

Co-firing Coal: Feedlot and Litter Biomass Fuels

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Abstract

Reburn with animal waste yield NO_x reduction of the order of 70-80 %, which is much higher than those previously reported in the literature for natural gas, coal and agricultural biomass as reburn fuels. Further, the NO_x reduction is almost independent of stoichiometry from stoichiometric to upto 10 % deficient air in reburn zone. As a first step towards understanding the reburn process in a boiler burner, a simplified zero-dimensional model has been developed for estimating the NO_x reduction in the reburn process using simulated animal waste based biomass volatiles. However the first model does not include the gradual heat up of reburn fuel particle, pyrolysis and char combustion. Hence there is a need for more rigorous treatment of the model with animal waste as reburn fuel. To address this issue, an improved zero-dimensional model is being developed which can handle any solid reburn fuel, along with more detailed heterogeneous char reactions and homogeneous global reactions. The model on “ NO_x Reduction for Reburn Process using Feedlot Biomass,” incorporates; a) mixing between reburn fuel and main-burner gases, b) gradual heat-up of reburn fuel accompanied by pyrolysis, oxidation of volatiles and char oxidation, c) fuel-bound nitrogen (FBN) pyrolysis, and FBN including both forward and backward reactions, d) prediction of NO_x as a function of time in the reburn zone, and e) gas phase and solid phase temperature as a function of time. The fuel bound nitrogen is assumed to be released to the gas phase by two processes, a) FBN evolution to N_2 , HCN, and NH_3 , and b) FBN oxidation to NO at the char surface. The formulation has been completed, code has been developed, and preliminary runs have been made to test the code. Note that, the current model does not incorporate the overfire air. The results of the simulation will be compared with the experimental results. During this quarter, three journal and four conference publications dealing with utilization of animal waste as fuel have been published. In addition a presentation was made to a utility company interested in the new reburn technology for NO_x reduction.

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1. INTRODUCTION

Biomass is a general term describing a variety of waste products such as wood waste material (saw dust, wood chips, etc), crop residues, and animal wastes. In general, any solid fuel other than fossil derived coal, oil or natural gas is considered a biomass fuel. The overall objective of the program is to develop a database on cofiring of coal and biomass fuels, which primarily include the feedlot biomass, and litter biomass fuels.

What is the rationale behind the co-firing of coal: feedlot and litter biomass fuels? Since 1978, the average number of animal units has increased, and hence animal waste generation has increased by 56% (for cattle) and 176% (for layer). Large concentrated animal feeding operations (CAFO) have expanded all over the country including Texas. The Texas Panhandle region covering adjacent users of Oklahoma and New Mexico is the largest cattle feeding region in the nation, producing about 7.2 million fed cattle annually (which is almost 32% of the fed cattle produced and slaughtered in the U.S.), and contributing approximately \$14 billion per year to the regional economy. The cattle feeding industry in the Texas Panhandle area is growing at the rate of approximately 100,000 head of feedlot capacity per year. Each animal fed leaves approximately one ton of collectable manure (or 2 lb per cattle per day) containing 35% moisture and 65% solids (combustibles + ash). Broiler producers under contract from Poultry integrators raise these birds for slaughter in broiler houses that may occupy 10,000 to 30,000 birds per house. Sanderson Farms process more than 50 million broiler/ year (broiler life 41 days, 1.25 tons per 1000 birds processed). They kill approximately a million chicken per week. Most of their broiler houses are located within a 70-mile radius of their feed mill in Franklin and Robertson County, Texas. In the USA alone approximately 8 billion heads are produced for slaughter annually. With an average litter production of 0.20 lb per day per bird, poultry waste production is estimated to be approximately 15 million tons per year, out of which almost 600,000 tons is generated in Texas (1998). Totally about 110 million tons of cattle manure (Feedlot Biomass, FB) and poultry manure (Litter Biomass, LB) are produced annually on a dry matter basis out of which 10 million dry tons of livestock and poultry waste are produced in Texas alone.

In many cases, the production of manure is in excess of the availability of farmland application. While the land application of manure either from cattle or poultry as fertilizer has been the expedient solution, the problem with this remedy is that manure is a relatively dilute nutrient source, sharply increasing the transportation cost from the confinement facility to the site of application. Depending on transportation costs, beyond a certain radius, manure cannot compete with commercial fertilizer as a nutrient. If the rate of land application for the manure as the fertilizer is not reduced, air and water quality problems will become more serious. The stock piled waste poses economic and environmental liabilities. Hence the animal bio-waste from CAFO's can lead to ground water contamination and air pollution problems with release of CH₄, NH₃, H₂S, amides, volatile organic acids, mercaptans, esters, and other chemicals. Some states have actually enacted moratoriums on the construction of new facilities, until the local regulatory authorities satisfy the ability of disposition of the manure locations based on a rigorous nutrient balance or even more stringent criteria.

So a viable solution to the disposal problem is to use the feedlot and litter biomass as fuels for energy conversion. Various technologies, that utilize feedlot biomass as a sole energy source, are summarized in tabular form (Annamalai *et al.*, 1987). Some of these technologies have met with limited technical success. The limitations were primarily due to reliance on

feedlot biomass as the sole-source of fuel despite its highly variable properties (i.e. ash %, moisture %, salts etc.) and associated flame stability problems.

Since feedlot and litter waste could be readily combusted in the presence of high heat value coal, most of these problems could be eliminated by blending waste/biomass with coal and firing in existing boiler burners. A state of art review on cofiring has been recently undertaken (Sami *et al.*, 2001). The review summarizes various biomass fuels, properties and their combustion behavior, existing literature on co-firing, fundamental concepts related to coal: biomass blend combustion, and modeling studies.

The properties, performance, and emission data for coal, coal: FB and coal: LB blends on cofiring and fixed-bed gasification data for FB, LB, coal: FB and coal: LB blends were reported in previous DOE quarterly reports and partly published in recent articles (Sweeten *et al.*, 2003; Annamalai *et al.*; 2003a, 2003b). Even though fuel N increased for blended fuels, the NO_x emission did not increase. Further the reburn tests with FB and LB revealed reduction of NO_x of the order of 80 %. A provisional US patent # 60/278,277 was obtained and application for permanent patent is under review.

In order to explain the significant reduction of NO_x with animal waste based biomass as reburn fuels, fixed bed modeling effort was substituted with zero dimensional reburn model reported in Quarterly Progress report # 10. The previous zero dimensional model developed for estimating NO_x reduction during the reburn process using simulated biomass volatiles was the first step towards understanding the reburn process in a boiler burner. Since the results of the earlier simplified model were encouraging, the need for a more rigorous treatment of the model was thought to be necessary. The current progress report concerns with formulation of rigorous reburn model which accounts for mixing of cold reburn supply with hot NO containing main-burner gases, reburn fuel particle heat up, pyrolysis, N evolution, homogeneous reactions of volatile matter and nitrogenous compounds, heterogeneous char reactions etc.

