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Coal combustion models: A review

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Abstract.
Computational Fluid Dynamics has been used for optimisation of industrial applications with some level of success. The modest accuracy provided by some of the combustion models in use has left some room for research and improvement. Coal is presented as a fuel with complex chemical properties due to its fossil fuel nature. The devolatilization process of coal is investigated with special attention to the best models that can handle heavy and light volatiles found in coal. The heterogenous char combustion is also presented paying attention to the nature of the char particle during the combustion process. The other processes such as drying, homogenous volatile combustion, radiation models, particle tracking models and turbulent models are investigated in a general manner as they rarely vary with the type of fuel being investigated. A summary of the industrial applications that have successfully utilised the CFD models for optimisation of coal combustion are presented thus helping in drawing the final conclusion.
Keywords: Coal; Combustion; Computational Fluid Dynamics, Devolatilization

1　Introduction

Solid fuels are the main source of energy in large scale power plants with coal contributing most of the energy through combustion. Coal has multiple chemical and physical properties depending on where it is extracted. As such coal can be classified as a rock, sediment, conglomerate or a biological fossil with a complex colloidal system[1]. In as much as the coal structure varies according to the region where it is extracted, generally coal is made up of Carbon, Hydrogen, Oxygen, Sulphur and Ash. Table 1 presents a summary of the thermo chemical properties of coal[2].

Table 1. Thermo-chemical properties of coal[2]

Moisture content, w-%	Net calorific value, J/kg	Ash content, %	C, % (on dry basis)	H, %	N, %	O, %	S, %	Cl; K; Ca
6-10	26-28.3	8.5-10.9	76-87	3.5-5	0.8-1.5	2.8-11.3	0.5-3.1	Trace

Pollution has always been an issue with coal fired boilers though different measures have been proposed over the years to reduce these emissions. This has been due to emissions such as SOx, NOx, CO and CO_2 which are harmful to the environment and the ecosystem. Considerable research has gone into improving the pre, during and post combustion processes of coal combustion but the underlying fact is that the cost of experimental work on large scale plants is high[3][4]. Zimbabwe and South Africa have the highest dependence on coal thermal power plants compared to other forms of energy in Southern Africa. The installed capacity of coal thermal power plants in South Africa is around 40 000MW whilst that of renewable sources and low carbon fuels is around 9300MW[5][6].

The most common way of harnessing energy from coal is through combustion since it is highly exothermic and self-accelerating. Computational Fluid Dynamics (CFD) comes into play with its ability to capture combustion parameters that can later be used for optimisation. For combustion modelling, there has to be knowledge of the theory behind fluid mechanics, heat and mass transfer, chemical kinetics and thermodynamics which makes it a complex task to capture all the physics into one model. The general equations that need to be solved are the conservation equations (mass, momentum and energy)which are

adapted for ANSYS Fluent through the finite volume method of solving equations. The equations formed have the ability to capture the turbulent characteristics of combustion[7].

Combustion of coal in air is considered multiphase as solid phase (discrete phase) and gaseous phase (continuous phase) interact. As with all solid fuel combustion models, the Discrete Phase Model (DPM) or Particle Phase Model is the overall term used to describe all the models that capture the particle-particle and continuum-particle interaction of trajectories, momentum, heat transfer and mass transfer to and from the particles. For coal going through combustion, the first stage is particle drying which means specific equations have to be drafted for this process. The following process is the devolatization process which has always been an area of argument both experimentally and through modelling. The combustion of the products of devolatilization, char and volatiles, then follows leading to heterogenous models for char combustion and homogenous combustion for volatile combustion[8][9]. This paper is going to give insight into the current Computational Fluid Dynamics models used to analyse combustion of coal only.

2 Coal Drying Models

Drying models take an important role especially for cases when there is a considerable amount of moisture in the coal i.e. wet coal combustion. Drying as a water vaporisation process, tends to be affected by the local pressure and temperature within the combustion chamber[10]. Coal generally contains less surface moisture but more of inherent moisture which makes it difficult to remove all the water molecules at this stage. However, most drying models for coal assume complete removal of moisture. As long as the particle temperature is less than the vaporisation temperature, it is assumed that no volatiles are released but only H_2O molecules when they reach their local water vaporisation temperatures. Typically, the energy conservation equation is given in equation (1)[11]:

$$m_p c_{p,p} \frac{dT_p}{dt} = hA_p(T_\infty - T_p) + \varepsilon_p A_p \sigma\left(\theta_R^4 - T_p^4\right) - Q_v$$

(Error! Bookmark not defined.1)

Where m_p, $c_{p,p}$, T_p, A_p, ε_p are the particle mass, specific heat capacity, temperature, surface area and emissivity respectively. T_∞, h, and Q_v are the continuous phase local temperature, convective heat transfer coefficient and heat transfer due to vaporisation respectively. After the coal has lost its surface H_2O, diffusion has to occur due to a concentration gradient from the particle surface. Modelling of the diffusion coefficient is dependent on the coal particle diameter which makes it easier to model coal particles as they are assumed to be spherical during modelling[11][12].

