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

*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

abbreviation	explanation for the abbreviation	CFD	Computational Fluid Dynamics

2. Data generation

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

2.1. 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 $620MW_e$ utility scale boiler. The computational domain is modelled on a symmetry plane half way through the depth of the boiler. This was done to reduce the cell count Figure () highlights the computational domain. The validation of the model and mesh specifics are provided in the works of Rawlins et al (REFERENCE).

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

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

The P1 radiation model was used to resolve the radiative field in the domain. Particle transport was modelled using a multiphase approach with further details provided in the validation study of Rawlins et al(REFERENCE). The combustion follows a four step sequential process, beginning with the evaporation of moisture in the fuel, followed by devolatilization of the volatiles, which made use of single rate model, finally the phenomena of char burnout would follow making use of the kinetic/diffusion model of Baum and Street (REFERENCE). For the gas-phase reactions the turbulence-chemistry interaction was approximated using the eddy dissipation-finite rate model. A summary of the combustion models used by the CFD model are provided in Table ().

Table 1
CFD model utilized combustion model summary

Model	Equation	Constants
Devolatilization - Single rate (REFERNCE)	$\frac{dm_{vol}}{dt} = R_{vol}(m_{0,vol} - m_{vol})$, $R_{vol} = A_{vol} exp\left(\frac{E_{a,vol}}{RT_p}\right)$	$A_{vol} = 2 \times 10^5 [s^{-1}]$, $E_{a,vol} = 6.7 \times 10^7 [J/kmol]$
Char burnout - Kinetic/diffusion model (REFERCNE)	$\frac{dm_{char}}{dt} = -A_p p_{O_2} \frac{R_{diff} R_c}{R_{diff} + R_c}$	$A_c = 0.0053 [kg/m^2 sPa]$, $E_{a,c} = 8.37 \times 10^7 [J/kmol]$
Gaseous reactions - Eddy Dissipation Model (REFRECNE)		

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 convergence criteria for the simulation model was set to 1e-3 for the continuity equation, 1e-4 for the velocity equations and 1e-6 for the remaining transport equations.

2.2. Simulated dataset

3. Model development

3.1. Network based model integration

3.2. Hyper parameter tuning

table of NN and MDN data comparison for tuning

Table 2
Hyperparameter search space for fully connected NN and MDN models

Parameter	NN search space	MDN search space
Number of distributions	-	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 3
Design of experiments input ranges for simulations

Input variable	Min	Max	Units
Fuel flow rate for mills 1 to 6			kg/s
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

4. Results and discussion

5. 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.