

## SYSTEMS BASED CFD MODELLING OF PACKAGE STEAM BOILERS

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**ABSTRACT** Dynamic thermo-fluid models of fire-tube steam boilers can be used to optimise the design and operation of equipment, resulting in possible energy and emissions savings. This work presents the development of a dynamic boiler model of a 4-pass wetback fire-tube boiler, using the commercial 1-dimensional CFD tool Flownex<sup>®</sup>. The thermal model includes all relevant heat transfer and fluid flow phenomenon between the combustion flue gasses and the boiler water/steam. The predicted exhaust flue gas temperatures at different operating pressures are compared favourably to the performance data for a PFTA500-4 boiler, with accuracy improvements over previous modelling studies in the literature. Finally, the transient simulation capabilities of the model are demonstrated for a case of varying steam demand levels, with PID control algorithms implemented to control the feedwater control valve on the mass flowrate of fuel to the boiler. The modelled control system will be further refined in future work to include oxygen trim control over the air/fuel ratio. The completed model will be integrated into larger steam generation and distribution steam networks in Flownex, to assist industrial companies in South Africa in improving their energy efficiency.

## INTRODUCTION

In South Africa, steam boiler systems are used extensively for industrial process heating at temperatures below 230 °C. Although a limited number of large water-tube boilers produce steam in the sugar and paper industries, most plants in the country utilise smaller fire-tube boilers. According to Joubert et al. (2016), the total installed capacity of fire-tube boilers in South Africa is approximately 10.6 GW<sub>th</sub>. These steam systems typically consist of a central boiler house with multiple package boilers connected in parallel to a main steam header. Steam systems are in general highly dynamic in nature and the control of multiple boilers to meet a dynamic plant load is not always straightforward. Based on the author's experience in industry doing steam system audits, there is a significant potential to optimise steam generation, distribution and end-use in South African industry. Dynamic heat transfer modelling of steam systems from generation to end-use can provide data to identify and quantify interventions (either operational or equipment modification) to improve plant performance, thus reducing energy costs and emissions.

In practice, many steam optimisation tools (e.g. Steam System Modelling Tool<sup>1</sup>) are based on a steady-state, steady-flow, analysis of energy and mass balances in a steam system. This approach is well suited for quick calculations, but it is not able to account for the dynamic nature of many plants. For example, when there is a sudden reduction in steam demand, the pressure in the main header will begin to rise.

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<sup>1</sup> The steam system modelling tool forms part of the MEASUR software package that is freely available from the US Department of Energy and can be download <https://www.energy.gov/eere/amo/measur>

This will be detected by the control system, which will reduce the firing rate on the boilers. Once a dynamic model of the steam system exists, it can be used to test different design concepts and control strategies in a virtual environment before making any modifications to plant equipment. Such modelling can also provide an estimate of the potential savings, whilst also identifying any potential challenges that could disrupt production.

This paper presents the development of a network-based Computational Fluid Dynamics (CFD) model of a fire-tube boiler for dynamic simulations. The model is developed in the commercially available software package Flownex<sup>®</sup> and is validated against performance data for the Johnston PFTA 500-4 boiler, with natural gas as the fuel. The boiler model that is presented in this paper will form part of a broader steam system model in Flownex that is being developed by the Council for Scientific and Industrial Research (CSIR) to assist companies with continuous improvement of their steam systems.

## MODELLING METHODOLOGY

**Boiler description.** The analysis presented in this paper is based on a 4-pass wetback boiler design, as shown in Figure 1. Combustion of the fuel and air stream takes place in the furnace pass, where the heat transfer is predominantly by radiation to the inner furnace wall. The flue gas is then moved through a further 3 passes, where heat is exchanged via convection with the inner boiler tube walls. The specifications for the boiler geometry are based on the Johnston PFTA 500-4 boiler, as the manufacturer provides detail about the geometry of the design, as well as the thermal performance for benchmarking the model. The dimensions of the PFTA 500-4 are presented below in Figure 2. At maximum load, this boiler can generate up to 7.6 t/h of saturated steam at pressures up to 25 barg. The Flownex model can be easily modified to account for differing boiler geometries and number of passes.

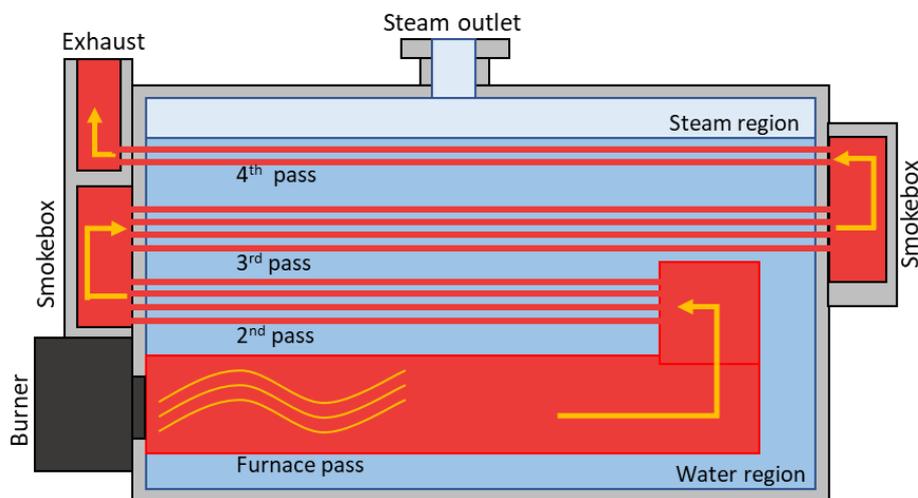
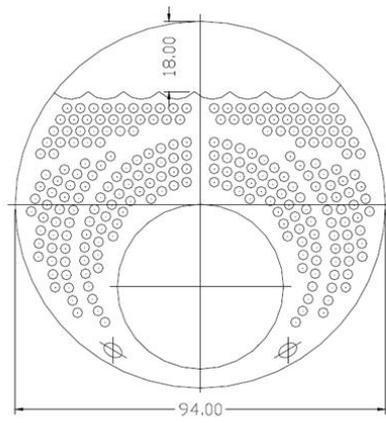


Figure 1: Diagram of 4-pass, wetback, fire-tube boiler.