3 Coal Devolatilization Models

Devolatization happens when a fuel loses its volatile components, which takes place when the coal particle is heated in the absence of oxygen. The same energy equation that is modelled during coal drying is called upon with a minor change which recognises the heat of vaporisation for the coal volatiles during the devolatilization process. When coal is heated up during particle drying and devolatilization, it softens up and swells which affects the devolatilization process unlike for biomass. To account for this effect, a swelling coefficient (C_{sw}) is introduced which basically compares the size of the particle before and after swelling as a function of particle diameter and volatile mass fractions, as shown in equation (2)[12].

$$\frac{d_p}{d_{p,0}} = 1 + (C_{sw} - 1) \frac{(1 - f_{w0})m_{p,0} - m_p}{f_{v0}(1 - f_{w0})m_{p0}}$$

(Error! Bookmark not defined.2)

The parameters f_{w0}, m_{p0}, f_{v0} and d_{p0} represent the initial mass fraction of evaporating/boiling material (if wet combustion is modelled), initial particle mass, initial mass fraction of volatiles in the bulk gas and initial particle diameter respectively. The other parameters m_p and d_p represent similar properties after swelling. The reason for the sheer vast number of devolatilization models, is because the process uses assumptions when modelling using CFD[8]. For example, simple models focus on the volatile yield rate whilst complex models focus on both the yield rate and the composition[10]. The devolatilization models used for coal are described next.

3.1 Constant Rate Model

This model assumes volatiles are released at a constant rate, thesame as a constant rate chemical reaction, as represented in equation (3)[8]:

$$-\frac{dm_p}{dt} = A_0 . f_{v,0}\left(1 - f_{w,0}\right)m_{p,0}$$

(Error! Bookmark not defined.3)

where A_0, f_{v0}, and $m_{p,0}$ denote the rate constant, initial volatile mass fraction in the particle, and initial particle mass, respectively. Pillai[10] managed to define the rate constant for different coal species under combustion as 12 s^{-1}.

3.2   Single-Rate Kinetic Model

From a chemical kinetics background, this model takes the first order reaction approach to represent the devolatilization process as represented by equation (4) and (5)[13]. The equation is modelled as a function of the volatiles remaining in the particle.

$$-\frac{dm_p}{dt} = k(m_p - (1 - f_{v0})(1 - f_{w0})m_{p0})$$

(Error! Bookmark not defined.4)

$$k = A_1 e^{-\left(\frac{E}{RT}\right)}$$

(Error! Bookmark not defined.5)

For both coal modelling, as supported by Tabet[8], this model offers the best compromise for determining volatile yield rate hence its use for most industrial applications. Different exponents have been proposed by researchers to improve on the accuracy of this model in predicting devolatilization. Because of this, the model is specific to the coal being tested and the parameters cannot be transferred to other coal species applications[14]. The pre-exponential factor and activation energy can be obtained by means of the Functional Group-Depolymerisation Vaporisation Cross linking code which is closely linked to the FG-DVC model[15].

3.3   Two Competing Reactions Model

This model appreciates that volatiles can be classified so they must be treated differently. Because coal has both heavy volatiles and light volatiles, the devolatilization rates are treated differently. The light volatile matter with higher H/C ratio will be released at low temperatures whilst the heavy volatile matter with low H/C ratio is released at high temperatures. Heavy volatile matter has higher release rate at high temperatures than light matter. This model was refined by Kaboyashi[16]as shown in equation (6) so it can be adapted for CFD.

$$\frac{m_v(t)}{(1 - f_{w,0})m_{p,0} - m_a} = \int_0^t (\alpha_1 k_1 + \alpha_2 k_2)\, exp\left(-\int_0^t (k_1 + k_2)dt\right)dt$$

(Error! Bookmark not defined.6)

Where k_1 and k_2 are the competing rates that control devolatilization over different temperature ranges. The parameters $m_v(t)$, α_1, α_2 and m_a represent volatile yield up to time, mass stoichiometric factor for low temperatures, mass stoichiometric factor for high temperatures and mass of ash in particle. By separating the devolatilization process, the model tends to be more accurate than the single rate kinetic model. However the limitations are shared with the single rate kinetic model as it cannot predict the volatile compositions and can only be used for the same coal species under study[9], [17].