2. EXECUTIVE SUMMARY

Reburn technology is a process where the NO_x produced by coal fired main burners is reduced with additional burners called reburners fired with natural gas or coal as reburn fuel under slightly fuel rich conditions. When animal waste was used as a reburn fuel, the reduction of NO was found to be of the order of 80 % and almost independent of stoichiometry upto 10 % deficient air. In order to understand the mechanisms governing NO reduction, a reburn model is presented here to predict the capture of NO_x by reburn fuel. The main fuel flow typically supplies 80-90 % of required thermal output while the remainder is supplied by reburn fuel. Thus, given the rating of the burner and heating values, the flow rates of main fuel and reburn fuel can be calculated. The main fuel $CH_xO_yN_x$ is fired along with air and “x” moles of NH₃ to simulate the desired amount of NO_x. The “x” value is calculated assuming complete oxidation of NH₃ into NO and H₂O. Flame temperature and species mass fractions are calculated assuming complete combustion and given % of heat loss. The hot NO containing main gases are assumed to mix with cold reburn fuel stream. An exponential mixing model is used to simulate the mixing of main burner product gas jet along with the reburn jet in the reburn zone. As the reburn jet mixes with hot main gases, temperature of gas increases which in turn heats up the particles in the reburn jet. The solid particle in the reburn stream is assumed to undergo pyrolysis producing char, volatiles, fuel bound nitrogen (FBN) compounds and ash; further the char along with char N reacts heterogeneously to produce CO, CO₂, CH₄, NO etc.

The pyrolysis and evolution of FBN are assumed to be first order and volumetric while the heterogeneous reactions occur with constant density. The volatile matter is assumed to consist of CO₂, CH₂, and H₂ while the gaseous N compounds released by particles include HCN, NH₃, and N₂. The mass fraction of each species evolving from fuel nitrogen can be given as input into the code, or the empirical curve fit data for coal and biomass can be used to calculate the product distribution of N into the gas phase. The global reaction schemes are used to depict the NO formation and destruction process in the reburn zone. Upto 5 homogeneous reactions involving FBN, 4 homogenous reactions involving oxidation of volatiles (CO, H₂, CH₂, CH₄) and 6 heterogeneous reactions (C+1/2 O₂ producing CO and CO₂, C+CO₂, C+H₂O, C+H₂, C+NO) are used in the model. Blowing corrections are used in determining the species concentration at particle surface. Homogenous and heterogeneous reactions along with the mixing cause increased gas temperature and change in NO concentration. The input to the code are: a) Main burner: total heat throughput of the boiler burner, % heat input in main burner, heat loss from main burner, ultimate and proximate analysis, LHV of the fuel, percentage of excess air (main burner equivalence ratio), temperature, NO concentration required to be simulated; b) Reburner: Fuel property, ultimate and proximate analysis, initial particle size, LHV of the fuel, FBN pyrolysis distribution (optional), specific heat and density of the fuel, heat of pyrolysis of the volatile matter, distribution of O₂, CO₂, and N₂ in the reburn gas being supplied along with the reburn fuel, c) Reburn Zone: reburn equivalence ratio. The output results are particle dia d_p , density ρ_p , particle burn rate \dot{m}_p , gas phase temperature T_g , particle temperature T_p , and mass fraction of species Y_k including NO distribution in the reburn zone as a function of time. Note that the current model accounts for combustion of main fuel and reactions between reburn fuel and main-burner gases. Due to the small-scale test facility, the experimental data have been generated without 'overfire' air, so an 'overfire' air model has not been incorporated into the code.

3. EXPERIMENTAL

For the current quarter, no experiments were run. However, a part of the data generated from experiments and reported in previous progress reports has been published (Sweeten *et al.*, 2003, Annamalai *et al.*, 2003a and 2003b).

4. THEORETICAL

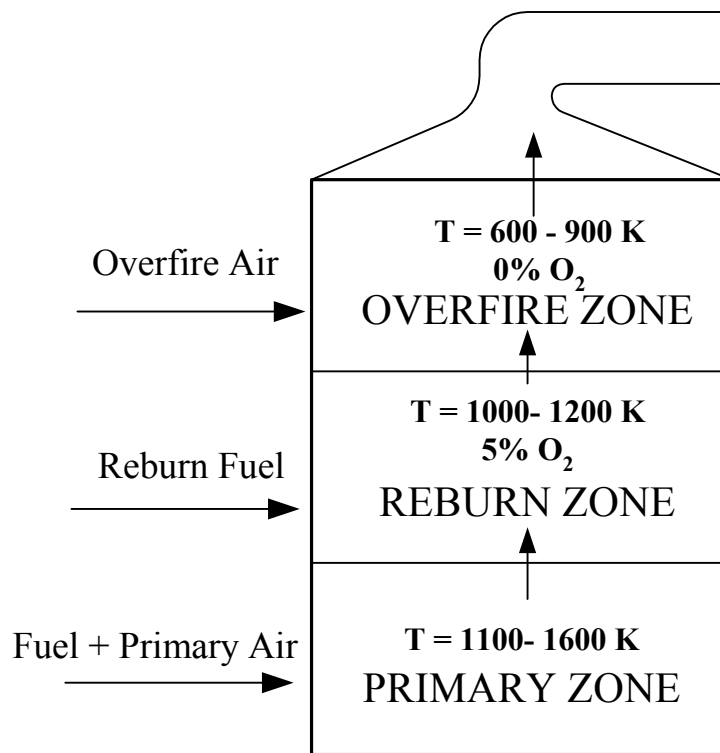
In typical coal fired boilers, reburn fuel is injected into the upper furnace region. The overall furnace process occurs in 3 main zones in a boiler. They are,

1. Primary zone
2. Reburn zone
3. Overfire zone

Table 1 and figure 1 explain the processes that occur in all the 3 zones in a coal fired boiler furnace.

Table 1: Reburn Process

Zone	Process
Primary Zone	NO_x forms due to the combustion process of main fuel.
Reburn zone	NO_x is reduced with injection of reburn fuel. N_2 and HCN are formed.
Burn out Zone	Unreacted fuel, CO, HCN are burnt due to the addition of additional air after the reburn zone.

**Figure 1: Schematic of a typical Reburn process**

The current model accounts for combustion of main-burner fuel and reactions between reburn fuel and main-burner gases, however it does not include an overfire model. The difference between the current and older model is the capability to handle any solid fuel, along with more detailed modeling including heterogeneous and homogeneous global reactions. The solid fuel makes the inclusion of pyrolysis of volatile matter and fuel bound nitrogen (FBN), and char oxidation reactions necessary. The fuel bound nitrogen is assumed to be released to the gas phase by two processes, a) FBN evolution to N_2 , HCN, and NH_3 , and b) FBN oxidation to NO at the char surface. Figure 2 shows the various processes experienced by the reburn fuel.

