A SIMPLIFIED NON-LINEAR MODEL OF NOx EMISSIONS IN A POWER STATION BOILER

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ABSTRACT

When considering NO_X development in power stations, experiments show that its formation is slower than the combustion process. Therefore in this paper the modelling of NO_X emissions is decoupled from the combustion process. A NO_X model for Kilroot Power Station in Northern Ireland is then derived from the extended Zeldovich mechanism. The physical parameters in the model are determined from experiments. The comparison of the simulated values with the real measurements is also presented.

INTRODUCTION

The fuel crisis in 1970s led to the study of boiler modelling and control aiming to utilise fossil fuel effectively. Recently atmospheric pollution become a global concern. For this reason, the environmental impact of power plant emissions attracts increasing attention. Nitrogen oxides (NO_X) is one of the principal pollutants emitted from power plant. It contributes to photochemical smog, damages the ozone layer, and causes acid rain. Current legislation [UK Environment Protection Act (1992) and the US Clean Air Act Amendment (1990)] requires that power plants make significant reductions in pollutant emissions; especially NO_X [1]. NO_X can be reduced by operational modifications or by installing new equipment.

The thrust of this paper is the development of a simple NO_X, or more accurately a NO model, which can be used for boiler control and optimisation.

The options when considering new equipment include Low NO_X Burners (LNB), Natural Gas Reburning (NGR), Selective Catalytic Reduction (SCR), and Selective Non-catalytic Reduction (SNCR). Among them LNB is commonly used by power stations since it is relatively cheap and easy to install. However low NO_X burners can cause incomplete combustion, alter steam temperatures and reduce boiler performance [2].

Operational modifications can also reduce NO_X production. In this respect fuel/air ratio and secondary air distribution are the significant factors influencing NO_X emissions. From observation of operational procedures at Kilroot Power Station, it is evident that some operators can successfully reduce NO_X emissions by altering the secondary air entering the furnace region. However, since the physical, thermodynamic, and chemical processes occurring within a fossil fuelled boiler are complex, how the operational parameters affect NO_X emissions are still unclear.

Boiler models are useful to predict the influence of equipment design and operational changes. The models used for design are often those based on one or three-dimensional computational fluid dynamics (CFD). CFD models are founded on fundamental physical principles and can thus predict fluid flow and heat transfer properties within boilers under specified operational conditions. Submodels such as combustion, turbulence, and NO_X formation can be added as subroutines [3]. These models are still under development and since these models are complex and expensive to develop, they are not suitable for control system design.

For an operating power plant, the models describing the relationships between NO_X emissions and operational parameters is important. Operational relationships may be obtained from simple lumped parameter input-output models. These models can be derived analytically from basic principles and/or empirically from tests. Åström and Eklund [4] and, Åström and Bell [5] working from first principles derived simplified dynamic steam and water side models for a drum boiler. These models can be used to guide power plant operations or in simulation and control system design. Basic combustion models [6,7] have been used for laboratory furnace simulation and control system design. However NO_X formation is not included in any of these models. This paper attempts to address this omission.

KILROOT BOILER AND FUEL ANALYSIS

NIGEN-Kilroot Power Station, Northern Ireland, is a cyclic power plant with two generating units. Each unit has a dual fired (oil or coal) drum boiler and produces full load 300 MWe with oil firing or 200 MWe with coal firing. The boiler was designed to supply its turbine with steam at a temperature of 540°C and up to a pressure of 162 bar. There is one burner box on each corner. Each burner box contains nine separate sections of which four are oil burners, four are pulverised fuel burners and one is an auxiliary secondary air nozzle. All of the sections tilt in unison through ±25°, relative to the horizontal.

The research work was based on boiler unit 1 with oil firing. The composition of the fuel oil is listed in TABLE 1.

TABLE 1 - Fuel oil analysis results (%weight).

C	H	O	N	S	Ash
87.4	9.5	0	0	3.0	0.1

MODELLING OF NO_X EMISSIONS

NO_X emissions from practical combustion devices comprise NO, NO_2, and N_2O. The emissions of these species are governed by both formation and removal rates. Since the major portion of NO_X has been found to be NO [8, 9], the modelling of NO_X emissions in this paper solely considers NO formation.

The three principal sources of nitrogen oxide emissions in combustion are: oxidation of atmospheric nitrogen, often termed the *thermal NO* formation mechanism; *prompt NO* formation, and oxidation of nitrogen-containing compounds in the fuel, termed the *fuel NO* mechanism [10]. The relative importance of these three NO emissions from a particular combustion device depends on operating conditions and on fuel composition.