3.4   Chemical Percolation Devolatilization (CPD) Model (1990)

The CPD model characterises the devolatilization behaviour of rapidly heated solid fuels based on the physical and chemical transformations that take place within the fuel structure. This makes the model have the ability to predict the composition of volatiles [8]This model can be classified as a phenomenological model as it is not based on the Arrhenius equation. The approach is based on taking coal as being represented like a lattice that has aliphatic bridge connections. The bridges break during the devolatilization process but not at the same temperature[14].

3.5   Functional Group (FG) Devolatilization Model (1979)

As the previous CPD model, this model is able to predict the volatile composition produced though it is based on elemental and functional groups that make up the coal structure. Ma et al[18] managed to employ the model with satisfactory results for a 0.5 MW Pulverized Furnace Test Facility. The fuels that were used

were coal, milled wood, Palm Kernel Extract and Olive Miscanthus with a substitution of 15 to 20% on an energy basis[18].

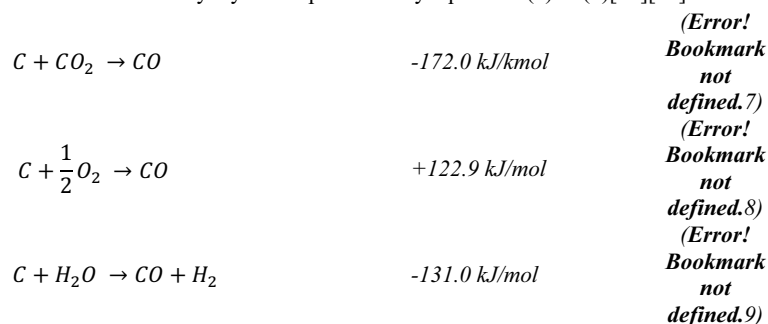*3.6   Functional Depolymerisation Vaporisation and Crosslinking Devolatilization model (1990)*

This model combines the Functional Group (FG) model for gas evolution and the statistical Depolymerization, Vaporization, and Cross linking (DVC) model. The FG subroutine is used to describe the gas evolution of the elemental and functional group compositions of the tar and char by use of chemical kinetics[19].The DVC subroutine is employed to determine the amount and molecular weight of macromolecular fragments, the lightest of which evolves as tar and the heavier ones to metaplast. This process of evolving involves depolymerisation, cross-linking and transport. Cross-linking in the DVC subroutine is computed by assuming that this event is correlated with CO_2 and CH_4 evolutions predicted in the FG subroutine for tar formation[14][20]. Alvarez et al[21]validated their experimental results which showed a deviation of ±5%.

3.7   Other Devolatilization Models

The use of these models is limited in industrial applications because either they have not been sufficiently validated yet or they require a lot of computational power to execute These include, Universal Devolatilization Process Model the FLASHCHAIN Model and the Distributed Activation Energy Devolatilization Model (DAEM). The FLASHCHAIN Model is a phenomenological model that can predict the volatile contents and requires knowledge of the ultimate analysis of the coal. The principle is based on four generic structural components that are used to characterise coal, labile bridges, aromatic nuclei, char links and peripheral groups. Labile bridges are considered important as well because their evolution determines the tar and gas yields which in-turn determines that volatile yield rate[14]. The Distributed Activation Energy Devolatilization Model (DAEM) assumes that the devolatilization process is comprised of independent reactions that occur parallel to each other. What is important is that these reactions all have unique properties such as order of reaction as well as activation energy. This approach makes the model more accurate than the single rate kinetic model and the two competing kinetic reactions though the limitations are shared [22]. The Universal Devolatilization Process Model is developed from the framework of the competing two step model with the difference being in the determination of the kinetic parameters[23].