**Previous studies.** A number of 3D CFD studies of fire-tube boilers have been conducted to investigate and optimise various aspects of the boiler design, including turbulent flames, combustion kinetics, radiation and convective heat transfer (Gutiérrez Ortiz, 2011). Although such modelling can yield critical insight into design of the boiler, a 3D CFD approach is generally not suited to dynamic simulations with an extended simulation time, due to the computational cost of the modelling. Various steady state and dynamic models of the heat transfer within a fire-tube boiler are presented in the literature (Bisetto, et al., 2015; Rahmani & Dahia, 2009; Sørensen, et al., 2003). These models typically involve discretising furnace and convection passes into sub elements and solving the governing energy equations for flue gas, tube wall and water/steam side. Rahmani & Trabelsi (2014) developed a steady state boiler model, which was validated specifically against the Johnston PFTA 500-4 boiler that is considered in this work.



1<sup>st</sup> Tube Pass – 90 tubes  
 2<sup>nd</sup> Tube Pass – 74 tubes  
 3<sup>rd</sup> Tube Pass – 68 tubes  
 Total Tubes – 232  
 (2.5" Tubes)

**Boiler specifications:**

Nominal thermal power: 4.9 MW  
 Maximum steam generation: 7.6 t/h  
 Maximum operating pressure: 25 bar<sub>g</sub>  
 Internal flooded water volume 14.744 m<sup>3</sup>  
 Nominal water volume: 12.045 m<sup>3</sup>  
 Furnace diameter: 1066.8 m  
 Furnace combustion volume: 5.091 m<sup>3</sup>  
 Total heating surface area: 237.5 m<sup>2</sup>  
 Number of convective tubes: 232

Figure 2: Specifications of Johnston PFTA 500-4 fire-tube boiler.

In general, there are a limited number of studies that consider the governing mass and momentum equations in the fire-tube boiler in conjunction with the energy equation. The solution of the full governing conservation equations for fluid flow and heat transfer is required to develop a comprehensive dynamic boiler model that can be used to optimise boiler operation. For example, if the response of a control system needs to be optimised for a specific scenario, it is necessary to model how the pressure in the boiler drum will respond to variations in steam demand, feedwater flowrate, fuel input and air/fuel ratio. Gutiérrez Ortiz (2011) presents a dynamic model of a fire-tube boiler based on the first principles of mass, energy and momentum conservation, which were solved in the Matlab environment. The model was further used to study the transient response of an 800 HP fire-tube boiler with fuel-oil as the energy source. Tognoli, et al. (2018) utilised the model of Gutiérrez Ortiz to demonstrate the PID control of feedwater flowrate and fuel input to a fire-tube boiler, using boiler pressure and water level as a setpoint.

**Flownex modelling.** Flownex<sup>®</sup> Simulation Environment is a commercial 1-dimensional CFD tool capable of modelling systems of flow and heat transfer. In this software, components are used to represent thermodynamic processes, such as flow distributions, heat transfer and combustion all with appropriate correlations. Flownex components are connected in between nodes forming a network and the conservation equations of mass, momentum and energy are solved for this integrated multi-physics network in a 1D coordinate system, where:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho V) = 0 \quad (1)$$

$$\frac{\partial (\rho V)}{\partial t} + \frac{\partial (\rho V^2)}{\partial x} = -\frac{\partial P}{\partial x} - \rho g \frac{\partial z}{\partial x} - \frac{f \rho |V| V}{2d} \quad (2)$$

$$\frac{\partial (\rho (h_0 + gz) - P)}{\partial t} + \frac{\partial (\rho V (h_0 + gz))}{\partial x} = \dot{Q} - \dot{W} \quad (3)$$

Flownex has been successfully applied to the dynamic simulation of different steam systems (Rossouw, 2016; le Grange, 2018). These studies demonstrate the ability of Flownex to accurately resolve the heat transfer and fluid flow in equipment such as boilers, heat exchangers, deaerators, pumps, and turbines. However, the focus of prior investigations has typically centred around large water-tube boilers for electricity generation. In terms of fire-tube boilers for steam production, no previous work was found using Flownex.

Combustion model. The natural gas combustion occurring in the first pass exiting the burner is modelled using components to represent the tube geometry, combustion, different modes of heat transfer into the surrounding water region and the boiler shell with two-phase water. The reactants are modelled discretely according to the mass fractions of fuel constituents. The air and fuel mixing is done on a node and this mixture is used in the combustion model. Flownex contains an adiabatic flame temperature component, which is based on the NASA CEA (chemical equilibrium for applications) library to calculate the flue gas composition and resulting maximum temperature from the chemical reaction of a certain mixture. As natural gas typically consists of more than 90% vol. methane, the fuel in this work was modelled as methane.

A natural gas flame that has a well-controlled air/fuel mixture does not typically produce soot. Therefore, the direct luminous flame radiation can be neglected as its contribution is much lower than the gas radiation from the combustion products (primarily H<sub>2</sub>O and CO<sub>2</sub>). The furnace chamber is assumed to be filled with a grey emitting, absorbing and isotopically scattering fluid medium with a grey furnace wall (Gutiérrez Ortiz, 2011).

