Highlights

Validation of an integrated data-driven surrogate model and a thermo-hydraulic network based model to determine boiler operational loads using a fully connected mixture density network

B.T. Rawlins,Ryno Laubscher,Pieter Rousseau

- Development of mixture density network using simulation data.
- Model based on validated CFD model of a 620 MW_e sub-critical boiler.
- Surrogate model prediction errors are below 10%.

Validation of an integrated data-driven surrogate model and a thermo-hydraulic network based model to determine boiler operational loads using a fully connected mixture density network

B.T. Rawlins[a,*], Ryno Laubscher[b] and Pieter Rousseau[a]

[a]*Department of Mechanical Engineering, Applied Thermal-Fluid Process Modelling Research Unit, University of Cape Town, Library Road, Rondebosch, Cape Town, 7701, South Africa*

[b]*Department of Mechanical Engineering, Stellenbosch University, Banghoek Road, Stellenbosch, 7600, South Africa*

ARTICLE INFO

Keywords:
Mixture density network
Surrogate modelling
Boiler operation

ABSTRACT

A data-driven surrogate model is proposed for a $620MW_e$ sub-critical power boiler. The surrogate model was developed using computational fluid dynamic (CFD) simulation data. The simulation data covered a varied range of inputs.

1. Introduction

The use of neural networks for the modelling of energy systems has been awesome. Optimization of a plant is extremely fun. Using the surrogate model development the model can be developed

*Corresponding author
rwlbra001@myuct.ac.za (B.T. Rawlins); rlaubscher@sun.ac.za (R. Laubscher); pieter.rousseau@uct.ac.za (P. Rousseau)
ORCID(s):

Nomenclature

λ $[W/mK]$ Thermal conductivity
μ $[Pa.s]$ Viscosity
$abbreviation$ explanation for the abbreviation
CFD Computational Fluid Dynamics
E $[J/kg]$ Total energy
p $[Pa]$ Pressure
S $[kg/m^3]$ Mass source term
S_h $[W/m^3]$ Energy source term
S_k $[kg/m^3]$ Species source term
S_m $[N/m^3]$ Momentum source term
T_g $[K]$ Gas temperature
u $[m/s]$ Directional velocity
Y_k $[kg/kg]$ Mass fraction of species k

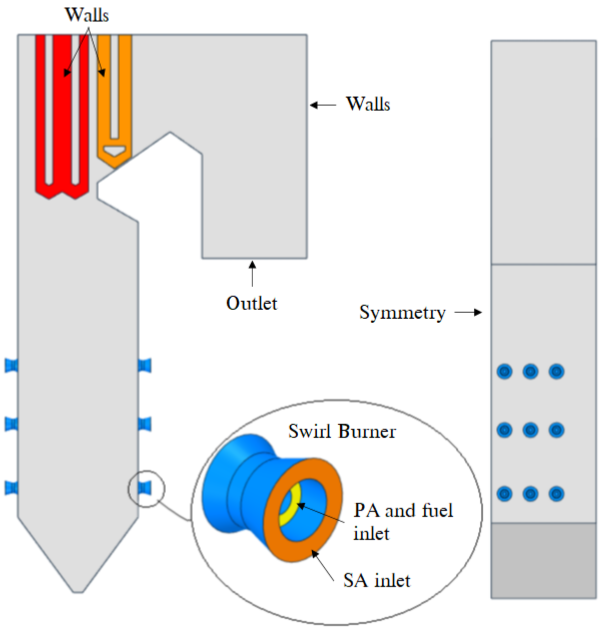
2. Applicable machine learning theory

3. Data generation

A steady-state multiphase non-thermal equilibrium CFD model was used to generate the target data, which was subsequently used for training/development of an appropriate surrogate model.

3.1. CFD model setup

The current study makes use of the commercial CFD software package ANSYS® Fluent 2019 R3 to resolve the fluid flow, heat transfer and combustion processes for a $620MW_e$ utility scale coal fired boiler. The computational domain is modelled on a symmetry plane half way through the depth of the boiler. Figure 1 highlights the computational domain and defines the important boundary conditions.



Boundary conditions		
Name	Type	Specify
Outlet	Pressure outlet	-
Symmetry	Symmetry	-
Walls (Grey, red and orange)	Convection []	Free stream, temperature and heat transfer coefficient
PA and fuel inlet	Velocity	Axial velocity
SA inlet	Velocity	Axial & tangential velocity

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Figure 1: CFD model geometry and boundary condition descriptions.

