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

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- 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

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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

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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, and was subsequently used for training/development of an appropriate machine learning 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 $620MW_e$ utility scale boiler burning a pulverised fuel. 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 and illustrates the important boundary conditions.

(INSERT FIGURE)

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).

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

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 with further details on the modelling is 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 moisture in the fuel, followed by devolatilization of the volatiles, the phenomena of char burnout would follow, finally the gas phase reactions can commence. The char oxidation reaction was set so that the product species is CO. For the gas-phase reactions the turbulence-chemistry interaction was approximated using the eddy dissipation model. A summary of the combustion equations and constants are provided in Table 1 for the interested reader.

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

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

Table 2
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

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 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

design of experiments (DOE) was conducted to generate a set of 180 simulation cases.
Use inputs based on
High low values for DOE what mapping etc

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. Data pre-processing

4.2. Hyper parameter tuning & final model selection

table of NN and MDN data comparison for tuning

Table 3
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

5. Results and discussion

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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