The net radiant heat transfer ( $\dot{Q}$ ) between the gas mixture and the enclosed surface of the boiler can be calculated using Eq.(4) (Incorpera & De Witt, 1996), with the gas emissivity and absorptivity based on the Leckner correlation, which is applicable to carbon dioxide and water vapour combustion products and is readily available in Flownex.

$$\dot{Q} = \sigma A(\varepsilon_f T_f^4 - \alpha_f T_w^4) \quad (4)$$

The Leckner correlation is a function of the mixture pressure, component partial pressures, the mean beam length, the gas temperature, and wall temperature. Using this correlation, the gas mixture emissivity and absorption can be calculated. The equation for the gas emissivity and absorptivity are given in Eqs.(5-6) as a function of the emissivity/absorptivity of H<sub>2</sub>O and CO<sub>2</sub> and the Leckner correlation coefficient. For a more detailed description of the Leckner correlation calculations, refer to Modest (2003).

$$\varepsilon_f = \varepsilon_{H_2O} + \varepsilon_{CO_2} - \Delta\varepsilon \left( p_{H_2O} L_b \frac{T_w}{T_f}, p_{CO_2} L_b \frac{T_w}{T_f} \right) \quad (5)$$

$$\alpha_f = \alpha_{H_2O} + \alpha_{CO_2} - \Delta\varepsilon \left( p_{H_2O} L_b \frac{T_w}{T_f}, p_{CO_2} L_b \frac{T_w}{T_f} \right) \quad (6)$$

The combustion flame model in Flownex is a point chemical equilibrium model and does not take spatial effects into account. As described by Gutiérrez Ortiz (2011), the heat is not released instantaneously at the burner inlet, but rather fractionally along the flame length. Previous authors applied linear, parabolic, or exponential heat release profiles along the flame length. In this work the fractional heat release profile recommended by Rahmani and Trabelsi (2014) is used, where:

$$F(x) = \frac{6}{L_f} \left( \frac{x}{L_f} - \frac{x^2}{L_f^2} \right), \quad \text{for } 0 \leq x \leq L_f \quad (7)$$

The Flownex combustion model is used to calculate the total heat release rate from the fuel and associated combustion products for the flue gas. The energy released is then divided along the discretised length of the flame, according to Eqs.(7-8).

$$\dot{Q}_{flame}(x) = F(x)\dot{Q}_{total}, \quad \text{for } 0 \leq x \leq L_f \quad (8)$$

Boiler tube heat transfer segment model. The heat transfer network from the flowing combustion gasses inside the boiler tubes to the water/steam is presented in Figure 3. Flownex allows the creation of a compound component that incorporates these various sub-element heat transfer and pressure drop models. In order to increase accuracy, each pass was discretised into several segments, as stated in the previous section. The network presented in Figure 3 was used for the furnace pass and the convective passes.

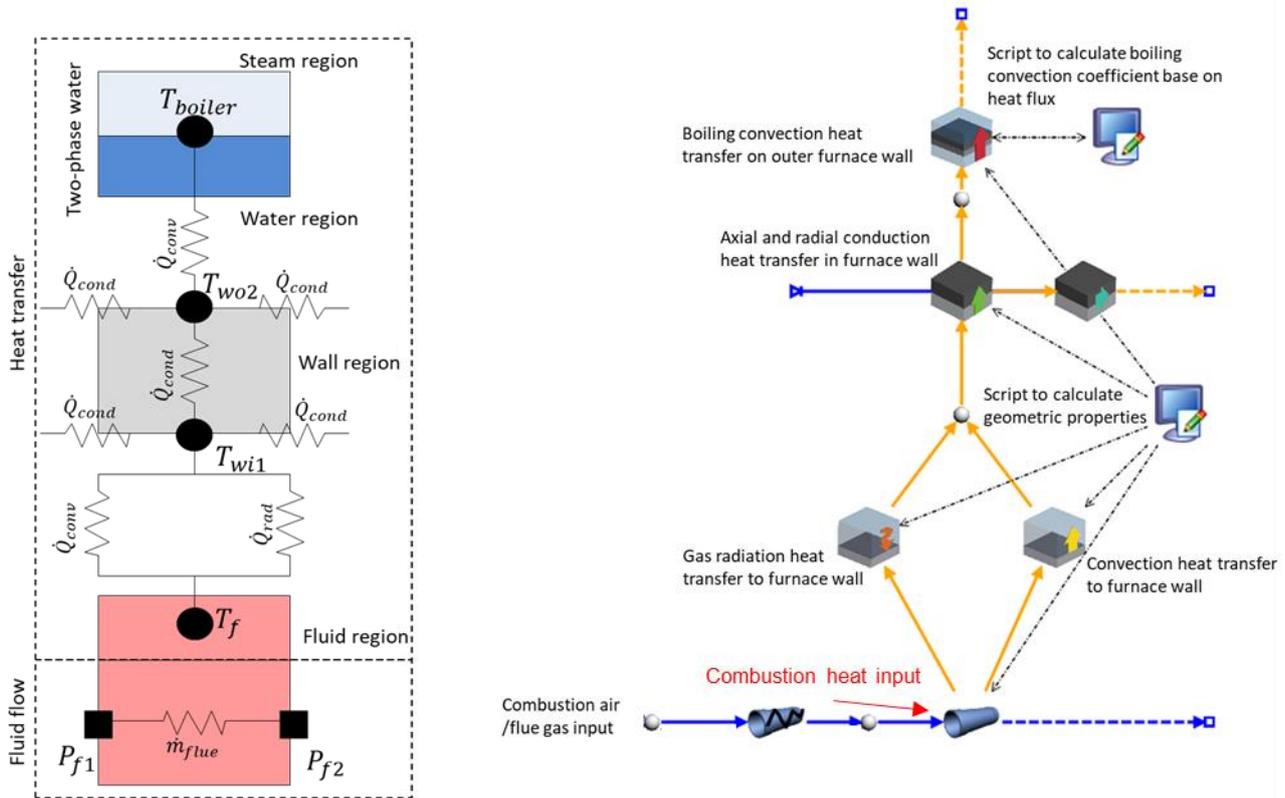


Figure 3: Flownex model of boiler tube heat transfer segment.