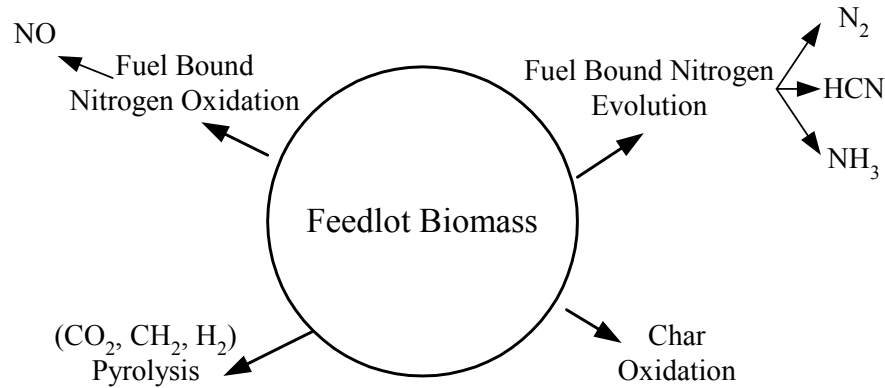
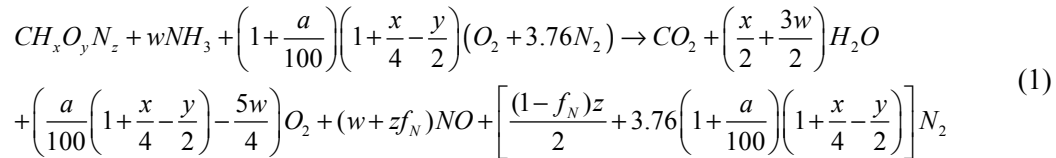


Figure 2: Schematic of typical solid fuel combustion during the reburn process

4.1. Main Burner Modeling

The main burner is modeled to burn any fuel having an empirical formulae $CH_xO_yN_x$ along with NH_3 to simulate the desired amount of NO_x entering the reburn zone. The NH_3 injection is dependent on the amount of NO_x required down stream of the main burner. The assumptions in the main burner modeling are:

- The main burner fuel $CH_xO_yN_x$ is assumed to oxidize completely in the main burner zone.
- The production of NO_x is solely attributed to the complete oxidation of NH_3 introduced with the main fuel. The model ignores Thermal and Fuel NO_x formation. The equation represents the overall reaction in the main burner zone.
- In case NO_x is produced by certain % of conversion of N in fuel to NO (can be specified as an input to the code), then one may set NH_3 moles to be zero ($w = 0$).



For a given thermal throughput (boiler rating), and fraction of total heat throughput through the main burner, the mass flow rate of fuel in the main burner is calculated as

$$\dot{m}_{fuel} = \frac{HTP_{f,MB} \times R_{Boiler}}{LHV_{MB}} \tag{2}$$

The temperature of the burnt gases leaving the main burner is calculated taking into account the heat loss in the main burner zone. The heat loss from the main burner zone is defined as a fraction of the Lower Heating Value (LHV) of the main burner fuel.

The temperature is calculated from the energy balance between the inlet and outlet of the main burner. Assuming that the main burner fuel, the primary air, and NH_3 enter the main burner at room temperature (298 K), the energy balance equation is given as

$$H_{in,mainburner} = H_{out,mainburner} + Q_{loss} \quad (3)$$

where Q_{loss} assumes positive values for losses.

$$H_{in,mainburner} = h_{f,fuel} + h_{t,fuel} + \frac{\dot{m}_{NH_3}}{\dot{m}_{fuel}} (h_{f,NH_3} + h_{t,NH_3}) + \frac{\dot{m}_{air}}{\dot{m}_{fuel}} (h_{t,air}) \quad (\text{kJ/kg of main burner fuel supplied}) \quad (4)$$

$$\dot{m}_{fuel} = \dot{m}_{MB} \quad \text{'MB' main burner} \quad (4a)$$

$$h_{t,fuel} = \int_{T_{ref}}^{T_{MB,in}} c_{p_k} dT, \quad h_{t,fuel} = h_{NH_3,fuel} = h_{air,fuel} = 0 \quad \text{if } T_{MB,in} = 298 \text{ K}$$

The $h_{f,fuel}$ is calculated from the LHV of the main burner fuel.

$$h_{f,fuel} = \frac{(\bar{h}_{f,CO_2} + \frac{x}{2} \bar{h}_{f,H_2O})}{MW_{fuel}} + LHV_{MB} \quad (\text{kJ/kg of main burner fuel supplied}) \quad (5)$$

where \bar{h} , is in kJ/kmole

The heat loss in the main burner expressed as a fraction of the LHV of the main burner fuel, is calculated as

$$Q_{loss} = d \times LHV_{MB} \quad (\text{kJ/kg of main burner fuel supplied}) \quad (6)$$

Therefore from equation 3,

$$h_{f,fuel} + h_{t,fuel} + \frac{\dot{m}_{NH_3}}{\dot{m}_{fuel}} (h_{f,NH_3} + h_{t,NH_3}) + \frac{\dot{m}_{air}}{\dot{m}_{fuel}} (h_{t,air}) = \frac{\dot{m}_{prod,MB}}{\dot{m}_{fuel}} \left(\sum_k Y_k h_{T,k,MB} \right) + d \times LHV_{MB} \quad (7)$$

where

$$\dot{m}_{prod,MB} = \dot{m}_{NH_3} + \dot{m}_{MB} + \dot{m}_{air} \quad (8)$$

The mass fraction of the individual species 'k' is calculated as,

$$Y_{k,MB} = \frac{X_{k,MB} MW_{k,MB}}{\sum_k X_{k,MB} MW_{k,MB}} \quad (9)$$

$$h_{T,k,MB} = h_{f,k,MB} + \int_{T_{ref}}^T c_{p_{k,MB}} dT \quad (10)$$

Therefore, the equation (7) can be written as

$$\sum_k Y_{k,MB} \left(h_{f,k,MB} + \int_{T_{ref}}^T c_{p,k,MB} dT \right) = \frac{\dot{m}_{MB}}{\dot{m}_{prod,MB}} \left[(1-d)LHV_{MB} + \frac{h_{f,CO_2} + \frac{X}{2} h_{f,H_2O}}{MW_{fuel}} + h_{t,fuel} + \frac{\dot{m}_{NH_3}}{\dot{m}_{MB}} (h_{f,NH_3} + h_{t,NH_3}) + \frac{\dot{m}_{air}}{\dot{m}_{MB}} (h_{t,air}) \right] \quad (11)$$

The temperature of the product leaving the main burner zone can be calculated from equation (11). A simple iterative scheme like the Newton Raphson method may be used for this purpose.

