47

JOURNAL OF THEORETICAL AND APPLIED

MECHANICS

No 1 1997

*Journal of Theoretical
and Applied Mechanics
Sofia, 1997, Year XXVII, No 1*

NUMERICAL MODELLING OF IN-FURNACE NO_x REDUCTION TECHNOLOGIES FOR PULVERISED COAL COMBUSTION

J. L. T. AZEVEDO, L. M. R. COELHO, M. G. CARVALHO

1. Introduction

The development and application of numerical models for large scale combustion equipment has been mainly developed within the 80's, while their use to the evaluation of combustion modifications for NO_x formation control became more common in the 90's. In addition to the NO_x emissions, the models allow the evaluation of the effect of combustion modifications on burnout and heat flux distribution which are important boiler performance characteristics. Review articles on the development of models for boiler furnaces [1] and specifically for coal fired boilers [2, 3] exist and therefore reference is given only to studies concerning the use of models to predict the reduction of NO_x emissions from pulverised coal fired boilers.

Fiveland and Latham [4] predicted NO emissions from a pilot scale and from a boiler furnace to analyse the influence of replacing standard cell burners by low NO_x cells using overfire air. The grid used for the three dimensional calculations, although limited by computational costs, represents well air staging at the burners. The model sensitivity to the operating conditions and the geometrical parameters is good when compared with the experimental results. Comparisons were performed with local experimental values of properties showing a reasonable agreement. Schnell and co-workers [5] presented results of numerical simulations to analyse the modification of a tangentially fired boiler from unstaged to air staged combustion using a tertiary air feed. The burners were considered in detail with 100 control volumes at the boiler wall for each burner. The inlet conditions were defined from a separate calculation with more refined grids including the burner throat. Predicted local concentrations of oxygen, temperature and NO close to the furnace exit are in good agreement with measured values.

Antifora et al [6] performed a numerical study comparing the combustion behaviour and NO formation for a front wall fired boiler using the upper row of burners out of service, without gas flow or with overfire air. The model only accounts for NO formation from volatiles and the influence of neglecting or considering mixture fraction fluctuations is analysed. The results show that the model tends to overpredict NO emissions although the predicted reduction in NO emissions is in agreement with the experimental results. Both these effects are larger when considering the fluctuations in the mixture fraction. At IST a numerical study was performed [7] comparing the use of both overfire air and the use of the lower row of burners out of service with the basic case of all burners in operation for a front wall fired boiler. The model was able to predict the reduction of NO emissions using burners out of service in both locations.

The present paper considers the use of rows of burners out of service for partial load and considers the evaluation of a retrofit configuration for reburning with natural gas for a front wall pulverised coal fired boiler. In the following section the numerical model used at IST is briefly described. Section 3 presents results of the model application and in the last section conclusions are given along with the identification of further model developments.

2. Description of the model

The numerical model is based on the solution of transport equations for main chemical species (O_2, CO_2, CO, H_2O and volatile species), enthalpy, the three gas momentum components and for the turbulent kinetic energy k and its dissipation rate ε. Pressure is calculated from the continuity equation using the Piso algorithm. The source term due to the heat transferred by radiation is calculated using the discrete heat transfer model considering scattering and a suitable package to evaluate the radiative properties of the gas-particle mixture [8]. The coal particles are described by a stochastic Lagrangian procedure to integrate the equation of motion and the energy balance, together with the consideration of physical models. The coal evolution is described in sequence by drying, pyrolisys and char combustion, considering the particle diameter constant with density variation. For volatile release a first order rate is used and the volatile yield has been assumed to be 1.35 the volatile matter from the proximate analysis. For char combustion a first order kinetic rate combined with a diffusion resistance is used.