In the post flame region in the furnace and convective passes no further heat input is added, and the flue gas only loses heat to the tube walls via convection and gas radiation. For tube passes 2 to 4, there are between 68 and 90 boiler tubes connected in parallel, which are captured in geometry applied to the flow and heat transfer elements.

The fluid volume and pressure drop are represented by the pipe component in Flownex. The pressure drop flow relationship is calculated from the Darcy-Weisbach equation primary losses, given by:

$$\frac{\Delta P}{L} = f \frac{\rho V^2}{2d} \quad (9)$$

The Flownex network contains components for internal convection, fluid radiation, axial and radial conduction as well as external pipe convection on the water-side. Heat is transferred to the inner tube wall via convection and gas radiation. As described in the previous section, the Leckner correlation is used to calculate the flue gas emissivity and absorptivity which is then used to calculate the gas radiation.

The internal convection is modelled with the Dittus-Boelter correlation for the convective heat transfer coefficient with geometry obtained from the pipe component. This equation is shown in Eq.(10). From the correlations provided in Flownex, Dittus-Boelter demonstrated the best accuracy during testing. Flownex allows the specification of custom correlations and could be modified to test other models but was not part of the scope of this study. Axial and radial convection are treated simply as heat transfer resistance based on material thickness and conduction properties for the boiler tubes.

$$h_{conv} = \frac{k_f}{d} 0.023 Re^{0.8} Pr^{0.3} \quad (10)$$

The approach by Rahmani & Trabelsi (2014) was adopted to model the water-side convective heat transfer coefficient, using the Gorenflo correlation, which is based on tube surface heat flux and boiler shell pressure. The equation used for this convective heat transfer is given as:

$$h_{boil} = 5580 \left( 1.73 P_b^{0.27} + P_b^2 \left( 6.1 + \frac{0.68}{1 - P_b^2} \right) \right) \left( \frac{q}{20000} \right)^{0.9 - 0.3 P_b^{0.15}} \quad (11)$$

The increase in heat transfer coefficient due to boiling fluid surround neighbouring heat transfer tubes is taken into account by a modified heat transfer coefficient:

$$h_{boil}^* = h_{boil} \left( 1 + \frac{1}{2 + q/1000} \right) \quad (12)$$

The boiler shell, in which two-phase water and steam separates, is modelled using a two-phase tank component in Flownex. Pipes are connected to this component by specifying the connection height and sub-cooled water and steam can therefore be extracted at the correct location such that a realistic water level can be calculated and verified.

Flownex offers a script component where a user may program certain calculations using input and output variables from other components. For the model in this study, scripts were used to calculate geometric properties where required by heat transfer correlations as well as to calculate the external pipe convection coefficient as described.

Number of segments used in furnace pass. Due to the steep temperature gradients and changing flue gas composition in the first furnace pass, this region of the boiler had the highest influence on the heat transfer calculations. Increasing the number of segments that are used to discretise the furnace (especially the flame length) increases the resolution and thus the accuracy of the heat transfer solution, whilst simultaneously increasing computational cost.

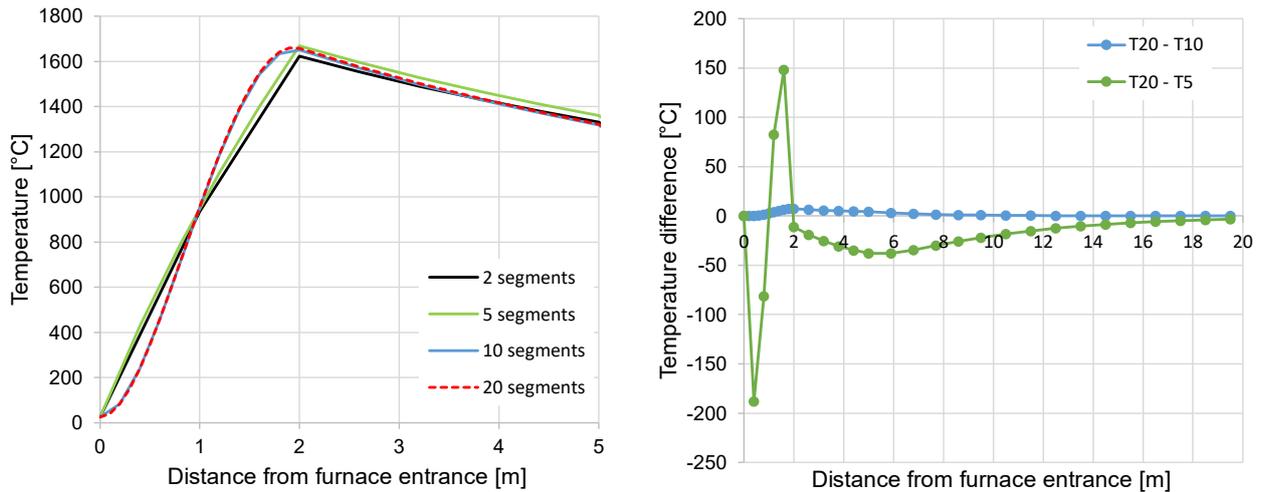


Figure 4: The flue gas temperature recorded when varying the number of segments in the furnace pass (left), and the difference between the different temperature curves (right).

