MODELLING OF GAS-FIRED BOILER SYSTEMS FOR BUILDING/HVAC PLANT SIMULATION

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ABSTRACT

The current models of boilers and furnaces which are used in HVAC system simulation programs are primarily concerned with calculating the heat output of the device and its fuel consumption. The formulation of the models relies heavily on empirical terms which are derived from manufacturers' data or testing programmes.

Detailed simulation. of the combustion process involves solution of the flow-field. and chemical reaction rate equations by CFD simulation. The computational intensiveness involved renders this approach infeasible for integration into plant simulation. programs.

The objective of this research is to investigate the feasibilty of increasing the functionality and integrity of boiler models to include combustion and pollutant formation processes whilst retaining their usability within HVAC simulation environrnents.

INTRODUCTION

The fossil fuel-fired boiler is a highly significant component of primary plant in buildings, from the point of view of its energy consumption and also its contribution to emissions to the environment. This significance has not been reflected in the rigour and functionality of the boiler models that are used in contemporary building and heating, ventilation and air-conditioning (HVAC) plant simulations. The output of currently available boiler models is generally limited to calculating the energy input to the building system and the fuel consumed.

Concern about the levels of emissions from combustion systems together with a steady movement towards carrying out total environmental impact analyses of new developments suggests that a more comprehensive type of boiler model, capable of generating output such as NO_x, CO, SO_x levels would make a valuable contribution to the role played by simulation in the analytical phase of the design process.

The objective of this research project is to investigate the extent to which the functionality of boiler models can be increased to include combustion-related effects without compromising their usefulness when incorporated within HVAC system simulation programs.

CONTEMPORARY BOILER MODEL

1) Simplified Models

The first empirical models incorporated into HVAC system simulation programs were typically based on curve fits of operating efficiency against load [1, 2]. This allowed connection of the model to the appropriate system variables (flow and return temperatures, water mass flow rate) but there was minimal representation of the processes within the component.

Many of these shortcomings have been addressed by recently described models such as the ASHRAE Primary Toolkit [3] and Liège [4] boiler models. The level of modelling was raised to include a more complete representation of the system variables and some modelling of the internal process within the component. This can be summarised as:

- an adiabatic combustion chamber with a one-step global (complete) reaction producing an undissociated adiabatic flame temperature.
- A heat exchanger (utilising an empirical (UA) value) extracting useful heat from the combustion products.

- A secondary heat exchanger to model heat losses from the casing to the environment.

This formulation allows a more realistic relationship to be established between the boiler's operating conditions and its predicted performance. It does not, however, predict effectively the change in performance when the boiler is operating under continuous modulating control. There is no intrinsic ability to account for the performance when the boiler is fired by different burners and emissions prediction is limited to CO_2 rates.

Little attention has been paid to the 'internal' calculation of heat transfer coefficients, as is commonplace, for example, in heating/cooling coil models. Whilst there is no reason why this should not be feasible in the post-flame gases, there are a number of difficulties raised. Local evaluation of the fluid thermal properties can be computationally intensive [5] and there is little reliable data on, for example, flue gas viscosities.

(2) CFD-based Models

The combination of chemical reaction modelling with flow field prediction afforded by contemporary (research and commercial) CFD codes has led to significant advances in combustion modelling. Most of this activity has been carried out in the propulsion field and there has been comparatively little work done on stationary systems.

The reported work has been focused on the gas-side processes of combustion and heat transfer to the walls and is not extended to the overall modelling of the component. Notwithstanding the contemporary computing power it is not feasible to solve a comprehensive set of combustion equations simultaneously with the flow field. As the formation of pollutant species does not involve significant energy changes compromise solutions such as post-processing [6] and extent of reaction interpolation [7] have been employed.

This research is aimed at bridging the gap between the two approaches outlined above to develop boiler models which can provide representation of the combustion characteristics such as NO_x, SO_x and CO emissions, together with a more detailed modelling of heat transfer processes whilst remaining sufficiently compact to be incorporated into building/HVAC plant simulation programs.