The NO_x post-processor is based on De'Soete [9] mechanism considering the solution of balance equations involving NO and its precursors (HCN and NH_3). For the reburning study the model was extended according to Chen [10] including a different set of kinetic coefficients for the competitive reactions involving HCN for rich conditions together with the consideration of a reaction path for the reduction of NO by hydrocarbons. Hydrocarbon species for the reburning mechanism are considered from the natural gas and from volatile species where a fixed fraction was considered (20% in this study). Volatile nitrogen is assumed to produce 65% HCN and 35% NH_3 with each specie being submitted to the competitive reaction scheme proposed by De'Soete. The NO_x post-processor also considers the thermal Zeldovich mechanism [11] and the heterogeneous reduction of NO by char [7]. The char nitrogen products are considered as NO (25% weight of nitrogen) and molecular nitrogen. The fraction of NO formed from char nitrogen should be modelled with further detail as a function of local conditions following single particle model simulations [12]. In previous work [4, 5, 7] HCN was considered from char nitrogen which can be partially justified as mainly CO is produced during the char burnout process. This provides the definition of a competitive reaction path for HCN enabling the predicted NO to be more sensitive to operating conditions [7, 13].

3. Study of industrial applications

3.1. Cases tested and operating conditions

The numerical results given in this paper refer to two boiler studies. The first study is concerned with the use of rows of burners out of service and is used to show the model performance compared with global values measured at the boiler. The second application consists on a feasibility study to evaluate the use of reburning technology for an existing pulverised coal fired boiler.

The numerical study considering the use of rows of burners out of service was carried out for a boiler from the Pego power station (Portugal) which is equipped with 16 low NO_x burners located at the front wall arranged in four rows. The computational domain is defined for the combustion chamber of the boiler up to the arch level and the simulations were carried out using a grid comprising 29 × 23 × 74 control volumes to represent half of the boiler with symmetry conditions at the middle plane.

To implement reburning in an existing boiler, alternative design solutions and operating parameters have to be compared in order to optimise boiler performance. In the feasibility study presented here only a design solution is analysed to evaluate the effect on NO_x formation and on thermal performance. For the reburning configuration the existing burner arrangement was assumed and NH_3). For the reburning study the model was extended according to Chen [10] including a different set of kinetic coefficients for the competitive reactions involving HCN for rich conditions together with the consideration of a reaction path for the reduction of NO by hydrocarbons. Hydrocarbon species for the reburning mechanism are considered from the natural gas and from volatile species where a fixed fraction was considered (20% in this study). Volatile nitrogen is assumed to produce 65% HCN and 35% NH_3 with each specie being submitted to the competitive reaction scheme proposed by De'Soete. The NO_x post-processor also considers the thermal Zeldovich mechanism [11] and the heterogeneous reduction of NO by char [7]. The char nitrogen products are considered as NO (25% weight of nitrogen) and molecular nitrogen. The fraction of NO formed from char nitrogen should be modelled with further detail as a function of local conditions following single particle model simulations [12]. In previous work [4, 5, 7] HCN was considered from char nitrogen which can be partially justified as mainly CO is produced during the char burnout process. This provides the definition of a competitive reaction path for HCN enabling the predicted NO to be more sensitive to operating conditions [7, 13].

3. Study of industrial applications

3.1. Cases tested and operating conditions

The numerical results given in this paper refer to two boiler studies. The first study is concerned with the use of rows of burners out of service and is used to show the model performance compared with global values measured at the boiler. The second application consists on a feasibility study to evaluate the use of reburning technology for an existing pulverised coal fired boiler.

The numerical study considering the use of rows of burners out of service was carried out for a boiler from the Pego power station (Portugal) which is equipped with 16 low NO_x burners located at the front wall arranged in four rows. The computational domain is defined for the combustion chamber of the boiler up to the arch level and the simulations were carried out using a grid comprising $29 \times 23 \times 74$ control volumes to represent half of the boiler with symmetry conditions at the middle plane.