The general conservation equations, which include, continuity, momentum, energy and species, were solved using a Eulerian approach. The subsequent equations are stated in Equation (1).

Table 1
Summary of combustion models and constants used in the CFD model

Model	Equation/s	Constant/s
Devolatilization		
Single rate kinetic model	$\frac{dm_{vol}}{dt} = R_{vol}(m_{0,vol} - m_{vol})$, $R_{vol} = A_{vol}exp\left(\frac{E_{a,vol}}{RT_p}\right)$	$A_{vol} = 2 \times 10^5[s^{-1}]$, $E_{a,vol} = 6.7 \times 10^7[J/kmol]$ - [5]
Char oxidation		
Diffusion/kinetic - [2]	$\frac{dm_{char}}{dt} = -A_p p_{O_2} \frac{R_{diff} R_c}{R_{diff}+R_c}$, $R_c = A_c exp\left(\frac{E_{a,c}}{RT_p}\right)$, $R_{diff} = \frac{5\times10^{-12}}{d_p}\left(\frac{T_g+T_p}{2}\right)^{0.75}$	$A_c = 0.0053[kg/m^2sPa]$, $E_{a,c} = 8.37 \times 10^7[J/kmol]$ - [5]
Gaseous reactions of volatiles and CO		
Eddy dissipation model - [1]	$R_{k,r,P} = \vartheta_{k,r} M_{w,k} AB\rho\frac{\varepsilon}{k} min\left(\frac{\sum_p Y_p}{\sum_j \vartheta_{j,r} M_{w,j}}\right)$, $R_{k,r,R} = \vartheta_{k,r} M_{w,k} A\rho\frac{\varepsilon}{k} min\left(\frac{Y_R}{\varepsilon_{R,r} M_{w,R}}\right)$	$A = 4.0,\ B = 0.5$

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\begin{aligned}
&\frac{\partial}{\partial x_i}(\rho\bar{u}_i) = S \\
&\frac{\partial}{\partial x_i}(\rho_{eff}u_iu_j) + \frac{\partial\overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\mu\left\{\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3}\delta_{ij}\frac{\partial u_i}{\partial x_i}\right\}\right] + \frac{\partial}{\partial x_i}(-\rho\overline{u_i'u_j'}) + S_m \\
&\frac{\partial}{\partial x_i}(u_i[\rho E + p]) = \frac{\partial}{\partial x_j}\left[\lambda\frac{\partial T_g}{\partial x_j}\right] + S_h \\
&\frac{\partial}{\partial x_i}(\rho u_j Y_k) = -\frac{\partial}{\partial x_j}(\vec{J}_k) + \sum_r R_{j,r} + S_k
\end{aligned}
\tag{1}
$$

The resolution of the Reynolds stress term found in the momentum equation, $-\rho\overline{u_i'u_j'}$, was approximated using the Boussineq equation [6]. In the present study the realizable k-ϵ turbulence model was utilized to address the turbulence closure problem, this model was selected for its applicability in modelling the effects of coal-fired swirl burners [3].

The P1 radiation model was used to resolve the radiative field in the domain. Particle transport was modelled using a multiphase approach, further details on the approach are provided in the validation study of Rawlins et al [4]. The combustion follows a four step sequential process, beginning with the heating and evaporation of the moisture present in the fuel, followed by the devolatilization process where the volatiles are liberated from the solid particle, succeeded by the phenomena of char burnout, and finally the gas phase reactions would commence. The char oxidation reaction product species was set to that of carbon monoxide (CO). For the gas-phase reactions the turbulence-chemistry interaction was approximated using the eddy dissipation model (EDM). A summary of the combustion equations and constants are provided in Table 1.

The simulations were solved using the SIMPLE pressure–velocity coupling scheme. The pressure term was discretized using the PRESTO! scheme. Momentum, species and energy equations were discretized using the second-order upwind scheme and the turbulent kinetic energy and dissipation rate using the first-order upwind scheme. The numerical mesh was generated using quadrilateral elements consisting of 6 million cells. The convergence criteria for the simulation model was set to 1×10^{-3} for the continuity equation, 1×10^{-4} for the velocity equations, 1×10^{-6} for the remaining transport equations, and 1×10^{-4} for monitored key parameters.