Prompt NO is usually formed in a fuel rich combustion environment. Since excess air is always provided in the boiler to ensure complete combustion, the contribution of prompt NO to total nitrogen oxide emissions is negligible. However, for boilers with low NO_X burners (Kilroot boiler does not have any low NO_X burners), the relative importance of prompt NO to nitrogen oxide emissions may increase due to combustion staging. Fuel NO is formed from the oxidation of the nitrogen compounds in fuel. Since there is no nitrogen contained in the fuel oil (see TABLE 1), this NO can also be neglected. Therefore the thermal NO is the principal source of nitrogen oxide emissions at Kilroot.

The formation of thermal NO is determined by a set of chemical reactions known as extended Zeldovich mechanism [11]. The principal reactions are:

$$O + N_2 \Leftrightarrow NO + N \tag{1}$$
$$N + O_2 \Leftrightarrow NO + O \tag{2}$$
$$N + OH \Leftrightarrow NO + H \tag{3}$$

The rate coefficients for the forward reactions (1)-(3) are K_1, K_2, K_3, and for the corresponding backward reactions are K_{-1}, K_{-2}, K_{-3}. Invoking the steady-state approximation for the N-atom concentration, that is $d(N)/dt \cong 0$, and assuming the partial equilibrium for the reaction

$$H + O_2 \Leftrightarrow OH + O \tag{4}$$

the NO formation rate may be expressed [10]

$$\frac{d(NO)}{dt} = 2K_1(N_2)(O) \frac{1-(NO)^2/K(O_2)(N_2)}{1+K_{-1}(NO)/[K_2(O_2)+K_3(OH)]} \tag{5}$$

where $K = (K_1K_2)/(K_{-1}K_{-2})$, ( ) denotes volume concentration.

Within the boiler furnace, since the formed NO is immediately taken away from the high temperature region by flue gas, it is reasonable to assume that (NO) << $(NO)_{equilibrium}$. Therefore the NO formation rate in the furnace can be expressed as

$$\frac{d(NO)}{dt} = 2K_1(N_2)(O) \tag{6}$$

In this equation, the (O) can be related to the (O_2) from the assumed equilibrium condition of reaction [8]

$$0.5O_2 \Leftrightarrow O \tag{7}$$
$$K_o = (O)/(O_2)^{1/2}$$

and Equation (6) becomes

$$\frac{d(NO)}{dt} = 2K_1K_o(N_2)(O_2)^{1/2} \tag{8}$$

Since (O_2) is the oxygen concentration after combustion, it can be calculated from the combustion equations

$$C + O_2 = CO_2 \tag{9}$$
$$S + O_2 = SO_2 \tag{10}$$
$$2H_2 + O_2 = 2H_2O \tag{11}$$

Noting that the volume of 1 mol ideal gas is 22.4×10^{-3} m^3, the oxygen consumed in the combustion, or the theoretical oxygen volume flow, is

$$\dot{V}_{f.O_2} = (1.87C + 0.70S + 5.6H)W_f = \beta W_f \tag{12}$$

where C, S, H are respectively the carbon, sulphur, hydrogen percentage in weight in fuel; W_f is the fuel mass flow.

Further, the stoichiometric air mass flow can be derived

$$W_{a.st} = \frac{\dot{V}_{f.O_2}}{0.21 v_a} = \frac{\beta W_f}{0.21 v_a} \tag{13}$$

where v_a is the specific volume of air.

When the gas volume flow $\dot{V}_g$ is approximated by $v_a W_a$, where W_a is air mass flow, the oxygen concentration after combustion can be expressed as

$$(O_2) = \frac{0.21\dot{V}_a - \dot{V}_{f.O_2}}{\dot{V}_g} \cong \frac{0.21 v_a W_a - \beta W_f}{v_a W_a} \tag{14}$$

Finally from Equation (13), the oxygen concentration becomes

$$(O_2) = \frac{\beta}{v_a}\left(\frac{W_f}{W_{a.st}} - \frac{W_f}{W_a}\right) = \frac{\beta}{v_a}(\lambda_{st} - \lambda) \tag{15}$$

where λ is the fuel to air ratio and λ_{st} is the stoichiometric fuel to air ratio.