DESCRIPTION OF THE MODEL

(1) Scheme

The modelling scheme which forms the basis of this work is summarised by the flow diagram of Fig 1.

There are four zones, each with an idealised residence time distribution:

- an adiabatic combustion zone
- a combustion chamber containing post-flame gases with radiative and convective heat transfer to the walls
- a multi-pass counterflow heat exchanger (convective heat transfer only)
- the flue system (a cross-flow heat exchanger with unmixed fluid on the flue gas side).

Losses to the environment from the water jacket are modelled as a subsidiary cross-flow heat exchanger.

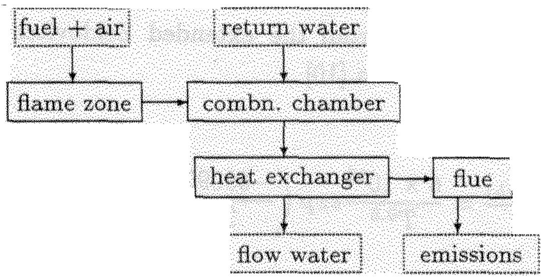

Figure 1: Flow Diagram for Boiler Model

(2) Flame Zone

The key to a simplified model of this type is the way in which the flow/mixing characteristics can be represented in a way which preserves computational economy with reproduction of the characteristics of different burner types. This has been effected in the one-dimensional approach adopted here by modifying the composition and temperature of the species entering the flame zone.

This is carried out by defining a mixing distribution function $\Phi(T, x)$ which is at present derived empirically from burner test data. This function essentially forms the triggering mechanism for the equations used to model the combustion process: a null value corresponds to plug flow in the flame zone with no backwards propagation of species or enthalpy. In this limiting case, there is no ignition or propagation of the flame.

To accomodate the prompt-NO mechanism in the modelling of NO_x formation a two-step combustion model is used [8]

$$\frac{-d[CH_4]}{dt} = 10^{10}\left(\frac{RT}{P}\right) exp\left(\frac{-12019}{T}\right)[CH_4][O_2] \tag{1}$$

$$\frac{d[CO_2]}{dt} = 10^{10}\left(\frac{RT}{P}\right) exp\left(\frac{-12019}{T}\right)[CO][O_2] \tag{2}$$

At each time step the appropriate concentrations and the gas temperature are updated and the prompt-NO formation calculated from [9]

$$\frac{d[NO_{pr}]}{dt} = fKT^n[O_2]^\alpha[N_2][CH_4]^\beta exp\left(\frac{-Ea}{RT}\right)$$

and thermal NO from the extended Zeldovitch mechanism equation [10]

$$\frac{d[NO_{th}]}{dt} = \frac{6 \times 10^{16}}{T^{0.5}} exp\left(\frac{-69090}{T}\right)[O_2]_e^{0.5}[N_2 \tag{3}$$

All calculated rates have the units (mol $\mathrm{cm}^{-3}\,\mathrm{s}^{-1}$). The equations are solved using a finite time-step with the energy changes evaluated at each time step for equations 1 and 2. The energy changes associated with NO formation are small and are not evaluated.

(3) Combustion Chamber

The combustion chamber is discretized in the direction of gas flow. No further combustion modelling takes place; however the formation of thermal NO continues in the post-flame gases and is modelled in each segment by solving equation 3. A good predictive model for CO formation in the combustion chamber is difficult to devise in a simplified model. Carbon monoxide is formed much faster than it decays, and with a reaction time constant of approximately 2 ms under typical conditions, can be regarded as being in equilibrium.

The equilibrium concentration of CO is calculated at the mean temperature in the combustion chamber (typically 1700K) and is taken to be 'frozen' at this level by the rapid quenching in the heat exchanger.