Therefore using equations (9) and (11) the mass fraction of the species in the product gas leaving the main burner zone and the temperature of the same can be calculated. The mass flow rate of a species 'k' leaving the main burner can be calculated as

$$\dot{m}_{k,MB} = \dot{m}_{prod,MB} \times Y_{k,MB} \quad (12)$$

4.2. Reburn Fuel Model

Table 2: Fuel properties of coal and Feedlot Biomass

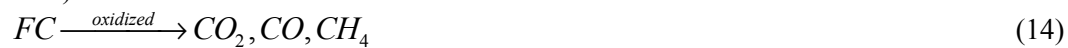
Parameter		Wyoming Coal	Feedlot Biomass
Proximate Analyses (as received)	Dry loss	21.23	10.88
	Volatile Matter	32.58	56.97
	Fixed Carbon	41.92	17.33
	Ash	4.28	14.83
Ultimate Analysis (DAF Basis)	Carbon	75.63	50.08
	Hydrogen	4.76	5.98
	Oxygen	18.10	38.49
	Nitrogen	1.14	4.58
	Sulfur	0.37	0.87

Table 2, shows the properties of coal, feedlot biomass used for the simulation (Sweeten *et al.*, 2003, Priyadarsan *et al.*, 2003a, and Priyadarsan *et al.*, 2003b). Freeman *et al.*, 2003, have reported that Feedlot biomass can be used as an effective reburn fuel, to reduce the NO_x emissions from boiler burners. The chemical formula of the reburn fuel is given as $CH_{X1}O_{Y1}N_{Z1}$. The composition of the reburn fuel is assumed to be

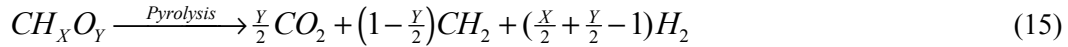
$$CH_{X1}O_{Y1}N_{Z1} \xrightarrow{\text{composition}} FC + VM + FBN + Ash \quad (13)$$

The different components of the solid fuel react differently.

FC is assumed to consist of pure carbon and gets oxidized via heterogeneous reactions (X – XV).



Solid fuel pyrolysis is through finite kinetics, which depends on the type of reburn fuel. The volatile matter composition is assumed constant throughout the pyrolysis period of the fuel. The composition of the volatile matter is determined from the ultimate analysis of the reburn fuel. A single reaction model has been assumed for determining the volatile matter release rate from the solid fuel into the gas phase. The details of the reaction model shall be covered later in the report. The volatile matter composition is determined as



where it is assumed that the product of pyrolysis are CO_2 , H_2 , and CH_2 .

In equation (15), it may seem unusual to use CH_2 as one of the products of pyrolysis. However, this became necessary due to the following reasons.

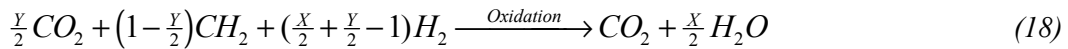
An attempt was made to make use of CH_4 , C_2H_2 , or C_2H_4 as product species, instead of CH_2 , but since the oxygen content of the biomass used is very high (Table 2), the coefficients for CH_4 , C_2H_2 , or C_2H_4 in equation (15), were negative, which is unrealistic. The choice of CH_2 seemed to satisfy equation (15) and the coefficient for CH_2 is positive. However, the heat of formation of CH_2 is not known a priori. It is determined by using the Heating Value (HV) of FC and the heat of pyrolysis of the VM (which is given as input by the user)

$$LHV_{RB, fuel, daf} = Y_{FC, daf} HV_{FC} + (1 - Y_{FC, daf}) (LHV_{VM, daf} + Hp) \quad (16)$$

In the above equation (16), the heat of pyrolysis of FBN has been neglected due to smaller amount of nitrogen compared to volatile matter. Using equation (16) the LHV of the VM can be determined as

$$LHV_{VM, daf} = \left[\frac{LHV_{RB, fuel, daf} - Y_{FC, daf} HV_{FC}}{(1 - Y_{FC, daf})} \right] - Hp \quad (\text{kJ/kg of VM}) \quad (17)$$

Since the pyrolysis products are assumed to be CO_2 , CH_2 , and H_2 , the heat of formation of CH_2 is determined as



Therefore heat of formation of CH_2 is calculated as,

$$\bar{h}_{f, CH_2} = \frac{\left(1 - \frac{y}{2}\right)\bar{h}_{f, CO_2} + \frac{x}{2}\bar{h}_{f, H_2O} + LHV_{VM, daf} MW_{VM}}{\left(1 - \frac{y}{2}\right)} \quad (\text{kJ/kmol}) \quad (19)$$

where \bar{h} , is in kJ/kmole



Fuel Bound Nitrogen (FBN) undergoes both pyrolysis (equation 20a) and heterogeneous oxidation (equation 20b) at the char surface. A single reaction model is used for the pyrolysis of fuel nitrogen. The details of the reaction rate shall be discussed later in the report.

FBN is oxidized and pyrolyzed from the particle surface. The pyrolysis products of FBN are (equation 20a) assumed to be N_2 , NH_3 , and HCN . The mass fraction of each species

evolving from fuel nitrogen can be given as input into the code, or the empirical curve fit data for coal and biomass can be used to calculate the product distribution of N into the gas phase. For coal, the curve fit has been done from the experimental data given by William *et al.*, 1945, and for biomass, it has been done from the experimental data given by Zhou *et al.*, 2000.

The ash is assumed to be inert and undergoes no chemical and physical change during combustion of the reburn fuel in the reburn zone and is assumed to be retained in the fuel.

The mass flow rate of the reburn fuel supplied to the burner is calculated from the fraction of the heat throughput through the reburn fuel in the boiler burner.

$$\dot{m}_{RB,daf} = \frac{(1 - HTP_{f,MB}) \times R_{Boiler}}{LHV_{RB,daf}} \quad (21)$$

$$\dot{m}_{RB,as\ received} = \frac{\dot{m}_{RB,daf}}{(1 - Y_{RB,ash})} \quad (22)$$

