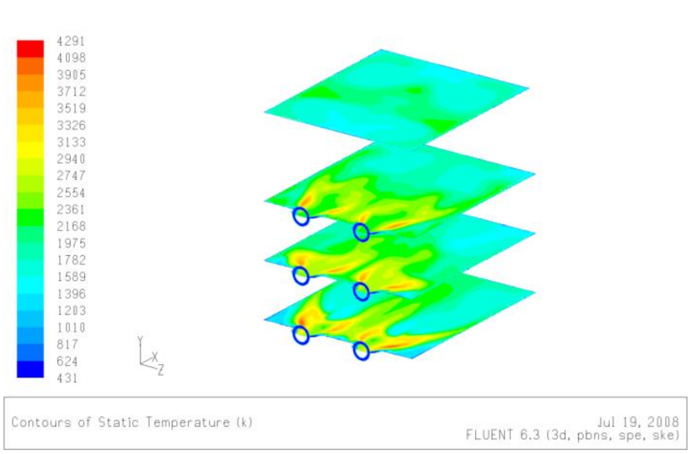

Figure 12 Conventional case - Static temperature (K) contours on the horizontal plane through the burners' axes and an arbitrary plane above the flame zone

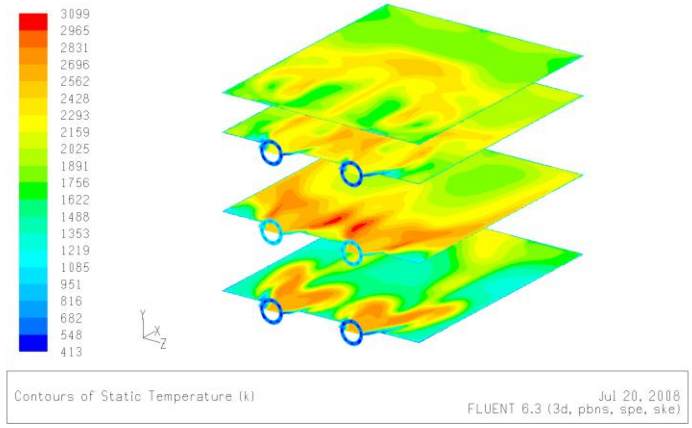

Figure 13 HiTAC case - Static temperature (K) contours on the horizontal plane through the burners' axes and an arbitrary plane above the flame zone

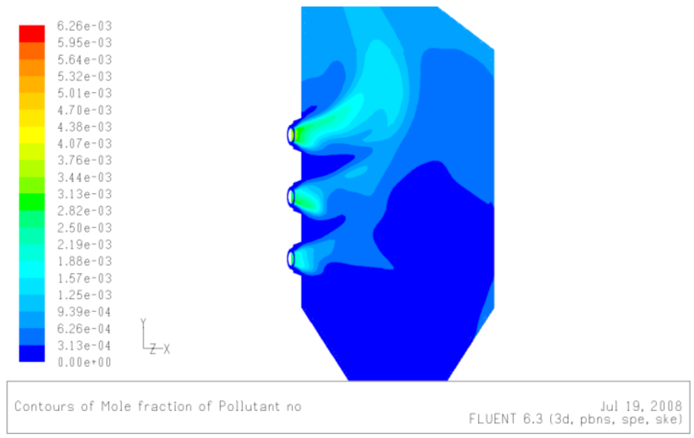

Figure 14 Conventional case - NO volume fraction distribution on the vertical plane passing though the burner axes

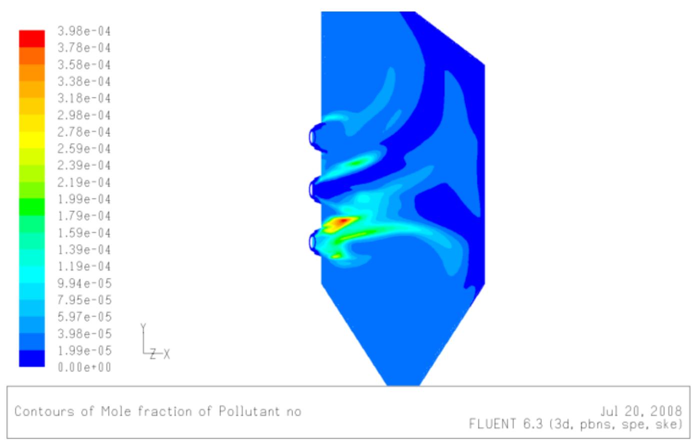

Figure 15 HiTAC case - NO volume fraction distribution on the vertical plane passing though the burner axes

CONCLUSIONS

The computer model results showed that the NOx emission levels are drastically lower when firing the boiler with methane as compared to firing it with heavy fuel oil. This result was to be expected as the Large Combustion Plant Directive [9] states two different limit values for the NOx emissions in large combustion plants, with that of gaseous fuels being lower than that of liquid fuels. The predicted result with methane as the fuel was 191 mg/Nm^3, which is much lower than the ceiling for gaseous fuels stated in the LCP directive, i.e. 300 mg/Nm^3. At the time, the DPS boiler did not, in actual fact, comply with this directive, since the measured NOx emission level was higher than the maximum level of 450 mg/Nm^3 allowed by the directive for liquid fuels. Hence it can be concluded that if the DPS boilers had to be converted to work on methane, the NOx emissions would be reduced to levels which comply with the Large Combustion Plant Directive.

When the boiler was simulated to work with HITAC technology and using methane as a fuel, the scaled NOx emission level was predicted to be equal to 93.8 mg/Nm^3 which is nearly half that predicted for the simulated ordinary combustion case (191 mg/Nm^3).

This work showed that it is possible to model high temperature air combustion with an off-the-shelf computational fluid dynamics software. The results from applying the model to the performance of one of Malta's power station boilers were quite interesting, although there still remains the issue of how to convert such a boiler to operate on gaseous fuels and HITAC technology.

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