Heat transfer from the gas to the combustion chamber wall is calculated by both radiation and convection. The radiation component is modelled as a cylindrical flame with unity view factor, using the mean gas temperature within the chamber:

$$Q_r = R_r A_w(\overline{T_g}^4 - T_w^4 \tag{4}$$

The gas-to-wall convective film coefficient is evaluated at each of the sectors by the following expression which allows for entry length effects and large temperature differences between the gas and the wall [11]:

$$\begin{aligned} Nu &= 0.0214(Re^{0.8} - 100)Pr^{0.4} \\ &\quad \left[1 + \left(\frac{d}{L}\right)^{0.67}\right]\left(\frac{T_g}{T_w}\right)^{0.4} \end{aligned} \qquad (5$$

A fixed water-side heat transfer coefficient is estimated from

$$Nu = 0.023(Re^{0.8}Pr^{0.4}) \tag{6}$$

giving a value of around 500 W m^{-1} K^{-1}. The thermal resistance of the metal wall is neglected.

(4) Main Heat Exchanger

The main heat exchanger (usually of the triple-pass type) is modelled as a standard counter-flow unit. Because of the decreased gas temperatures (typically 1300K) NO formation and radiation heat transfer are negligible in this component. Radiative and convective heat transfer are modelled as within the combustion chamber.

BOILER PERFORMANCE PREDICTION

(1) Global Performance

Initial evaluation of the output of this model has been made by modelling the performance of a cast iron, triple-pass gas-fired boiler equipped with a standard blast tube [12]. Comparison of the predicted global performance of the boiler with generic figures for this type of boiler obtained from a commercial testing programme [13] are shown in Table 1. The test figures were obtained with the boiler firing at its rated input (190 kW), a water return temperature of 71°C and a flow temperature of around 82°C.

	Predicted	Measured
NO_x (ppmv wet)	47.0	45.5
CO (ppmv wet)	32.0	33.6
Flue Gas Temp. (°C)	212	171

Table 1: Global Performance of Triple-Pass Boiler

The predicted emissions performance figures agree well with the measured values: however, the measurements only apply to a single operating point. It can be seen that the heat transfer performance of the device is under- estimated as evidenced by the exit gas temperature which is 50°C higher than the measured value: this corresponds to an under-prediction of the boiler eficiency of about 2%.

(2) Thermal Performance Characteristics

Most commercial-size boilers can operate under continuously modulated control. The limit on this is the *turn-down ratio* defined as:

$$\frac{maximum\ firing\ rate}{minimum\ firing\ rate}$$

both the air and fuel are modulated proportionately. As the fuel and air flow rates are reduced, the exit flue gas temperature should fall, with a corresponding increase in thermal efficiency. The residence time of the gases in the device gets longer, with a consequent increase in the 'size' of the heat exchanger.

Figs 2 and 3 show that the model correctly predicts these trends as the firing rate (expressed as a fraction of the rated input) is reduced.

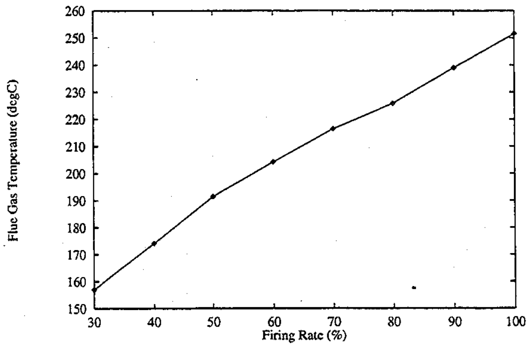

Figure 2: Variation of Flue Gas Temperature with Firing Rate

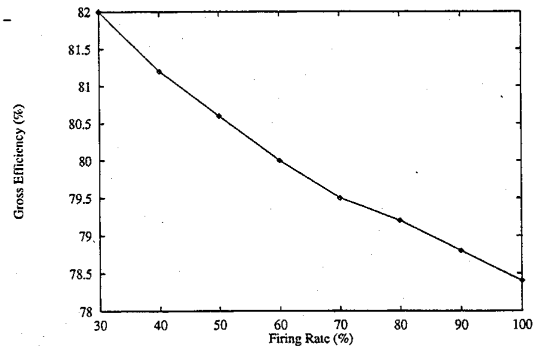

Figure 3: Variation of Gross Thermal Efficiency with Firing Rate

(3) NO_x Emission Characteristics

The formation of NO_x is strongly dependent on temperature and more weakly affected by oxygen concentration. As excess air leads to a reduction in flame temperature it is well-known that a peak in NO_x occurs on the lean side of the stoichiometric air:fuel ratio. The predicted NO_x emissions from the prototype triple-pass boiler at its maximum firing rate over a range of excess air levels is shown in Fig 4. A very strong peak can be seen at 2.5% excess air — typical operating conditions are within the range 12 – 15%. Experimental measurements covering this range of operation are not available at present.