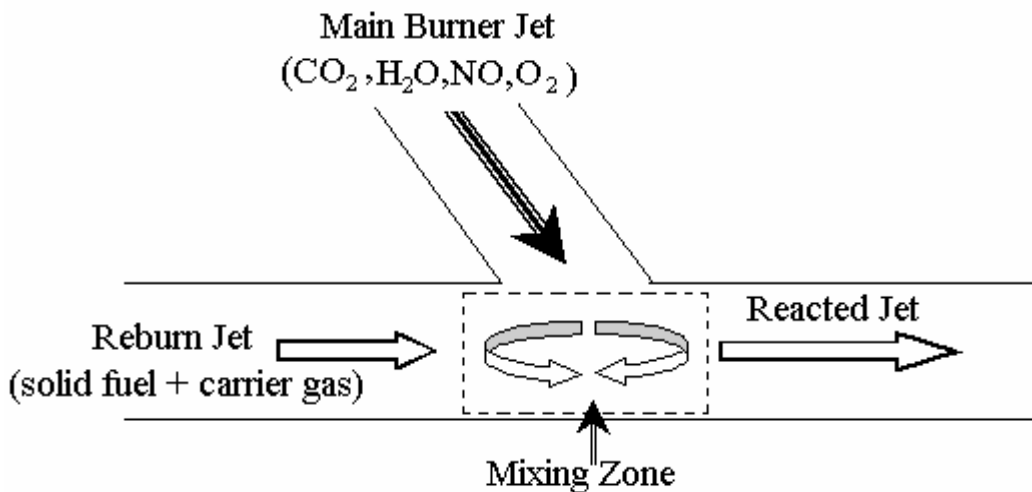


Figure 3: Schematic of the mixing model

4.3 Mixing Model Development

An exponential mixing model (Stickler *et al.*, (1983), Alzueta *et al.*, 1998) is used to simulate the mixing of main burner product gas jet along with the reburn jet in the reburn zone. Figure 3 shows a schematic of the mixing model used. In this model, the main-burner product gas jet is entrained into the reburn jet gradually, thus increasing the mass flow rate of the reburn jet. This particular model was used because of its simplicity to implement and more importantly in this model the reburn jet undergoes greater change in the stoichiometry during the mixing process and appears to lead to favorable results.

$$\dot{m}_{RB,t} = \dot{m}_{RB,t=0} + \dot{m}_{prod,MB} \left(1 - \exp\left(-\frac{t}{\tau_{mix}}\right) \right) \quad (23)$$

Therefore, the mass added to the reburn jet from the main burner jet in time period dt is

$$d(\dot{m}_{RB,t} - \dot{m}_{RB,t=0}) = d\dot{m}_{added} = \left[\frac{\dot{m}_{prod,MB}}{\tau_{mix}} \exp\left(-\frac{t}{\tau_{mix}}\right) \right] dt \quad (24)$$

Since the global ϕ_{RZ} is given an input to the code, the O_2 supplied along with the rebrun fuel is calculated as

$$\phi_{RZ} = \frac{\left(\frac{O_2}{RB \cdot fuel}\right)_{Stoichiometric,RZ}}{\left(\frac{O_2}{RB \cdot fuel}\right)_{Actual,RZ}} = \frac{\left(\frac{\dot{m}_{O_2}}{\dot{m}_{RB \cdot fuel}}\right)_{Stoichiometric,RZ}}{\left(\frac{\dot{m}_{O_2}}{\dot{m}_{RB \cdot fuel}}\right)_{Actual,RZ}} \quad (25)$$

$$\left(\frac{O_2}{RB \cdot fuel}\right)_{Stoichiometric,RZ} \quad \text{stoichiometric } O_2: \text{ reburn fuel ratio (mass basis)} \quad (25a)$$

$$\left(\frac{O_2}{RB \cdot fuel}\right)_{Actual,RZ} \quad \text{actual } O_2: \text{ reburn fuel ratio (mass basis)} \quad (25b)$$

$$\phi_{RS} = \frac{\dot{m}_{RB,daf} \left(\frac{MW_{O_2}}{MW_{RB,daf}}\right) \left(1 + \frac{X1}{4} - \frac{Y1}{2}\right) \phi_{RZ}}{\dot{m}_{RB,daf} \left(\frac{MW_{O_2}}{MW_{RB,daf}}\right) \left(1 + \frac{X1}{4} - \frac{Y1}{2}\right) - \phi_{RZ} Y_{O_2,MB} \dot{m}_{prod,MB}} \quad (26)$$

Therefore, the mass flow rate of O_2 supplied along with the solid reburn fuel is calculated as,

$$\dot{m}_{O_2,RS} = \frac{\dot{m}_{RB,daf} \left(\frac{MW_{O_2}}{MW_{RB,daf}}\right) \left(1 + \frac{X1}{4} - \frac{Y1}{2}\right)}{\phi_{RS}} \quad (27)$$

Since other gases like CO_2 , and N_2 are also supplied along with the reburn O_2 , the mass fraction or the composition of the gases supplied along with the reburn fuel are given as input in the code. The total mass flow rate of the gas phase supplied along with the solid reburn fuel is,

$$\dot{m}_{gas,RS} = \frac{\dot{m}_{O_2,RS}}{Y_{O_2,RS}} \quad (28)$$

Therefore, the mass flow rate of the gases supplied along with the solid reburn fuel are calculated as,

$$\dot{m}_{k,RS} = Y_{k,RS} \dot{m}_{gas,RS} \quad (29)$$

4.4. Chemical Reactions

4.4.1. Homogeneous Reburn Reactions

The reburn reactions take place in the gas phase where the NO is primarily reduced and formed due to interaction with other species. The global reaction scheme is used to depict the NO formation and destruction process in the reburn zone. The reactions considered are,

1) Hydrocarbon (HC) reduction: Chen *et al.*, 1996

where

$$CH_x = \sum_i C_i H_i = (CH_4 + C_2H_2 + C_2H_4 + \dots + CH_2) \quad (30a)$$

In this case

$$CH_x = \sum_i C_i H_i = (CH_4 + CH_2) \quad (30b)$$

In the above equations (30a and 30b) CH_2 is considered, as it assumed to be a product of the reburn fuel pyrolysis.

$$w_{NO,I} = -2.26 \times 10^9 X_{NO} X_{CH_x} \exp\left(\frac{-76233}{RT_g}\right) \quad (\text{kmol/m}^3\text{-s})$$

2) Ammonia oxidation: De Soete, 1975

$$w_{NH_3,II} = -4 \times 10^6 X_{NH_3} X_{O_2}^{b_{II}} \exp\left(\frac{-133900}{RT_g}\right) \quad (I/s) \quad (31)$$

where b_{II} the order of reaction with O_2 depends on X_{O_2} in the gas phase, and is calculated by a curve fit from the data provided by De Soete, 1975. It is calculated as

$$\begin{aligned} \ln(X_{O_2}) > -3, \quad b_{II} &= 0 \\ -5.671 \leq \ln(X_{O_2}) \leq -3, \quad b_{II} &= \text{curvefit} \\ \ln(X_{O_2}) < -5.671, \quad b_{II} &= 1 \end{aligned} \quad (32)$$

3) Ammonia reduction: De Soete, 1975

$$w_{NH_3,III} = -1.8 \times 10^8 X_{NH_3} X_{NO} \exp\left(\frac{-113000}{RT_g}\right) \quad (I/s) \quad (33)$$