In Equation (8), the (N_2) can reasonably be seen as constant due to the existence of large amounts of N_2 in the flue gas. Therefore Equation (8) can be written as

$$\begin{aligned}\frac{d(NO)}{dt} &= 2K_1 K_O (N_2)(\beta / v_a)^{1/2}(\lambda_{st} - \lambda)^{1/2} \\ &= \alpha(\lambda_{st} - \lambda)^{1/2}\end{aligned} \tag{16}$$

The reaction coefficient α determines the reaction rate. For evenly distributed gas mixture, it is a function of temperature alone; the higher the temperature, the faster the formation rate [12]. However, in the furnace region, the contacting between air and fuel is not evenly distributed, and this will inevitably affects the total NO formation rate. Thus the coefficient α should be regarded as a function of temperature and distribution.

Suppose all the secondary air damper positions are fixed during operation, the average temperature and distribution factor can be associated with fuel flow W_f and burner tilt position ξ. When fuel flow increases, the gas flow becomes more turbulent and hence improves the mixing process. Additionally, the temperature is raised due to the extra released heat. When burner tilt goes up, the heat transfer area is reduced, and hence the temperature in the reaction region goes up. In Kilroot boiler, the burner tilt position is measured in percentage. It can be adjusted from 10% (the lowest position) to 100% (the highest position). The middle position is therefore 55%.

Assuming that

$$\alpha = f(W_f, \xi) = \alpha_0 W_f^r \left(1 + \alpha_1 \frac{\xi - 55}{90}\right) \tag{17}$$

Equation (16) becomes

$$\frac{d(NO)}{dt} = \alpha_0 W_f^r \left(1 + \alpha_1 \frac{\xi - 55}{90}\right)(\lambda_{st} - \lambda)^{1/2} \tag{18}$$

This equation implies that the NO formation rate is zero when fuel flow is zero or the fuel/air ratio equals to the stoichiometric value, and this is in agreement with the NO formation mechanism.

EXPERIMENTS

The experiments were made on the boiler unit 1 at Kilroot Power Station in January 1995. Three tests were conducted for the purpose of determining the parameters in Equation (18).

Test A

The purpose of this test was to verify the relationships between NO concentration and $(\lambda_{st}-\lambda)$. During the test, the load was 240 MW, the fuel flow was about 16 Kg/s, and the burner tilt position was kept at 55%. The input fuel/air ratio was changed by altering the air flow. All required data was received from the Data Acquisition System and logged on a PC. The sampling rate was 1 minute and the duration of the test was 280 minutes.

Figure 1 shows the response of NO concentration to changes in λ. It can be seen that the NO concentration responds inversely to the changes in fuel/air ratio, which is in good qualitative agreement with Equation (18).

Test B

This test was mainly used to estimate parameter r. During the test, the load was changed, hence the fuel flow, the burner tilt position was kept constant at 75%, and there is also variations in the fuel/air ratio. The duration of the test was 170 minutes. Figure 2 shows the response of (NO) to changes in fuel flow and λ.

Test C

Parameters α_0 and α_1 can be estimated using this test. During the test, the fuel flow was constant, the burner tilt position was changed. There was also variations in fuel/air ratio. The duration of the test was 300 minutes. Figure 3 shows the response of (NO) to changes in burner tilt position and λ.

Parameter estimation
Using data from test A, the equation

$$(NO) = 3610(\lambda_{st} - \lambda)^{1/2} \tag{19}$$

is obtained. The measured data and the corresponding curve computed from Equation (19) are shown in Figure 4. A good agreement between them can be seen, which again indicates that the approximation made for Equation (14) is acceptable. The coefficient $\alpha_0(16)^r$ is determined from this test as 3610.

Figure 5 shows the result from test B. It can be seen that

$$y = 1982(W_f)^{0.25} \tag{20}$$

where $y = (NO)/(\lambda_{st} - \lambda)^{0.5}$

From Equation (20), the parameters can be written
$\alpha_0\,(1+\alpha_1 20/90) = 1982;\ r = 0.25$
and substituting the two parameters back into Equation (19) produces
$\alpha_0 = 1805;\ \alpha_1 = 0.441$
From test C, the relations between (NO) and burner tilt position ξ is determined. Curve fitting gives

$$y = 1806 + 791x \tag{21}$$

where
$y = (NO)/[W_f^{0.25}(\lambda_{st} - \lambda)^{0.5}]$
$x = (\xi - 55)/90$

Therefore the parameters α_0 and α_1 are found to be 1806 and 0.438 respectively which are very close to the values obtained from test A and B. The result is shown in Figure 6. It can be seen that these parameters give a good fit to the test data.