4   Coal Heterogenous Char Reaction Models

As soon as volatiles leave the coal particle, the coal would have softened up taking a spherical shape. This offers an easier approach to modelling of coal species as no effort is put on adjusting the models to suit the surface of different particles. Heterogenous char combustion is a surface process that requires high temperatures to react. Generally, the global reactions between Carbon and Oxygen result in the formation of Carbon Monoxide within the boundary layer as represented by equations (7) to (9)[24][25].

$$C + CO_2 \rightarrow CO \qquad \qquad \text{-172.0 kJ/kmol} \qquad \qquad \textit{(Error! Bookmark not defined.7)}$$

$$C + \frac{1}{2}O_2 \rightarrow CO \qquad \qquad \text{+122.9 kJ/mol} \qquad \qquad \textit{(Error! Bookmark not defined.8)}$$

$$C + H_2O \rightarrow CO + H_2 \qquad \qquad \text{-131.0 kJ/mol} \qquad \qquad \textit{(Error! Bookmark not defined.9)}$$

The task of bringing combustion models and industrial parameters together is affected by the issue of unburnt carbon which is the opposite of complete combustion assumed during combustion modelling. Because of this oversight, results from heterogenous char combustion models and experimental results end up in disagreement[14]. The coal heterogenous char reaction models that are of importance are discussed next.

4.1   Diffusion-limited rate model (1971)

The Diffusion-limited rate model is based on the works of Baum and Street[26]under the assumption that the surface reaction proceeds at a rate determined by the diffusion of the gaseous oxidant to the surface of the particle.

4.2   Kinetics / Diffusion-limited Model

As the name suggests, the char reaction is based on both diffusion of oxygen to the particle surface as well as the reaction kinetics that take place at the particle surface. For pulverised coal, below 773K the reaction rate is controlled by chemical reactions and above 1823K diffusion effects take precedence[8][9].Applicable to coal combustion, this model can be divided into two:

4.2.1   Field Char Oxidation Model. More adapted for coal because it has a spherical shape and it is
considered to be surrounded by a stagnant boundary layer through which oxygen must diffuse to
before reacting with the char[27].

4.2.2   Gibb Char Oxidation Model. More adapted for biomass combustion as it caters for the issue of
irregular shapes and pore existence within the fuel particle[10].

4.3   Smith Intrinsic Char Reaction Model (1982)

The works of Baum and Street[26] were modified by Smith[18] because char is known to be a porous substance meaning the pore diffusion rates need to be taken into account. This allows the chemical rate in this instance to be expressed as a function of intrinsic chemical and pore diffusion rates.

4.4   Multiple Surface Reaction Model

This model takes the approach of wall surface reactions, where the char particle depletes according to a set multiple reaction mechanism. However, the model has limitations in alternating between non-premixed, premixed and partially premixed combustion[10][28].

4.5   Multistep semi global kinetics char combustion model

Hurt and Carlo[29]proposed this model by studying the mechanism of O_2 itself and the effect it has on the global properties of the surface reaction such as activation temperature, activation energy and ratio between CO and CO_2. Combustion modelling of reaction kinetics is based on the assumptions that other intermediate reactions are more important than others thus the continued advent of multistep semi global kinetics as they seek to capture combustion parameters[30][31].
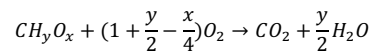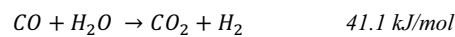
4.6   Boundary Layer Models

These models try to divide the zones of reaction around the char particle into different sections. The simplest is the single film model, which assumes that CO is the primary product of oxidation within the boundary layer represented as a single film around the particle (boundary layer). However, the burnout is usually over predicted with the single film. As a step further, Burke and Shumann[32] adopted the double film model for CFD which automatically assumed the existence of two distinct regions within the boundary layer. Specific reactions take place within each region. Makino and Law[32] developed the continuous film model which considers oxidation of C and CO within the boundary layer to CO_2 which comes at the expense of computational power and complexity. This in turn makes the continuous film model unattractive for engineering modelling applications[24][33].

5   Homogenous Volatile Matter Combustion Models

The volatiles released during devolatilization create a source for gaseous combustion. Volatiles carry almost 50% of the energy for coal. Ignition and flame stability, local temperature, species distribution and pollutant formation are all influenced by volatiles combustion. In CFD simulations, the volatile gases are lumped into one single "artificial" species, CH_yO_x or a few artificial species. Since homogenous combustion is a reaction between gases, homogenous combustion models are applicable to any type of fuel and the usual reactions are presented by equations (10) to (13). The reaction mechanisms used byhomogenous volatile matter combustion models are either global one step reaction mechanism, global two step reaction mechanism and Jones and Lindstedt 4-step mechanism[11][21].