4) HCN oxidation: De Soete, 1975

$$w_{HCN,IV} = -10^{10} X_{HCN} X_{O_2}^{b_{IV}} \exp\left(\frac{-280328}{RT_g}\right) \quad (I/s) \quad (34)$$

where b_{IV} the order of reaction with O_2 depends on X_{O_2} in the gas phase, and is calculated by a curve fit from the data provided by De Soete, 1975. It is calculated as

$$\begin{aligned}
\ln(X_{O_2}) > -3, \quad b_{IV} &= 0 \\
-5.671 \leq \ln(X_{O_2}) \leq -3, \quad b_{IV} &= \text{curvefit} \\
\ln(X_{O_2}) < -5.671, \quad b_{IV} &= 1
\end{aligned} \tag{35}$$

5) HCN reduction: De Soete, 1975



$$w_{NH_3,V} = -3 \times 10^{12} X_{HCN} X_{NO} \exp\left(\frac{-251000}{RT_g}\right) \text{ (I/s)} \tag{36}$$

4.4.2. Other Homogeneous reactions

Apart from the NO_x reaction, there are other homogeneous reactions, which tend to consume the O_2 present in the reburn zone.

6) CO oxidation: Williams, 2000



$$w_{CO,VI} = -4 \times 10^{14} [CO][O_2]^{0.25} [H_2O]^{0.5} \exp\left(\frac{-20202}{RT_g}\right) \text{ (kmol/m}^3\text{-s)} \tag{37}$$

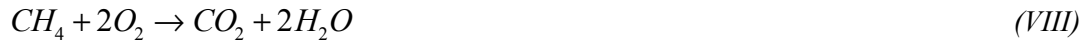
7) H₂ oxidation: Tsuji, 2002



$$w_{H_2,VII} = -10^{13.52} [H_2]^{0.85} [O_2]^{0.25} [H_2O]^{1.42} [C_2H_4]^{-0.56} \exp\left(\frac{-41000}{RT_g}\right) \text{ (gmol/cm}^3\text{-s)} \tag{38}$$

where CH_2 is used instead of C_2H_4 in equation (38)

8) CH₄ oxidation: Bartok, 1991



$$w_{CH_4,VIII} = -2.8 \times 10^9 [O_2]^{1.3} [CH_4]^{-0.3} \exp\left(\frac{-202600}{RT_g}\right) \text{ (kmol/m}^3\text{ s)} \tag{39}$$

9) CH₂ oxidation: Smoot and Smith, 1985

The kinetics for C_2H_4 may be used for calculating the reaction rate for CH_2



$$w_{CH_2,IX} = -10^{14.70} [CH_2]^{0.9} [O_2]^{1.18} [CH_4]^{-0.37} \exp\left(\frac{-50000}{RT_g}\right) \quad (\text{mol/cm}^3 - \text{s}) \quad (40)$$

4.4.3. Heterogeneous reactions:

The following heterogeneous reactions occur at the particle surface. The kinetic rate constants for the heterogeneous reactions are given as,

10) Carbon oxidation: Annamalai *et al.*, 1993



$$k_{C,X} = 1.6 \times 10^5 \exp\left(\frac{-20000}{T_p}\right) \quad (1/s) \quad (41)$$

11) Carbon Oxidation: Annamalai *et al.*, 1993



$$k_{C,XI} = 2.3 \times 10^7 \exp\left(\frac{-26200}{T_p}\right) \quad (1/s) \quad (42)$$

12) Carbon oxidation: Annamalai *et al.*, 1993



$$k_{C,XII} = 3.42 T_p \exp\left(\frac{-15600}{T_p}\right) \quad (1/s) \quad (43)$$

13) Steam carbon reaction: Bryden *et al.*, 1996



$$k_{C,XIII} = 1.67 \times k_{C,XII} \quad (1/s) \quad (44)$$

14) Methane formation: Schoeters, 1985



$$k_{C,XIV} = 3 \times 10^{-3} \times k_{C,XII} \quad (1/s) \quad (45)$$

15) C and NO reaction: Mitchel *et al.*, 1982



$$k_{C,XV} = 1.57 \times 10^5 \exp\left(\frac{-34000}{RT_p}\right) \quad (1/s) \quad (46)$$

The mass loss rate for each of the reactions X – XV, is calculated as

$$\dot{m}_{C,i} = \rho_w k_{c,i} Y_{kr,w}^{n_i} \pi d_p^2 \quad (47)$$

$$k_{c,i} = A_{c,i} \exp\left(\frac{-E_{C,i}}{RT_p}\right) \quad (48)$$

The total carbon consumption rate for a particle of size d_p is given as

$$\dot{m}_C = \sum_{i=X}^{XV} \dot{m}_{C,i} \quad (49)$$

In order to calculate heterogeneous reactions on the particle surface, the species concentration must be determined first. The species mass fraction at the particle surface ($Y_{kr,w}$) is calculated as follows.

With the assumption of a first order reaction ($n_i = 1$) at the particle surface, the analysis of the mass transfer across the frozen film yields the following expression for the species mass fraction at the particle surface (Du, 1995).

$$\frac{Y_{k,w}}{Y_k} = \left[\exp(X) - \sum_{i=10}^{15} \frac{v_{k,i} \rho k_{c,i} S n_i d_p (\exp(X) - 1)}{(X Sh \rho D)} \right]^{-1} \quad (50)$$

where

$$X = \frac{\dot{m}_p}{(Sh \rho D \pi d_p)} = \frac{h_m d_p}{\rho D} \quad (51)$$

$$\dot{m}_p = \dot{m}_V + \dot{m}_C \quad (51a)$$

$$Sh = 2 + 0.6 Re^{\frac{1}{2}} Sc^{\frac{1}{3}} \quad (52)$$

From the above equation (50), it can be seen that the oxygen mass fraction at the particle surface ($Y_{kr,w}$) is calculated in terms of the bulk gas mass fraction (Y_{kr}) next to the particles by a mass balance that accounts for the blowing effects (Stefan flow) from the particle and chemical reactions at the surface.

4.4.4. Volatile Matter release from the solid reburn fuel:

A single reaction model has been assumed for determining the volatile matter release rate from the solid fuel into the gas phase.

$$\frac{dm_{pyro}}{dt} = \left(\frac{V_{int} - V}{V_{int}} \right) A_{pyro,fl} \exp\left(\frac{-E_{pyro,fl}}{RT_p}\right) m_{part} \quad (53)$$

The activation energy for Wyoming coal (low sulfur coal) and feedlot biomass were calculated by Thien, 2002, and are tabulated in Table 3.