To implement reburning in an existing boiler, alternative design solutions and operating parameters have to be compared in order to optimise boiler performance. In the feasibility study presented here only a design solution is analysed to evaluate the effect on NO_x formation and on thermal performance. For the reburning configuration the existing burner arrangement was assumed

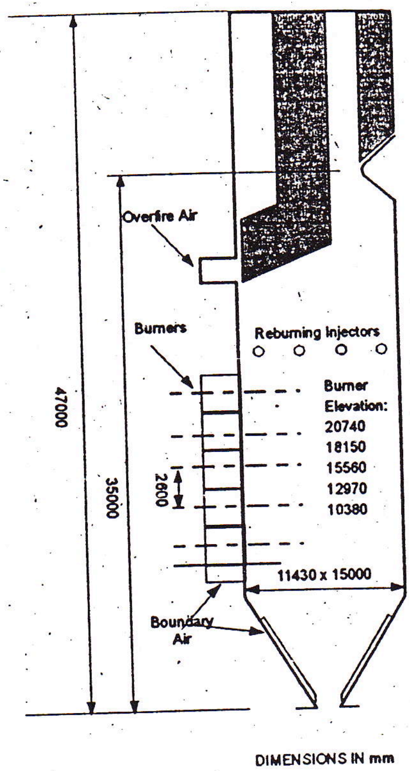

Fig. 1. Schematic representation of the Sines boiler for reburning configuration.

to be kept and additional inlet ports were defined for the boiler as schematically shown in Fig. 1. Four reburning injection ports have been considered at the side walls and six overfire air were considered in the front wall above the burners and close to the side wall. The calculations for the Sines boiler (Portugal) were performed considering as the furnace outlet a vertical plane above the boiler nose with a grid 28 × 37 × 116 for half the boiler with symmetry conditions.

Table 1 shows the main operating conditions for the cases reported in this paper (Pego and Sines boiler). For the Pego boiler partial load conditions are analysed using either the lower or upper row of burners out of service while other conditions for full load are available elsewhere [13]. For Sines the reburning configuration is compared with a base case where the upper (5^{th}) row of burners is out of service and used to feed staged air. Natural gas has been considered as the reburn fuel with a flow rate of 13.1 ton/h (80% CH_4 in weight) replacing 20% of the coal feed. To provide a better mixing it was assumed that natural gas is diluted with recirculated combustion products in order to provide a high inlet velocity (53m/s). The overfire air flow rate is 285 ton/h. All flow rates were defined to achieve approximately stoichiometric

Flow rates in ton/h	Pego Boiler – Partial Load		Sines boiler – Full load	
	Case L	Case U	Base Case	Reburning
Coal Flow	78.5	76.7	102.4	82.
ROOS	Lower (1st)	Upper (4th)	Upper (5th)	Upper (5th)
Secondary Air Flow	500.	496	545	396
Air Flow in ROOS	50.	49.	74.5	54.5
Primary Air Flow	173.	170.	289	217
Boundary Air Flow	80	80	155	155
Coal composition (As Received)	VM=25.6% FC=52.7% XC= 65.2% XS= 0.71%	ASH=13.6% H_2O=8.07% XH=3.48% XN=3.48%	VM=28.8% FC=51.0% XC=67.7% XS=0.94%	ASH=13.4% H_2O=6.77% XH=4.40% XN=1.54%

Table 1. Operating conditions of the test cases presented for the Pego and Sines boiler.

coefficients of 1.10, 0.9 and 1.20 respectively for the main combustion zone, reburning zone and final combustion zone. The location of the reburning and overfire air ports was chosen for this first configuration in order to achieve estimated residence times of 0.6 s and 0.8 s between the three zones considered.

3.2. Use of rows of burners out of service

The calculated velocity flow field, temperature and NO_x concentration in a plane across the burners are shown in Fig. 2 for the Pego boiler for both cases considered (L and U). The air velocity from the burners out of service are small compared with velocity close to the main burners as the inlet value is about half and the gas expansion due to temperature rise is slower. The flow is highly tri-dimensional but the figure allows the identification of a large recirculation in the ash pit zone which promotes upward flow close to the front wall. This can be seen from the oxygen distribution for case L where the flow from the lower burners is entrained. As a result of the swirl action part of this flow is deviated towards the lateral walls and oxygen from the underfire air is transported and mixed in the upper levels, promoting therefore air staging. Close to the back wall opposed to the burners, a low velocity region can be identified between the burner levels leading to low levels of oxygen concentration in that region as can be seen in Fig. 2. The deflection of the burner jets at the back wall, produces zones where char combustion is intense justifying the low levels of oxygen close to the back wall above and below the burner levels.