Summary
By considering the three tests, the corresponding parameters α_0, α_1 and r are chosen as 1806, 0.438, and 0.25 respectively. If the NO component in the flue gas is expressed as Y_{NO}, the global volume balance gives

$$\frac{dY_{NO}(t)}{dt} = 1806W_f^{0.25}(t)[1 + 0.438\frac{\xi(t) - 55}{90}] * [\lambda_{st} - \lambda(t)]^{1/2} - Y_{NO}(t) \tag{22}$$

SIMULATION

In the simulation, Equation (22) is solved using the input variables fuel flow, W_f, air flow, W_a, and burner tilt position, ξ. The output from the differential equation produces the concentration of NO in the flue gas. The specific parameters needed for the Kilroot boiler were calculated from boiler geometry and fuel analysis as

$V = 1958\ m^3$, $\lambda_{st} = 1/13.36$

There is a measurement time delay, that is

$$Y_{measured}(t) = Y_{simulated}(t - \Delta t)$$

In order to compare the responses from the model with measurements from the real plant, new data was collected. The input variables taken from the real plant are given in Figure 7. The computed model response compared to the measured one are given in Figure 8. A good correlation between measured and simulated values can be observed from the figure.

CONCLUSIONS

This paper has presented a model of NO emissions for a power plant boiler. It is modelled from the extended Zeldovich mechanism and require only a few physical parameters obtained from experiments. A set of new test data is used to compare the simulated values with real measurements. It is shown that good results are obtained from the model with real plant input variables. The model can also be used in other applications such as for optimising boiler operation and combustion control system design.

ACKNOWLEDGEMENT

The authors acknowledge the support provided by NIGEN-Kilroot Power Station and the permission to use their facilities.

REFERENCES

1. Holmes, R. and Mayes, I.W., 1994, "Progress report on the development of a generic NO_X control intelligent system (GNOCIS)", Coal R&D Program, Project Profile 103, ETSU, U.K.

2. Ruiz, P.F., 1993, "Clean coal technologies: future in the European Community energy scene", Energy World, 12, 1-8.

3. Nelson, R.K., Franklin, J.D. and Scherer, B.E., 1994, "Prediction of NO_X generation in coal fired boilers", Power-Gen Americas '94.

4. Åström, K.J. and Eklund, K., 1972, "A simplified non-linear model of a drum boiler-turbine unit", Int. J. Control, 16, 145-169.

5. Åström, K.J. and Bell, R.D., 1988, "Simple drum-boiler models", IFAC Power Systems Modelling and Control Applications, 123-127.

6. Dfannstiel, D., 1991, "Modelling and simulation of an industrial combustion process", Nonlinear Engineering Computations, 665-674.

7. Cretnik, J., Strmonik, S. and Zupancic, B., 1985, "A model for combustion of fuel in the boiler", Proc. of 3rd Symposium Simulations Technik, 469-473.

8. Glassman, I., 1987, "Combustion", Academic Press Inc., USA, 319-345.

9. British Electricity International, 1991, "Modern Power Station Practice", Pergamon Press, London, B, 26-28.

10. Bartok, W. and Sarofim, A.F., 1991, "Fossil Fuel Combustion: A Source Book ", A Wiley-Interscience Publication, 215-256.

11. Drake, M.C., Correa, S.M., Pitz, R.W., Shyy, W. and Fenimore, C.P., 1987, " Superequilibrium and Thermal Nitric Oxide Formation in Turbulent Diffusion Flames", Combustion and Flame, 69, 347-365.