A mesh dependency study was conducted to determine the effect of the number of elements along the flame length on the model results. Note that a 2 m flame length was assumed in this boiler model based on results from Rahmani & Trabelsi (2014). The predicted temperature profiles can be seen in

Figure 4 (left). To gain more insight into the difference between the 10 segments and 20 segments temperature curves, the difference between the curves was plotted in Figure 4 (right). The mesh study shows that the use of 15 segments is sufficient to accurately model the furnace pass with 10 flame, and 5 non-flame elements. In the convective tube passes the results converged quickly when more than 3 elements were used. In this work 5 elements were used to model each convective pass to generate a high resolution of temperature profiles along the path lengths.

A diagram of the full boiler model in Flownex is presented in Figure 5, where each heat transfer element shown in the network is represented by Figure 3. The flame elements include the addition of heat input, whilst the red pipe elements exclude addition heat input. Various pressure, temperature and mass flow boundary conditions are applied to the inlet and outlet nodes on the fire-side and water-side.

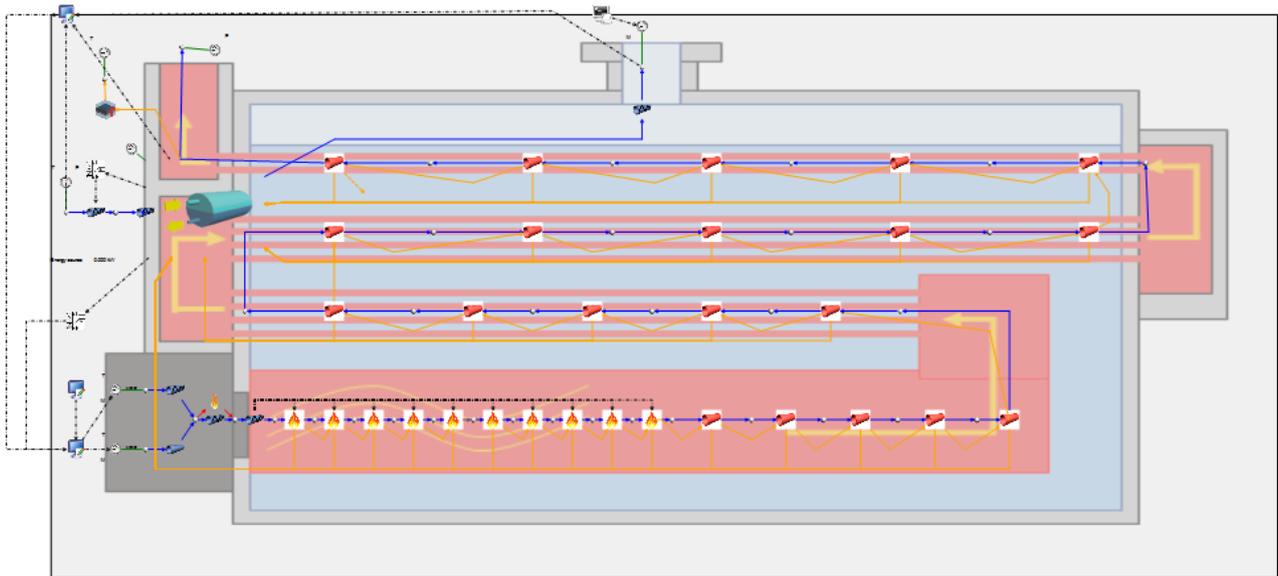


Figure 5: Complete boiler model

### MODEL VALIDATION

The Johnston company provides boiler provides performance data at different boiler operating pressures for the PFTA 500-4. This data includes the flue gas outlet temperature, the steaming rate, and the boiler efficiency. The boiler pressure directly affects the water/steam temperature and therefore the heat transfer within the boiler. The performance from the manufacturer data sheet data is presented in Table 1.

Table 1: PFTA 500-4 Boiler operating data (Johnston boiler company, n.d.)

Pressure [bar <sub>g</sub> ]	Flue gas Temp.[°C]	Efficiency [%]	Steaming rate [kg/h]
0.689	136.7	85.4	7883.3
3.447	168.9	83.9	7730.3
6.895	191.7	82.9	7647.6
10.34	207.2	82.2	7601.8
13.79	219.4	81.6	7573.2
17.24	230.0	81.2	7554.6
20.68	238.9	80.8	7542.8

The given operating parameters of boiler pressure and steaming rate were applied to the Flownex boiler model. Flownex has a built-in designer feature that was used to calculate the mass flow rate of fuel to achieve the desired steaming rate under different boiler operating pressures at steady state. The calculated values for the fuel flow rate are given in Table 2, along with the calculated efficiencies from the thermal boiler model.

Table 2: The Flownex boiler model simulation parameters and recorded values.

Model inputs		Designer calculated	
Pressure [bar <sub>g</sub> ]	Steaming rate [kg/h]	Fuel flow rate [kg/h]	Efficiency [%]
0.689	7883.3	376.87	84.3
3.447	7730.3	382.82	83.0
6.895	7647.6	387.09	82.1
10.34	7601.8	390.13	81.5
13.79	7573.2	392.54	81.0
17.24	7554.6	394.57	80.5
20.68	7542.8	396.34	80.2

The exit flue gas temperature and calculated boiler efficiency from the Flownex model are compared to the data provided by Johnston as well as the model of Rahmani & Trabelsi (2014) in Figure 6. In terms of exit flue gas temperature, the current model can predict the measured data from the manufacturer with a high degree of accuracy. In terms of the calculated boiler efficiency the Flownex model slightly underestimates the boiler efficiency under the given steaming conditions, however the trend is well captured. As the flue gas temperatures are correctly predicted it is surmised that the difference in efficiency could lie in the use of methane in the model, vs the natural gas composition that was used by Johnston during testing.