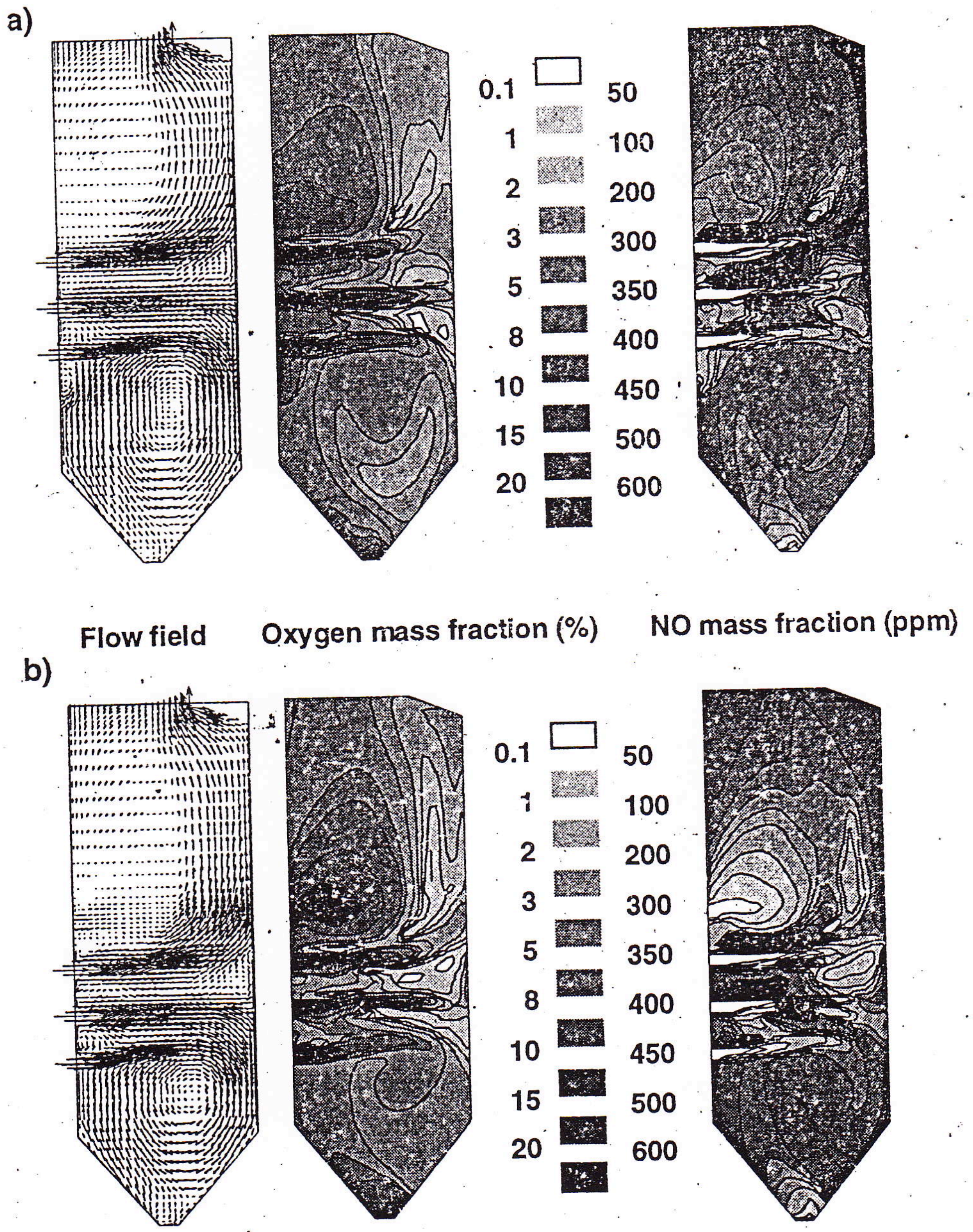

Fig. 2. Calculated flow field, oxigen and NO mass fraction for the partial load cases considered. a) Low row of burners and b) upper row of burners out of service