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$
          242.0 kJ/mol   *(Error! Bookmark not defined.10)*

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$ *283.0 kJ/mol*   *(Error! Bookmark not defined.11)*

$$CO + H_2O \rightarrow CO_2 + H_2$$ *41.1 kJ/mol*   *(Error! Bookmark not defined.12)*

$$CH_yO_x + (1 + \frac{y}{2} - \frac{x}{4})O_2 \rightarrow CO_2 + \frac{y}{2}H_2O$$ *(Error! Bookmark not defined.13)*

5.1   Eddy-Dissipation model
The model is based on the assumption that the chemical kinetic rate is directly proportional to the time required to mix reactants at the molecular level. Due to the turbulent nature of combustion, the eddy properties are responsible for giving the information concerning mixing time. A drawback of the EDM model is the lack of generality for the constants meaning validations are needed for each application process rather than having a global constant[10][34].

5.2   Finite Rate Chemistry model
This model is based on computing the chemistry reaction rates of the different species during the combustion process[8]. The finite rate kinetics model or finite rate chemistry model further makes the assumption that turbulence and chemistry do not interact leaving the chemical rate of reactions for the different species to provide the major information. As such the turbulent fluctuations aren't factored leaving the chemistry mechanisms contributing much of the information. However, since reaction kinetics or mechanisms need a lot of processing power to capture all the reactions involved, the model usual provides challenges on an industrial scale where vast data is provided[35].

5.3   Eddy Dissipation Concept (EDC) model
The Eddy Dissipation Concept (EDC) is an extension of Eddy Dissipation Model (EDM). As the EDM model is classified as a breakup model, likewise the EDC model depends on the eddies formed (fine structures) as mixing occurs at a micro scale[36]. The fine structures are demarcated by a parameter from the Kolmogorov scale which implies that reactions take place in the fine structures whilst the larger structures are considered inert until they break up into smaller eddies. However, gas phase combustion models like the EDC are originally developed for high-Reynolds-number conditions[35][37].

5.4   Equilibrium approach model
This model uses a Probability Density Function in the form of look up tables to describe the turbulence-chemistry interactions during the combustion process. As noted by Tabet et al[8], no individual species transport equations are solved but rather the mean and variance of the species mixture fraction are solved.

5.5   Mixed-is-reacted approach model
As the name suggests, once the fuel and the oxidant come into contact, products are formed. This model is also referred to as the equilibrium model because the mass fractions of fuels, oxidant and products are obtained by solving transport equations of mean and variance of the mixture fraction for each fuel. This model works best for applications with high Damköhler numbers (Da>>1), meaning turbulence occurs very quickly compared to the actual reaction [33].

6   Turbulence Models
Generally, turbulence models seek to solve the conservation equations consisting of mass, momentum, energy and species concentration equations for the case of combustion. To make the conservation equations easily solvable, a modified set of conservation equations is formed by introducing averaged and fluctuating components for each parameter. This gives rise to the Reynolds Averaged Navier Stokes equations which need different hypothesis to solve for the extra coefficients formed depending on the application. The most common hypothesis results in the formation of a two-equation model which is called the k-epsilon model. The other variations of k-epsilon model which have been successfully applied include the RNG k-epsilon

model and the Realizable k-epsilon model which mainly differ on the values and expressions used to represent the constants in the equations[10].

7   Heat Transfer Models

The dominant heat transfer mode during combustion is radiation which accounts for most of the energy needed for drying, devolatilization and char combustion. Likewise, the models used in CFD modelling vary in accuracy and computational power requirement depending on their industrial applications. The Radiative Transfer Equation(RTE) captures certain parameters related to radiation heat transfer which include frequency, position vector, direction vector, path length, absorption coefficient, scattering coefficient, Blackbody emission intensity, Spectral radiation intensity, local absolute temperature, solid angle, radiation intensity source term. Because modelling is associated with reducing an equation whilst capturing the essential physics, radiation models are formed based on what information is important [10][25].

7.1   Directional Models

Directional Radiation Models currently being used include The Discrete Ordinate model, P1 model (Differential Approximation model),Rosseland Model, Discrete Transfer Radiation Model, and The Monte Carlo model[10]. The Discrete Ordinate model reduces the entire solid angle into a finite number of solid angles, also known as discretization. The accuracy of this model depends on the number of solid angles one wishes to form which also increases the computational power required[38].The DO model also results in false scattering and ray effects which gives rise to lack of conservation of radiative energy. The P1 model expands the radiation intensity into an orthogonal series of spherical harmonics which then transforms the RTE into a set of simultaneous partial differential equations. Further approximations on the P1 model will give the Rosseland Model which appears as a simple conduction equation with all the parameters being temperature dependent. However, the Rosseland Model has its limitations near a boundary. The Discrete Transfer Radiation Model is less expensive computationally as surface radiation is assumed to be a single ray. However the accuracy of this model can be increased by tracing more rays to represent the surface[25].