3.2. Simulated dataset

As previously mentioned the aim this study is to illustrate the use of a data-driven surrogate model, integrated with a 1D process model, to predict the heat loads to the various heat exchanging components, the flue-gas composition and

Table 2
Design of experiments input ranges for simulations

Input variable	Min	Max	Units
Total fuel flow rate for mills 1 to 6	39.5	120.2	kg/s
Excess air	1.155	1.401	$\%$
Fuel proximate analysis moisture mass fraction, Y_{H_2O}	0.025	0.085	kg/kg
Fuel proximate analysis ash mass fraction, Y_{ash}	0.259	0.559	kg/kg
Platen SH fouling thermal resistance, R_{platen}	0.004	0.007	m^2K/W
Final SH fouling thermal resistance, R_{final}	0.01	0.017	m^2K/W

exit gas temperatures for a utility scale boiler using various high-level inputs. The inputs include the the following, the excess air ratio per burner, the total mill flowrate for the six mills in operation, the average steam temperatures for the platen and final superheaters, the fouling resistance for the platen and final superheaters, the composition of ash and moisture of the fuel and the gross calorific value of the fuel. Thus the input field has a dimensionality of $d_{input} = 14$.

A design of experiments (DOE) was conducted to generate a set of 180 simulation cases to obtain a representative set of results. The various model input ranges used in the DOE are given in Table 2. The ranges where selected to cover a wide range of operational loads with maximum continuous ratings (MCR) between 100% and 30%.

4. Model development

The present work makes use of two types of machine learning models, namely a standard artificial neural network (ANN) and a mixture density designated model connected to a standard ANN (MDN-ANN). The following section will discuss the hyper parameter tuning and final selected model configuration. The programming language Python 3.7.8 and the Tensorflow machine learning libraries were utilized in the present study.

4.1. Model configuration

4.2. Hyper parameter tuning & final model selection

table of NN and MDN data comparison for tuning

Table 3
Hyper-parameter search space for fully connected NN and MDN models

Parameter	NN search space	MDN search space
Number of distributions	-	2,3,4
Number of layers	2,3,4	2,3,4
Number of neurons per layer	10, 40, 80, 100	10, 40, 80, 100
Learning rates	1e-3, 1e-4, 1e-5	1e-3, 1e-4, 1e-5
Mini batch sizes	16, 32, 64	16, 32, 64

Table 4
ANN model selection results

Parameter	NN search space	MDN search space
Number of distributions	-	2,3,4
Number of layers	2,3,4	2,3,4
Number of neurons per layer	10, 40, 80, 100	10, 40, 80, 100
Learning rates	1e-3, 1e-4, 1e-5	1e-3, 1e-4, 1e-5
Mini batch sizes	16, 32, 64	16, 32, 64

Table 4 highlights the hyper-parameter search spaces for both the ANN and ANN-MDN model. The ANN-MDN has an added parameter namely the number of additional distributions the ANN-MDN would fit to the output data.

The hyper-parameter search was conducted in a sequential manner with the number of layers and neurons per layer being the initial step, after which the learning rates were varied, followed by the batch sizes. The ANN-MDN hyper-parameter tuning was conducted in a similar manner only that an additional step is required to establish the best amount of distributions.

5. Results and discussion

5.1. Multiple load validation

Validation includes the use of integrating the surrogate model with a network based-process model of the water/steam side of the utility boiler under investigation. A C# script is used to access the Python API available in the process modelling software, Flownex SE® 2021. This allows for predictions to be made using the trained MDN model. The most probable predictions are retrieved using the surrogate model script and transferred to the respective process model components. A schematic of the surrogate and process models integration is provided in Figure 2.

Measured plant data for a 100%, 81% and 60% MCR load ratings was made available and is to be used compare the accuracy of the integrated model.

5.2. Utility boiler response to poor fuel combustion

The fuel quality is an important factor when determining the Fuels with total moisture contents exceeding The following results illustrate the effects poor quality fuel has on the case studies boiler operational. The study made use of the developed surrogate model to investigate the steady state operation of the boiler burning poor quality coal. In this section the results of a study conducted

6. Conclusion

The present work has shown it is possible

CRediT authorship contribution statement

B.T. Rawlins: Methodology, Software, Validation, Formal analysis, Investigation,Writing original draft, Visualization.. **Ryno Laubscher:** Writing review & editing, Methodology, Resources, Conceptualization.. **Pieter Rousseau:** Writing review & editing, Resources, Conceptualization.