	Case L	Case U
Measured carbon in ash (%)	9.1	6.3
Calculated carbon ash (%)	3.0	1.1
Measured NO (ppm)	369	348
Calculated NO (ppm)	574.3	536.2

Table 2. Calculated and measured fraction of carbon in ash and NO concentration in the flue gases.

The calculated carbon in ash and NO_x emission are compared with experimental values in table 2. The unburned carbon in ash is underpredicted but the effect of modifying the burner row patterns is predicted by the model with larger values for the case of the lower row of burners out of service (case L) compared with the case of using overfire air (case U). The calculation of burnout is important to determine a correct oxygen distribution heat release in the boiler for the NO_x calculations. Burnout depends mainly on the kinetics for char combustion which were assumed and on the larger particles trajectories influenced by wall impacts.

The NO formation was considered using De'Soete [9] mechanism for the gas phase without considering Chen extension [10]. The predicted values of NO are overestimated compared with the experimental data available at the boiler outlet as found by others [6]. These differences are attributed to the limited grid resolution close to the burners when using a single grid system for the whole furnace. Improvements may only be performed with the use the decomposition of the furnace in domains with independent grids. The comparison of the calculated emissions shows lower values when the upper row of burners is used for overfire air (case U) compared with the other case in accordance with the experimental values and for other boiler studies [7, 13]. The use of the lower row of burners out of service also promotes air staging compared with the use of all burners in operation [13] but assuming a fixed amount of NO production from char the results are less sensitive than considering HCN formation from char nitrogen [7, 13].

3.3. Use of reburning with natural gas

For Sines the application of the reburning technology was addressed comparing the boiler performance for a base case and for the case of using natural gas as a reburning fuel.

Fig. 3 shows the flow field in a plane across the inner burners. From this figure it can be seen that the flow is not modified significatively in the burner

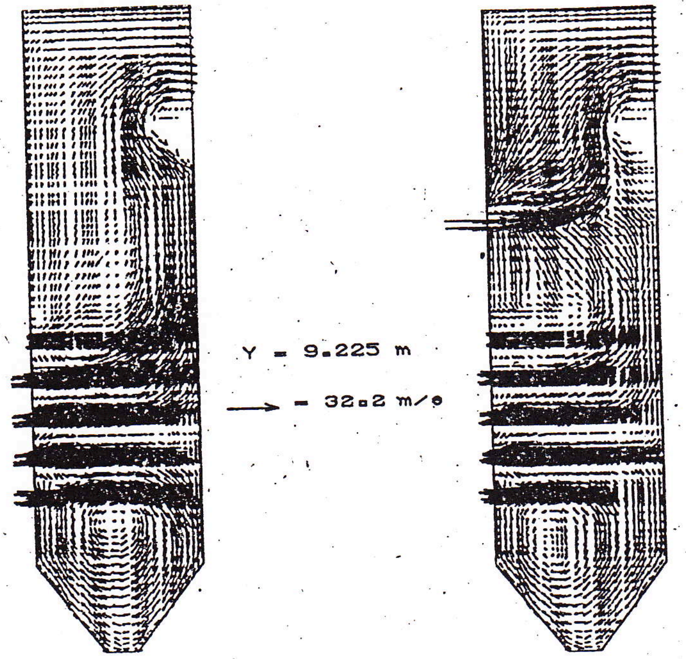

Fig. 3. Calculated flow field for the Sines boilet for the normal and reburning configuration in a plane crossing the inner burners.