12. Gardiner, W.C., 1984, "Combustion Chemistry", Springer-Verlag New York Inc., 361-418.

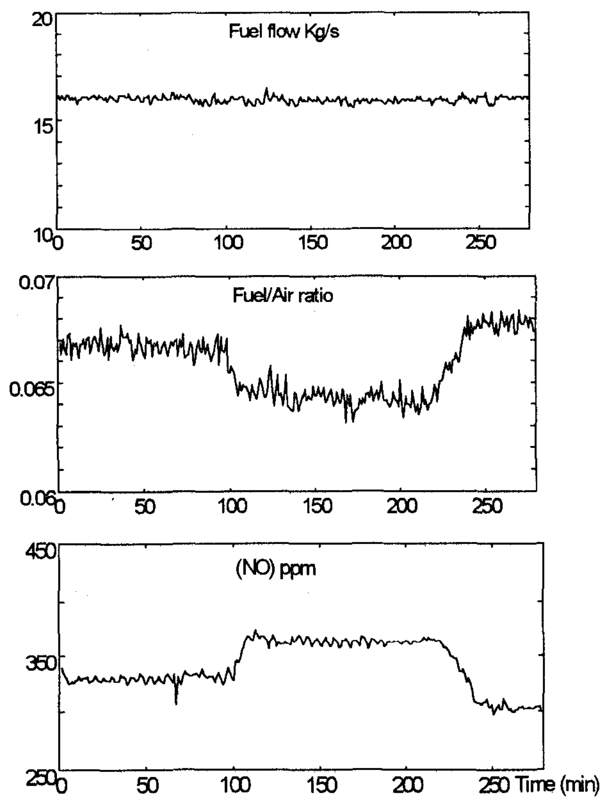

Figure 1: Test A showing response of (NO) to changes in fuel/air ratio.

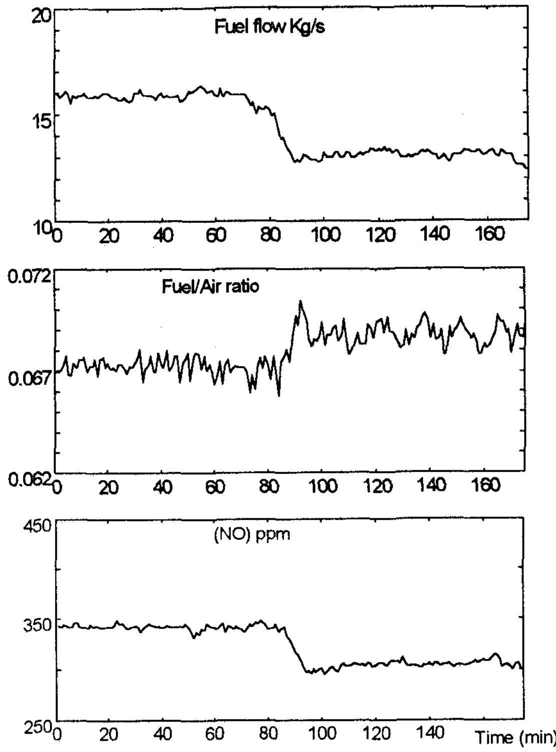

Figure 2: Test B showing response of (NO) to changes in fuel flow, fuel/air ratio.

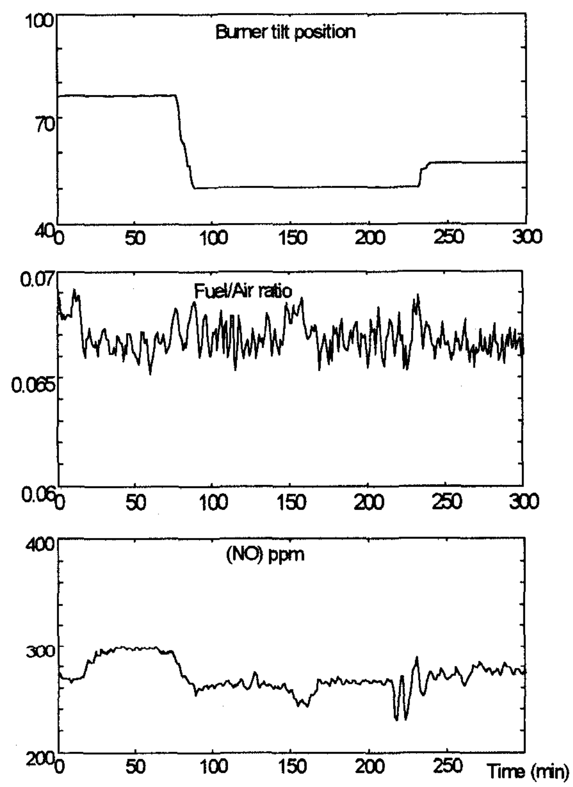

Figure 3: Test C showing response of (NO) to changes in burner tilt, fuel/air ratio.