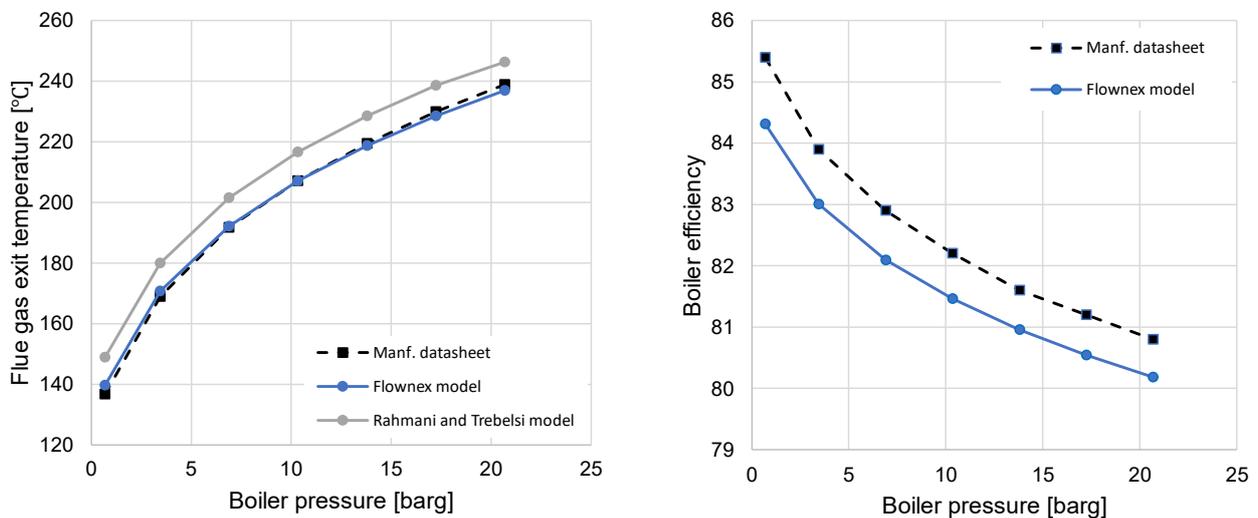


Figure 6: The model and manufacturer output for flue gas exit temperature (left) and boiler efficiency (right) for  $P_b = 21.68 \text{ bar}_g$ .

The flue gas temperature as a function of distance from the burner inlet is presented in Figure 7 (left). Along the assumed 2 m flame length the temperature of the gas rises rapidly reaching a maximum temperature of 1710 °C. As expected, the model results show that radiation is the dominant heat transfer mechanism in the furnace pass, whilst convection is dominant in passes 2 to 4. Due to the high temperature of the flue gas at the inlet to pass 2, gas radiation still plays a role in the heat transfer in this region. For passes 3 and 4 gas radiation is negligible as the gas temperature is significantly lower in these passes.

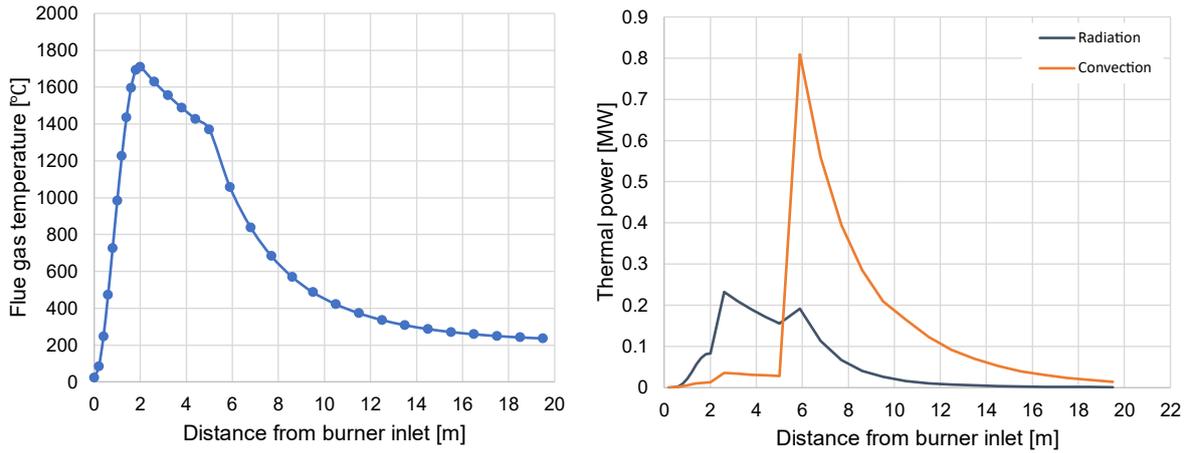


Figure 7: Temperature (left) and heat transfer (right) as a function of distance from the burner inlet, with  $P_b = 21.68 \text{ bar}_g$ .