Table 3: Pre exponential factors and Activation energy for coal and feedlot biomass using a single reaction model

Fuel type (ρ)	$A_{pyro,fl}$ (1/s)	$E_{pyro,fl}$ (kJ/kmol)
Coal	2.08×10^4 ⁺	32000 *
Feedlot Biomass	2.08×10^4 ⁺	18400 *

⁺ Mitchel *et al.*, 1982, * Thien, 2002, Thien *et al.*, 2003, and Annamalai *et al.*, 2003a

4.4.5. FBN pyrolysis rate:

A single reaction model has been assumed to determine the N release rate from the solid into the gas phase Mitchel *et al.*, 1982.

$$\frac{dm_{N-pyro}}{dt} = k_{N-pyro} \left(\frac{Y_N}{Y_{N,O}} \right) \left(\frac{V_{int} - V}{V_{int}} \right)^{0.364} m_{part} \quad (54)$$

$$Y_{N,O} = \frac{m_{N,O}}{m_O} \quad (55a)$$

$$Y_N = \frac{m_N}{m_O} \quad (55b)$$

$$k_{N-pyro} = 2.63 \times 10^5 \exp\left(\frac{-142675}{RT_p}\right) \quad (56)$$

4.4.6. FBN oxidation:

The FBN oxidation at the char surface is related to the char burning rate and is given as,

16) FBN oxidation at the fuel surface: Mitchel *et al.*, 1982



$$\frac{dm_{N-oxid}}{dt} = \left(\frac{m_N}{m_{part}} \right) \frac{dm_{C,XV}}{dt} \quad (57)$$

4.5. Governing Transient equations

1) Species balance equation:

The gas phase species balance or continuity equation for the control volume is,

$$\frac{dm_k}{dt} = S_{pyro,k} + S_{Htr,k} + S_{Hmr,k} + S_{N-pyro,k} + S_{N-oxid,k} \quad (58)$$

The source terms are calculated from the reaction kinetics mentioned earlier in the previous section.

The overall mass conservation equation for the gas phase is,

$$\frac{dm_{gas}}{dt} = \frac{dm_{pyro}}{dt} + \frac{d|m_C|}{dt} + \frac{dm_{N-pyro}}{dt} + \frac{dm_{N-oxid}}{dt} \quad (59)$$

2) Particle diameter:

Assuming, that the decrease in particle size is due to oxidation of FC on the char surface the particle diameter is calculated as,

$$\frac{d(d_p)}{dt} = -\frac{2\dot{m}_C}{\pi\rho_p d_p^2} \quad (60)$$

To keep the computation simple, only one uniform particle size is used as the initial diameter of the reburn fuel particle. The initial particle size is given as input by the user.

3) Energy equation for solid phase

The energy equation is used to calculate the particle temperature at the surface. Since the particle size is small (order of 100 μm), it is assumed to have uniform temperature. Thus, the surface temperature of the particle is also the bulk temperature of the particle.

$$m_{part} c_{part} \frac{dT_p}{dt} = -(\dot{q}_{conv} + \dot{q}_{rad}) + \dot{q}_{ch,p} \quad (61)$$

The source terms for the energy equations are calculated as

a) Convection term

Assuming quasi-steady state behaviour around the particle, the overall convective heat transfer rate between the particle and the gas is given as,

$$\dot{q}_{conv} = h(T_p - T_g) \pi d_p^2 F_B \quad (62)$$

$$F_B = \left(\frac{z}{e^z - 1} \right), \quad (Borman, 1998) \quad (63a)$$

$$z = \frac{\dot{m}_C + \dot{m}_V}{2\pi\rho_g D d_p} \quad (63b)$$

b) Radiation term

$$\dot{q}_{rad} = F_R \sigma_{SB} \epsilon (T_p^4 - T_{rad}^4) \pi d_p^2 \quad (64)$$

c) Chemical reaction term

The heat liberation rate due to chemical reactions at the particles is given as,

$$\dot{q}_{ch,p} = \sum_{i=1}^N \dot{m}_{C,i} HV_i + \dot{m}_{pyro} (H_p + HV_p) \quad (65)$$

4) Energy equation for gas phase

Gas phase energy equation is used to calculate the temperature of the gas phase.

$$\frac{d(m_{gas} h_{T,gas})}{dt} = \dot{q}_{conv} + \dot{q}_{rad} + \dot{q}_{ch} + \dot{q}_m \quad (66)$$

$$\dot{q}_m = (\dot{m}_c + \dot{m}_{pyro} + \dot{m}_{N-pyro} + \dot{m}_{N-oxid}) c_p (T_p - T_{ref}) \quad (67)$$

$$\dot{q}_{ch} = \sum_{i=1}^{IX} w_{hm,i} HV_i \quad (68)$$

4.6. Procedure

The current model formulation uses solid feedlot biomass as the reburn fuel. Reburn fuel pyrolysis, FBN evolution and oxidation, and global char reactions along with global homogeneous reactions have been incorporated into the model. The governing differential equations outlined in the previous section, shall be solved explicitly and integrated over time to determine the NO reduction in the reburn zone using feedlot biomass as the reburn fuel.

4.6.1 Input data

The following information discussed below is provided to the code as input.

Main Burner

- 1) Fuel property, ultimate and proximate analysis
- 2) Percentage of excess air
- 3) Inlet temperature
- 4) NO concentration required to be simulated in the reburn zone
- 5) Percentage of fuel N converted to NO
- 6) Total heat throughput of the boiler burner
- 7) Heat loss from the main burner
- 8) LHV of the main-burner fuel

Reburn Supply

Reburn fuel

- 1) Fuel property, ultimate and proximate analysis
- 2) Initial particle size
- 3) LHV of the reburn fuel
- 4) FBN pyrolysis distribution (optional)
- 5) Specific heat and density of the fuel
- 6) Heat of pyrolysis of the volatile matter

Reburn gas

- 1) Distribution of O₂, CO₂, and N₂ in the reburn gas being supplied along with the reburn fuel.

Reburn Zone

- 1) Equivalence ratio in the reburn zone

4.6.2. Output data

After simulation, the following information mentioned below is provided by the code as output.

- 1) NO distribution in the reburn zone as a function of time.
- 2) Gas phase temperature in the reburn zone as a function of time.
- 3) Temperature of the particle in the reburn zone as a function of time.
- 4) Distribution of other gas species in the reburn zone as a function of time.

5. RESULTS AND DISCUSSION

Results have not yet been obtained

6. CONCLUSION

No conclusion is presented since the results are not yet available.