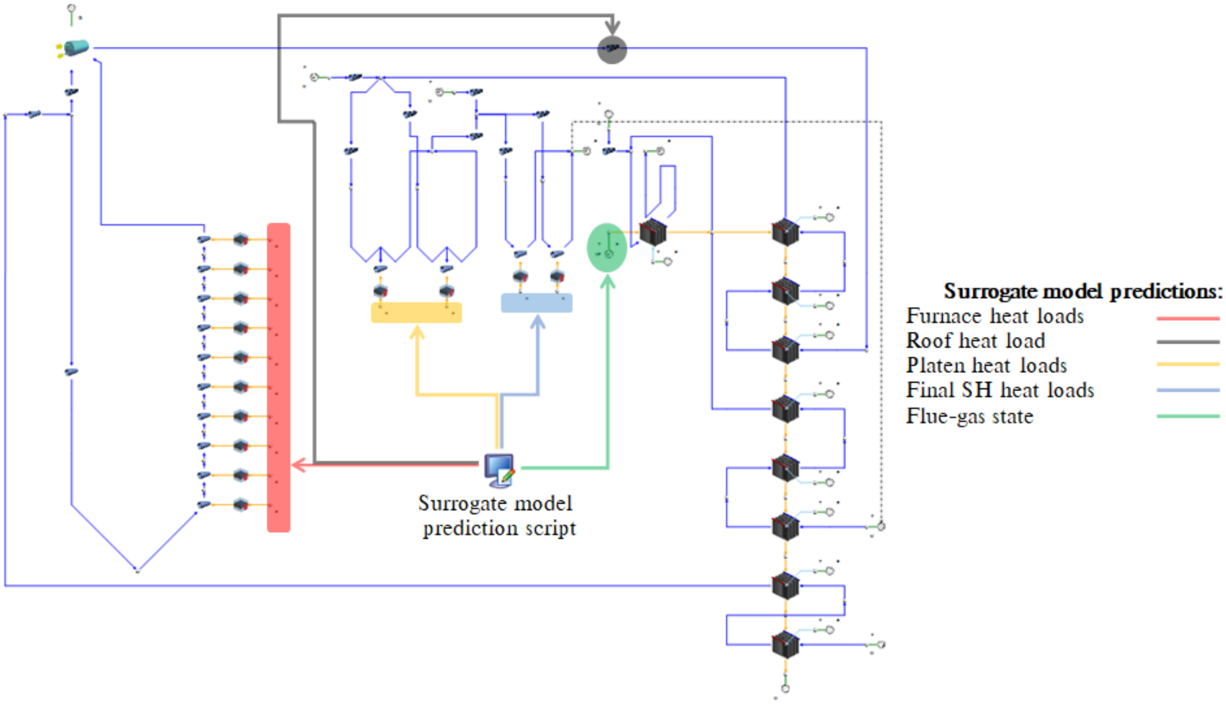

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Figure 2: Schematic of integrated surrogate and network based process model

References

[1] , 2021. ANSYS Fluent Theory Guide. 20 ed., Ansys Inc.

[2] Baum, M., Street, P., 1971. Predicting the combustion behaviour of coal particles. Combustion science and Technolodgy 3, 231.

[3] Modlinski, N., 2010. Computational modeling of a utility boiler tangentially-fired furnace retrofitted with swirl burners. Fuel Processing Technology 91, 1601–1608. doi:10.1016/j.fuproc.2010.06.008.

[4] Rawlins, B.T., Laubscher, R., Rousseau, P., 2021. Validation of a thermal non-equilibrium Eulerian-Eulerian multiphase model of a 620 MWe pulverized fuel power boiler., in: Skatulla, S. (Ed.), 12th South African Conference on Computational and Applied Mechanics (SACAM2020), MATEC Web of Conferences, Cape Town. doi:https://doi.org/10.1051/matecconf/202134700004.

[5] Sheng, C., Moghtaderi, B., Gupta, R., Wall, T.F., 2004. A computational fluid dynamics based study of the combustion characteristics of coal blends in pulverised coal-fired furnace. Fuel 83, 1543–1552. doi:10.1016/j.fuel.2004.02.011.

[6] Versteeg, H., Malalasekera, W., 2007. Introduction to Computational Fluid Dynamics, The finite volume method. Second ed., Pearson Prentice Hall. doi:10.1002/9781119369189.