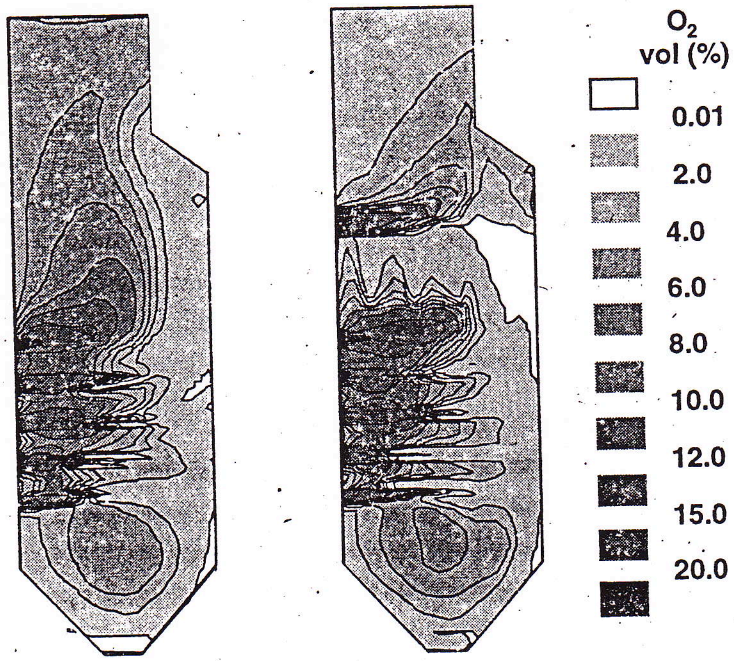

Fig. 4. Oxigen concentration distribution for the normal and reburning configuration.

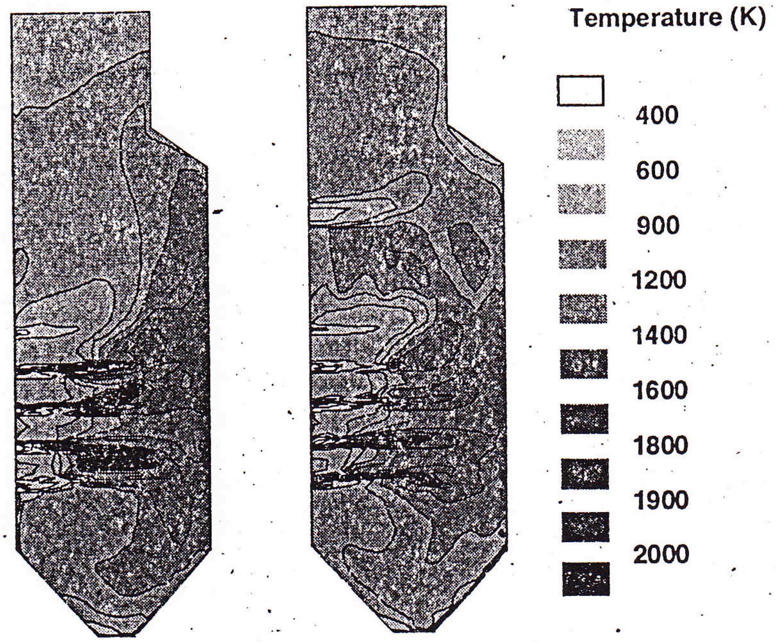

Fig. 5. Temperature distribution for the normal and reburning configuration.

zone. The upward flow above the burners has larger velocities in the inner burner plane due to the influence of the reburning injectors. Fig. 4 shows the oxygen contour profiles at vertical planes crossing the burners for the base and reburn configuration. The figure shows slightly higher oxygen consumption in the main combustion zone until the reburning injectors level where oxygen decreases quite substantially due to the natural gas combustion. This effect is stronger close to the back wall once it is the region where coal concentration is larger (as it is for the base case). The oxygen concentration at the outlet plane (not shown) has larger values close to the boiler centre for the base case while for the reburning case the higher values are close to the side wall as a result of the combustion being displaced to the centre of the boiler. The average oxygen concentration at the outlet is equivalent (3.9% for the normal case and 3.3% for reburning).