## DYNAMIC SIMULATIONS

The primary objective of this work is to develop a boiler model that can be used for dynamic simulations. This section presents a simplified example of a boiler control system in operation for a varying steam demand profile. As shown in Figure 8, the boiler is initially operating at steady state with a load of 3 t/h, which is then increased to 5 t/h and 7 t/h before decreasing again. Two PID controllers are integrated into the model to control the mass flowrate of fuel based on boiler pressure, and the feedwater flowrate based on the drum level. For each PID controller the output is a function of the measured error:

$$\text{Output}(t) = K_P e(t) + K_I \int_0^t e(\tau) d\tau + K_D \frac{de(t)}{dt} \quad (12)$$

As the steam demand increases the boiler pressure will begin to drop. This is detected by the control system which then increases the fuel flowrate. Currently it is assumed that the air/fuel ratio can be consistently maintained at 15%. Further models will look at decoupling the control of the combustion air fan from the fuel rate to be more representative of a real system. A second PID controller is used to control the valve position on the feedwater inlet. As the steam demand rises, the level in the boiler begins to drop. This is detected by the control system, which increases the rate of feedwater flow. The PID constants chosen for the fuel controller and the feedwater controller are given in Table 3.

The feedwater and fuel flowrate control systems do have an influence on each other. The feedwater is at a lower temperature than the two-phase mixture temperature in the boiler. Therefore, when the level is rising in the boiler, more fuel is required to maintain the boiler pressure. The boiler pressure also has a small influence on the feedwater flowrate. The upstream pressure to feedwater control valve is fixed, and only the opening fraction of the valve is controlled. Therefore, as the boiler pressure decreases the flowrate through the valve is slightly increased. Overall, Figure 8 demonstrates that the tuned PID controllers can control the boiler operation, with pressure variations below 0.15 bar.

Table 3: Chosen PID controller constants

	Fuel firing	Feedwater valve
$K_P$	$5 \times 10^{-4}$	20
$K_I$	$1 \times 10^{-6}$	0.1
$K_D$	0.01	10
setpoint	2168 kPa	2 m

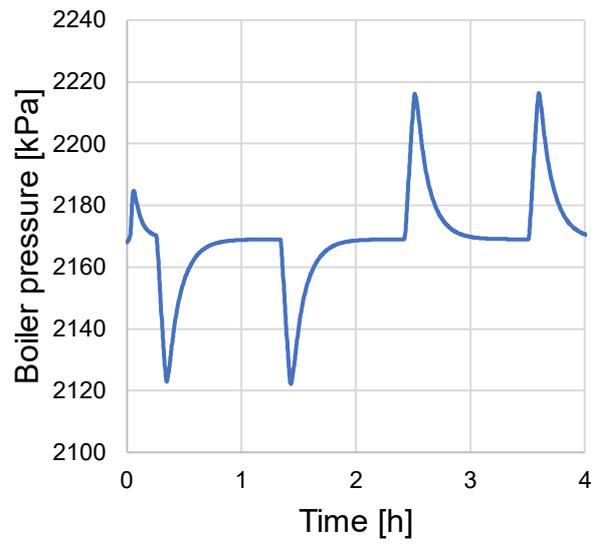
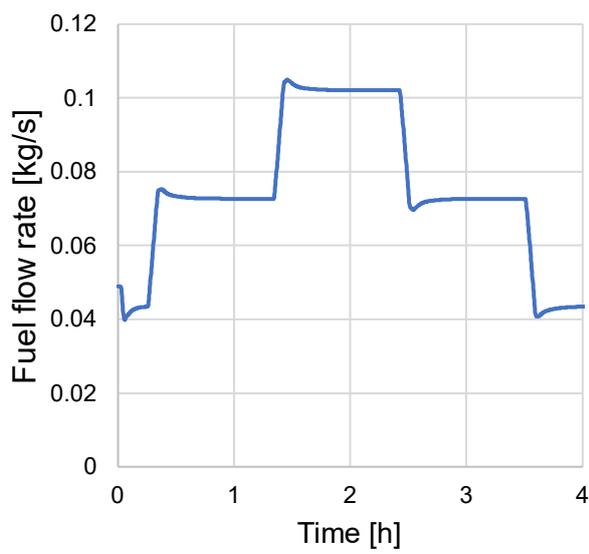
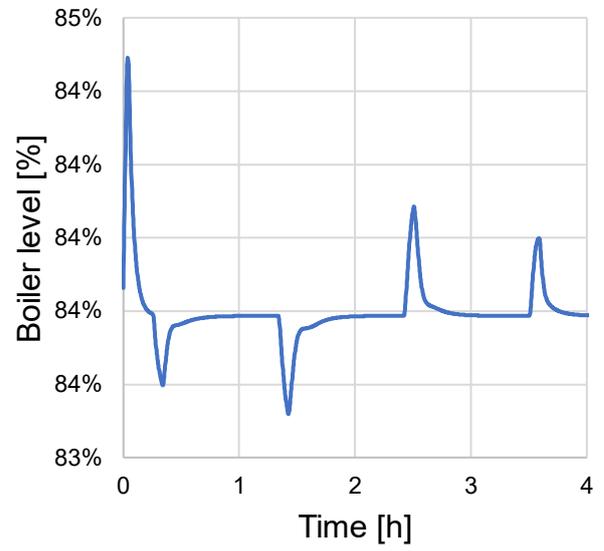
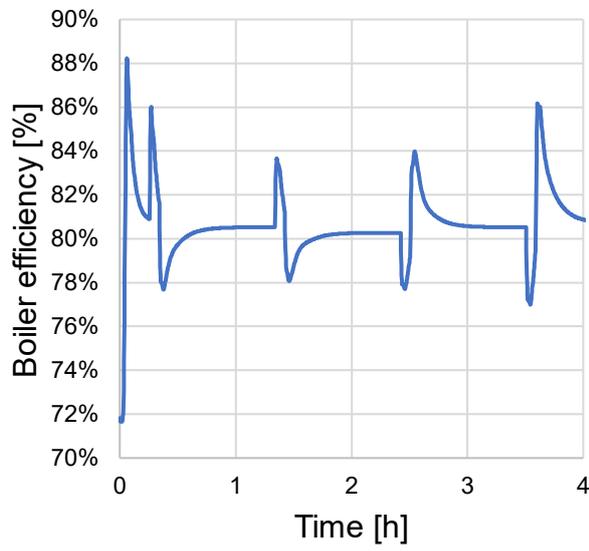
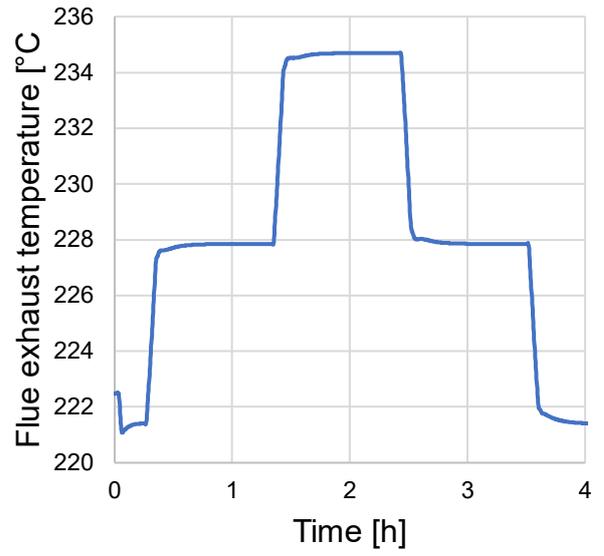
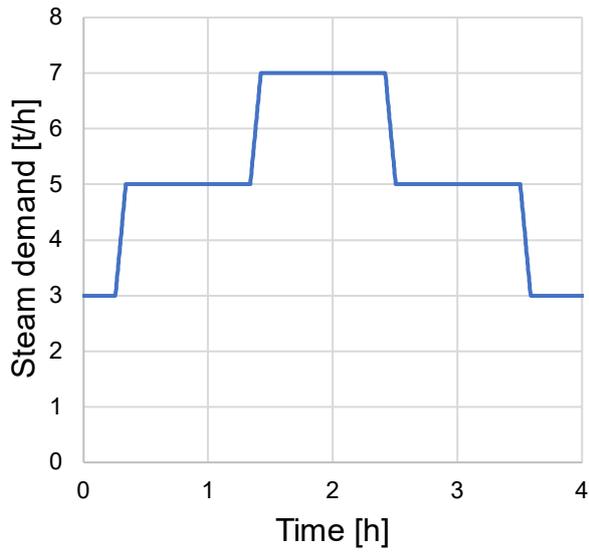