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9. LIST OF ACRONYMS AND ABBREVIATIONS

DAF: Dry Ash Free

FB: Feedlot biomass (Cattle manure)

FBN: Fuel bound nitrogen

FC: Fixed Carbon

LHV: Lower heating value

VM: Volatile matter

Nomenclature

a	excess air percentage supplied to the main burner zone
$A_{C,i}$	pre-exponential factor for reaction i
$A_{pyro,fl}$	pre-exponential factor for pyrolysis of fuels, 'fl': coal, or biomass
b_{II}	order of the reaction with O_2
c_{part}	specific heat capacity of the solid fuel particle
$c_{pk,MB}$	specific heat capacity of the main burner product gas species, 'k' (CO_2 , NO , H_2O , N_2 , O_2 .)
d	fraction of LHV of the main burner fuel lost from the main burner.
$E_{pyro,fl}$	activation energy for pyrolysis of fuels, 'fl': coal, or biomass, kJ/kmole
F_B	blowing correction factor
F_R	shape factor to account for shielding by other particles (assumed to be 1 in this case)
f_N	fraction of fuel N converted into NO
h	heat transfer coefficient for a particle of size dp , ($h = Nu \lambda / dp$), kW/m ²
	K
h_{f,CH_2}	heat of formation of CH_2 , kJ/kg

$h_{f,k}$	heat of formation of species k , kJ/kg
$\bar{h}_{f,k}$	heat of formation of species k , kJ/kmole
$H_{in,mainburner}$	enthalpy of the reactants entering the main burner at 298 K (main burner fuel, NH ₃ , and air), kJ
$H_{out,mainburner}$	enthalpy of the products leaving the main burner at T K (CO ₂ , H ₂ O, N ₂ , NO, O ₂), kJ
h_m	mass transfer coefficient, kg/m ² s
$h_{t,k}$	thermal enthalpy of species k , kJ/kg
$h_{T,k,MB}$	total enthalpy of the main burner product species, kJ/kg
$HTP_{f,MB}$	fraction of total heat throughput supplied through the main burner
HV_{FC}	heating value of FC, kJ/kg
$HV_{C,i}$	heating value of heterogeneous reactions
HV_i	heating value of i th homogeneous reaction
HV_p	heating value of the pyrolysis products, in the event volatiles oxidize in proportion to fixed carbon
H_p	heat of pyrolysis of the volatile matter
i	reaction number involving the species 'k'
$[k]$	concentration of species 'k' (kmol/m ³)
'k'	gas species O ₂ , CO, CO ₂ , CH ₄ , CH ₂ , H ₂ , H ₂ O, HCN, NH ₃ , NO, N ₂
$k_{C,i}$	specific reaction constant for reaction i , and
LHV_{MB}	lower heating value of the main burner fuel, kJ/kg
$LHV_{RB,fuel,daf}$	LHV of the reburn fuel on daf basis, kJ/kg
$LHV_{VM,daf}$	LHV of the VM on daf basis, kJ/kg
\dot{m}_k	mass flow rate of species k , kg/s
$\dot{m}_{gas,RS}$	Total mass flow rate of the gas supplied along with the solid reburn fuel
$\dot{m}_{RB,daf}$	mass flow rate of reburn fuel on daf basis
$\dot{m}_{prod,MB}$	total mass flow rate of the main burner jet
$\dot{m}_{RB,t=0}$	mass flow rate of the reburn jet at $t = 0$
\dot{m}_C	total carbon loss rate, kg/s
$\dot{m}_{RB,t}$	total mass flow rate of the reburn jet at time t
\dot{m}_V	total volatile loss rate
m_C	mass added to gas phase due to oxidation of FC (total carbon oxidation) in the solid fuel, kg
m_k	mass of species 'k', kg
m_N	mass of FBN remaining in the solid reburn fuel particle, kg
$m_{N,0}$	initial mass of FBN in the reburn fuel particle, kg
m_{N-oxid}	mass added to gas phase due to oxidation of fuel nitrogen at particle surface, kg
m_{N-pyro}	mass released from the solid fuel into the gas phase due to devolatilization of N in the solid fuel, kg

m_0	initial mass of the particle, kg
m_{part}	mass of the solid fuel particle, kg
m_{pyro}	mass added to the gas phase due to devolatilization of volatile matter in the solid fuel, kg
$MW_{k,MB}$	molecular weight of the main burner product gas species 'k' (CO ₂ , NO, H ₂ O, N ₂ , O ₂), kg/kmole
$MW_{RB,daf}$	molecular weight of the reburn fuel on daf basis, kg/kmole
MW_{VM}	molecular weight of VM
$N_{(S)}$	mass of FBN in the solid fuel particle, kg
n_i	order of reaction 'i' with respect to oxidizer
\dot{q}_{ch}	enthalpy added as result of homogeneous chemical reactions in the gas phase.
\dot{q}_m	enthalpy added to the gas phase due addition of mass from the particles
Q_{loss}	Heat loss from the main burner, $Q_{loss} < 0$ for heat loss from the main burner
R	Universal gas constant (8.314 kJ/kmol K)
R_{Boiler}	Rating of the boiler burner (kW)
S	mass source terms
$S_{Htr,k}$	heterogeneous reaction source term for species 'k'
$S_{Hmr,k}$	homogeneous reaction source term for species 'k'
Sn_i	equals to +1, if the species are produced for reaction i, and
Sn_i	equals to -1, if the species are consumed for reaction i
$S_{N-oxid,k}$	nitrogen oxidation source term for species 'k'
$S_{N-pyro,k}$	nitrogen pyrolysis source term for species 'k'
$S_{pyro,k}$	pyrolysis source term for species 'k'
t	time
T_g	temperature of the gas phase
$T_{MB,in}$	temperature of the main burner fuel entering the main burner
T_{rad}	radiative temperature surrounding the particle (assumed to be T_g in this case)
V	volatile matter already released into gas phase
V_{int}	initial volatile matter in the solid fuel
w	moles of NO required down stream of the main burner zone
$w_{hm,i}$	rate of i th homogeneous reaction (kg/s)
$w_{k,i}$	reaction rate of species 'k' in reaction number 'i'
X_k	mole fraction of species 'k' in gas phase
X_k	mole fraction of the main burner product gas species
Y_{ash}	ash fraction of reburn fuel on as received basis
$Y_{k,MB}$	mass fraction of product gases in the main burner, CO ₂ , NO, H ₂ O, N ₂ , O ₂

$Y_{kr,w}$	reactant 'kr' mass fraction at the surface of the particle, (ex. for reaction XII, reactant 'kr' is CO ₂ .)
$Y_{FC,daf}$	mass fraction of FC in the reburn fuel on daf basis
Y_N	mass fraction of nitrogen remaining in the fuel
$Y_{N,O}$	initial mass fraction of nitrogen in the fuel
ε	emissivity
ν	stoichiometric mass of species 'k' per unit mass of the carbon in reaction 'i'
ϕ_{RZ}	equivalence ratio in the reburn zone
ϕ_{RS}	equivalence ratio in the reburn supply zone
ρ_p	particle density
σ_{SB}	Stefan-Boltzmann constant
τ_{mix}	characteristic mixing time scale (sec)