The temperature distribution shown in Fig. 5 is more uniform for the reburning case due to the natural gas feed across the furnace and the lower coal flow rate leading to a more uniform heat release in the furnace. The heat fluxes at the lateral wall decrease as the flow is directed towards the centre of the boiler. The larger spreading of combustion due to the natural gas feed decreases the heat flux at the back wall increasing the contribution at the upper part of the front wall. The total heat flux to the boiler walls decreased from 201.4 to 183.2 MW as a result of the displacement of the combustion zone

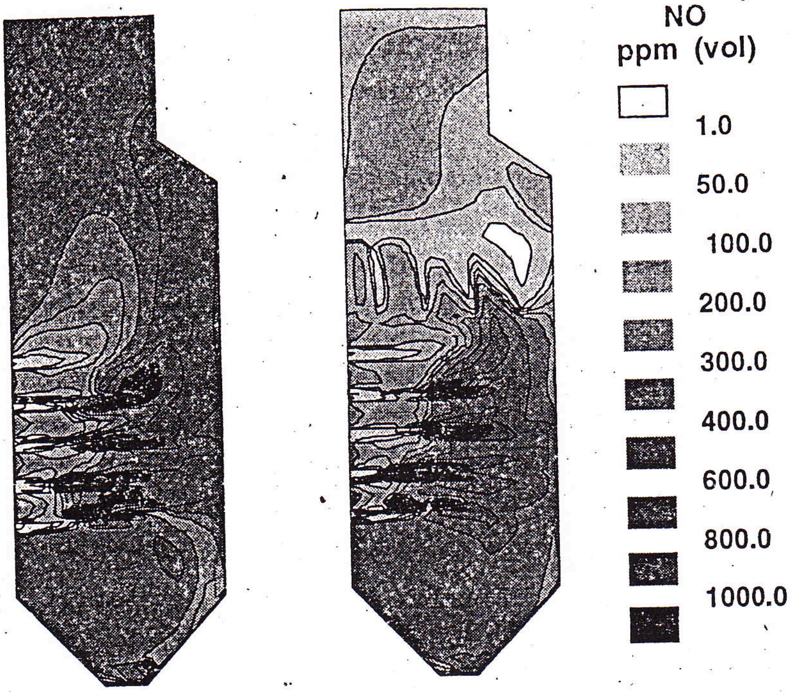

Fig. 6. NO concentration distribution for the normal and reburning configuration.

increasing heat transfer to the pannels from 43.2 to 71.2 MW. This information is important for boiler redesign and to optimise the operating conditions.

Fig. 6 shows the NO concentration distribution in a plane across the burners. The calculated results in the main combustion zone are similar with higher values of NO due to the higher oxygen and temperature for the base case where NO is formed close to the burners and close to the boiler nose due to char nitrogen. For the reburning case NO is destroyed by hydrocarbons from natural gas forming HCN with a larger peak concentration close to the boiler nose. This HCN is oxidised faster close to the front wall by the overfire air forming NO while close to the back wall this process is slower. The reaction mechanism considered [10] assumes a reduction of the HCN–NO reaction rate in reducing conditions and the production of HCN from the reburning step becomes important in both the base and reburning case. As a result the model predicts HCN concentrations at the boiler outlet with an average value of 96 ppm for the base case and 241 ppm for the reburning configuration. The calculated NO concentration at the boiler outlet is 135 ppm for the reburning case compared with 595 ppm for the base case. Considering the total nitrogen species (HCN and NO) at the outlet as a measure of NO_x emission and taking into account that the coal feed rate is reduced by 20% the nitrogen emission normalised by the coal flow rate is reduced by 28% for the reburning case.

4. Conclusions

Simulations were carried out for two front wall fired boiler concerning the use of two techniques to reduce NO_x emissions.