Figure 8: Results of dynamic simulation of boiler with PID control

## CONCLUSIONS AND FURTHER WORK

This paper has demonstrated the use of the one-dimensional, network based CFD approach, to modelling a 4-pass firetube boiler with natural gas as the fuel. The existing heat transfer and fluid flow components Flownex allowed for the rapid development of the boiler model, which can be further tailored to site specific applications with minimal development time. The model accurately predicted the measured exit flue gas temperature profiles at steady state for the Johnston PFTA500-4 boiler, across a wide range of operating pressures, with improvements in accuracy over the model of Rahmani & Trabelsi (2014). The overall boiler conversion efficiency at steady state is slightly underpredicted by the model by less than 1%. The ability of Flownex to solve the system in a dynamic state has been demonstrated for a simplified steam demand profile that is varied with time. A PID based boiler control system is used to control the feedwater flowrate in response to boiler level, and the fuel flowrate in response to boiler pressure. The tuned PID controllers can respond in a stable manner to varying demand.

The boiler component that has been developed will form one part of a larger steam generation and distribution network that is being developed in Flownex. This model will be applied to real world industrial plants to determine opportunities for steam system optimisation from generation to end-use. Further work will also focus on the development of a coal fired boiler model, which is more challenging to control than a gas fired model due to the thermal inertia involved in the boiler.

## NOMENCLATURE

### Roman numerals:

$A$	Boiler surface area	(m <sup>2</sup> )
$c$	Fluid specific heat capacity	(J/kgK)
$d$	Pipe diameter	(m)
$f$	Friction factor	( - )
$h_0$	Specific stagnation enthalpy	(kJ/kg)
$h_{boil}$	Boiling heat transfer coefficient	(W/m <sup>2</sup> K)
$h_{boil}^*$	Modified boiling heat transfer coefficient	(W/m <sup>2</sup> K)
$h_{conv}$	Convection heat transfer coefficient	(W/m <sup>2</sup> K)
$k_f$	Fluid thermal conductivity	(W/mK)
$L_b$	Mean beam length	(m)
$L_f$	Flame length	(m)
$p$	Partial pressure	(Pa)
$P$	Pressure	(Pa)
$\Delta P$	Pressure loss	(Pa)
$P_b$	Boiler steam pressure	(Pa)
$Pr$	Prandtl number	( - )
$q$	Tube surface heat flux	(W/m <sup>2</sup> )
$\dot{Q}$	Heat transfer rate	(W)
$Re$	Reynolds number	( - )
$T_f$	Gas mixture temperature	(K)
$T_w$	Wall temperature	(K)
$V$	Flow velocity	(m/s)
$\dot{W}$	Shaft power	(W)

**Greek numerals:**

$\alpha_f$	Gas mixture absorptivity	(-)
$\varepsilon_f$	Gas mixture emissivity	(-)
$\Delta\varepsilon$	Leckner correlation coefficient	(-)
$\rho$	Fluid density	(kg/m <sup>3</sup> )
$\sigma$	Stefan-Boltzman constant	(W/m <sup>2</sup> K <sup>4</sup> )
$\mu$	Fluid viscosity	(Pa.s)

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