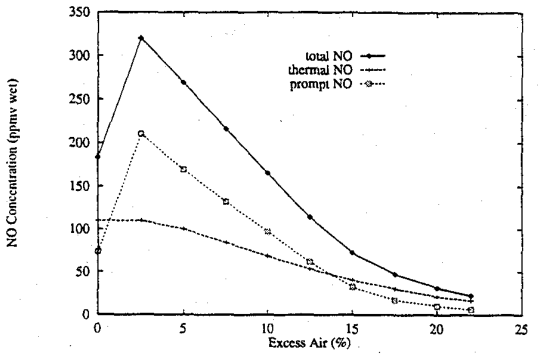

Figure 4: Predicted NO Formation with Excess Air

The variation of NO_x emissions with firing rate is dependent on burner design: for a typical blast tube burner, the curve is rather flat. Fig 5 shows that at typical operational excess air levels the model predicts an increase in NO_x levels as the firing rate is reduced. As conditions in the flame zone are substantially unchanged the prompt NO remains constant. Despite the smaller size of the post-flame high temperature zone, the longer residence time in this region leads to a higher predicted level of thermal NO. The test data [13] shows that some boilers exhibit an increase in NO_x emissions with a reduction in firing rate.

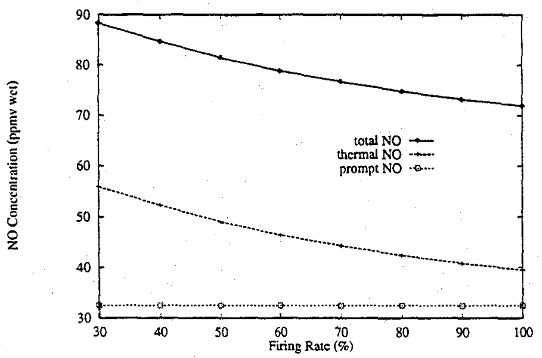

Figure 5: Predicted NO Formation with Firing Rate

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CONCLUSION

A three-component model to represent gas-fired boilers in system simulation programs has been proposed and implemented. The model uses geometrical information on the combustion chamber and heat exchanger of the prototype, together with a characterisation function which allows a concise, one-dimensional representation of the processes at the burner head. At present, this function is obtained by empirical means.

An intial comparison of the output of the model with tests carried out on commercial units has shown that the model has the capability to represent both trends and absolute values representing the thermal and emissions performance of such devices. The calculation of heat transfer processes within the boiler appears feasible, although the current model under-predicts the heat transfer by about 2%.

Future work will initially concentrate on refining the heat transfer prediction algorithm and on modelling as wide a range of boilers for which experimental data is available.

Further development will focus on obtaining the characterisation of the burner performance by CFD modelling; this will remove the remaining direct reliance on direct empiricism for boiler performance prediction.

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NOMENCLATURE

A	Area (m^2)
d	distance along tube (m)
Ea	activation energy (J mol^{-1})
f	constant
K	constant
L	length of tube (m)
n	number of carbon atoms in fuel
Nu	Nüsselt number
P	absolute pressure (bar)
Pr	Prandtl number
Q	heat flux (W)
R	universal gas constant (J mol^{-1} K^{-1})
Re	Reynolds number
R	heat transfer coefficient (W m^{-2} K^{-1})
	time (s)
T	temperature (K)
x	mol fraction
α, β	reaction order
Φ	burner mixing function

subscripts

g	gas
r	radiation
w	wall