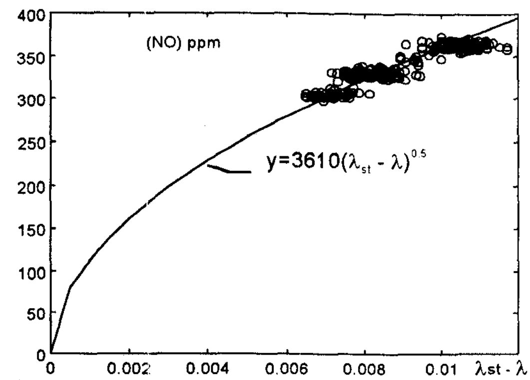

Figure 4: Results from test A, 'o' is test data, solid line is computed from Eq.(19).

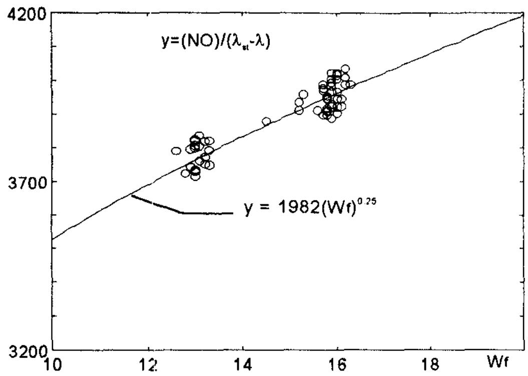

Figure 5: Result from test B, 'o' is test data, solid line is computed from Eq.(20).

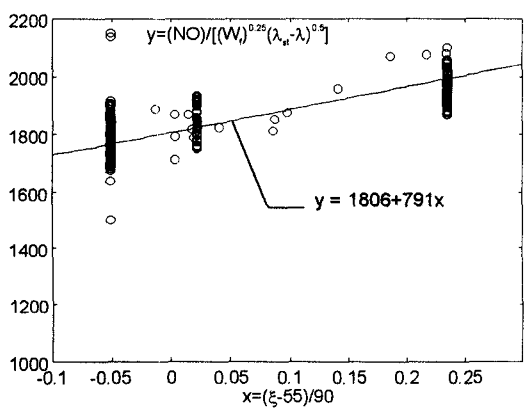

Figure 6: Result from test C, 'o' is test data, solid line is computed from Eq.(21).

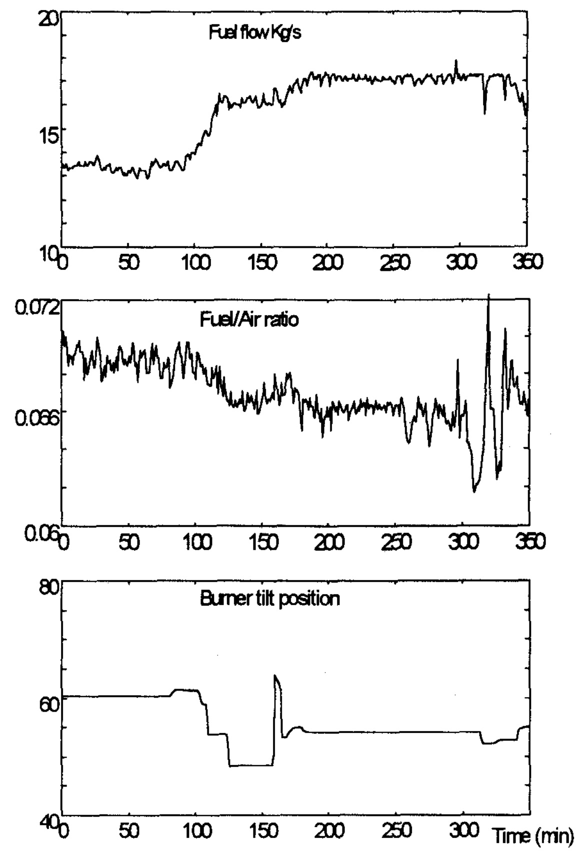

Figure 7: The model input variables (taken from plant).

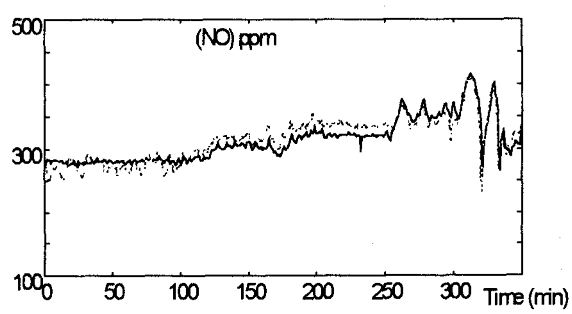

Figure 8: Comparison of plant measurements (solid) with model response (dashed).