In the first study the use of rows of burners out of service is analysed using the numerical model and the results are compared with experimental findings. For partial load the use of the upper row of burners with overfire air shows and confirms the potential for NO reduction only through modification of the operating conditions for an existing boiler.

The second study considers the use of reburning by natural gas. The calculated results allow to identify the effect of the boiler retrofitting on the NO emissions and on heat transfer which increases in the upper furnace region. The present paper shows the potential of the use of the numerical model for the optimisation of the operating conditions in the design phase of a boiler furnace retrofitting.

The model for NO formation extended for reburning conditions needs to be validated in particular on its use for rich conditions and on the formation of HCN. The contribution of char nitrogen also needs to be considered in more detail. The combustion calculation should also be extended to consider the chemical composition of volatile. Benefits from an improved NO_x formation model can be better evaluated using domain decomposition for industrial scale equipment to improve the simulation close to the burners.

Acknowledgements

The scholarship BD/3538/94 given by PRAXIS XXI to support the work from Eng. L. Coelho and the support of the EC through the project JOULE2, contract 0380 are acknowledged.

REFERENCES

[1] Coelho, P. J. The Mathematical Modelling of Utility Boilers. Part I: The Past, the Present and the Future, 3rd. European Conference on Industrial Boilers and Furnaces, Lisboa, 1995.

[2] Brewster, B. S., S. C. Hill, Radulovic, L. D. Smoot. In: Fundamentals of Coal Combustion for Clean and Efficient Use, Elsevier, 1993.

[3] Smoot, L. D. Modeling of Coal Combustion Processes. *Prog. Energy Combust. Sci.*, **10** (1984), 229-272.

[4] Fiveland, W. A., C. E. Latham. Use of Numerical Modeling in the Design of a Low-NO_x Burner for Utility Boilers. *Combust. Sci. and Techn.*, **93** (1993), 53-72.

[5] EPPLE, B., R. SCHNEIDER, U. SCHNELL, K. R. G. HEIN. Computerised Analysis of Low-NO_x Coal Fired Utility Boilers, 2nd Int. Conf. Combustion Technologies for a Clean Environment, Lisboa, 1993.

[6] ANTIFORA, A. M. SALA, L. VIGNENANO. NO_x Emissions from a Large Scale Coal-Fired Furnace, 2nd Int. Conf. Combustion Technologies for a Clean Environment, Lisboa, 1993.

[7] COIMBRA, C. F. M., J. L. T. AZEVEDO, M. G. CARVALHO. 3-D Numerical Model for Predicting NO_x Emissions from a Pulverised Coal Industrial Boiler. *Fuel*, **73** (1994), 1128-1134.

[8] DINHO, P., J. L. T. AZEVEDO, L. R. COELHO, M. G. CARVALHO. Modelling Radiation in Pulverised Coal Combustion, Eurotherm Seminar: Heat Transfer in Radiating and Combusting System, No **37**, Sallugia, 1994.

[9] DE SOETE, G. G. Overall Reaction Rates of NO and N_2 Formation from Fuel Nitrogen, 15th Int. Symp. on Combustion, The Combustion Institute, 1975, 1093-1102.

[10] CHEN, W. A Global Reaction Rate for Nitric Oxide Reburning, PhD thesis, Bringham Young University, 1994.

[11] CARVALHO, M. G., V. SEMIO, F. C. LOCKWOOD, C. PAPADOPOULOS. Predictions of Nitric Oxide Emissions from an Industrial Glass-melting Furnace. *J. Inst. of Energy*, **3** (1990), 39-47.

[12] VISONA, S. P., B. R. STANMORE. Modeling NO_x Release from a Single Coal Particle II. Formation of NO from Char-nitrogen. *Combustion and Flame*, **106** (1996), 207-218.

[13] COELHO, L. R., J. L. T. AZEVEDO, M. G. CARVALHO. Numerical Simulation and Comparison of NO_x Emissions from a Low NO_x Front Wall Fired Boiler for Different Operating Conditions, 3rd Int. Symp. on Coal Combustion, Beijing, 1995.