7.2   Spectral Models

Radiation can be described according to its level on the electromagnetic spectrum. CFD can also be manipulated to define models which are dependent on the electro-magnetic spectrum. The most common model associated with combustion is the Weighted Sum of Gray Gases Model. This model acknowledges that radiative absorption and emission from a gas is characterised by emissivity as a function of temperature and product of gas partial pressure and path length. The dominant emitters of radiation during combustion are CO_2 and H_2O as they are the products which attain the high temperatures. To simplify the input parameters required, look-up tables have been drafted for the emissivity of CO_2 and H_2O at different temperatures, partial pressures and characteristic length[33]. Other spectral models in existence but less robust are the Gray Model and the Multiband Model as they seek to treat the gases either as a single species at one energy level or by defined energy levels on the spectrum[10].

8   Particle Tracking Models

Newton's 2nd Law of motion stipulates that particle motion is due to forces acting on the particle. Hence integration of the momentum equation considering all the forces acting on the particle gives the particle trajectory. The forces expected to act on a solid fuel particle are drag, lift, gravitational forces and reaction forces (pressure gradient force and virtual mass forces) [39]. Each particle interacts with the fluid and other particles discretely. The multiphase flow (Solid and Gas) uses the Lagrangian Particle Tracking Model also known as the Particle Transport model. For pulverised fuel applications, drag force computation for coal particles is not complicated because they are considered spherical. This is a reasonable assumptions because during coal drying, the coal particle soften, swell and re-solidify to take the spherical shape in the process[1][8].The most basic and simplest models are usually sufficient to deal with most coal combustion applications. Two of the models that can be employed are the Schiller-Naumann Model[40] which uses less computational space and the Morsi and Alexander model[41]which is sensitive to the velocity at which the particles travel within the combustion chamber.

9   Summary of Models in Industrial Applications

Coal has been part of industrial power plants for a long time thus most boilers utilise coal as the primary fuel. CFD has also been a part of optimisation processes thus the models that have been successfully applied to industrial processes are presented in Table 2.

Table 2:Applications of CFD in coal combustion

Industrial Application	Combustion Models			Additional Physical Models	
	Devolatilization	*Heterogenous char combustion*	*Homogenous volatile combustion*	*Drag*	*Turbulence and Radiation*
1 MW combustion test facility in the Power Technology Centre (United Kingdom)[38]	FG-DVC devolatilization	Smith Intrinsic Char Reaction	2-step reaction mechanism; eddy dissipation	Haider and Levenspiel[42]	P-1 radiation RNGk−ε turbulence
150 MW commercial boiler(Chile)[9]	two competing rates	kinetic/diffusion surface reaction	eddy-dissipation	Morsi and Alexander[41]	discrete ordinates Standard k-ε and Realizable k-ε
Co-firing sludge in a 100MW pulverized coal-fired utility boiler (China)[43]	Single kinetic rate	Multiple-Surface-Reaction	2-step reaction, Finite-Rate/Eddy-Dissipation	-	P-1 radiation Realizable k-ε
Co-firing coal and Cynara cardunculus in a 350 MWe utility boiler(Spain)[33]	single rate kinetic		mixed-is-reacted single film	-	P-1 radiation standard κ−ε

10   Conclusion

A comprehensive review on the current combustion modelling practices with respect to the heating industry has been presented in this paper. The present work focused on pulverised coal applications as they seemed to be the most common. With regards to coal particle drying, the heat balance was presented in a general manner with most applications favouring to ignore the latent heat of water vaporisation. The mass balance was however universal as it is dependent on the diffusion of water molecules from the coal particle surface. Several coal devolatilization models were presented according to their capabilities. For applications which are only interested in the volatile yield rate, the single kinetic rate offers a compromise between computational power required and accuracy thus its preferred use over constant rate model, two competing rates model and the Distributed Activation Energy Devolatilization Model (DAEM). For applications that require knowledge of the volatile components, Functional Group-Depolymerization, Vaporization, and Cross linking (FG-DVC) model is favoured over Chemical Percolation Devolatilization (CPD) Model, Functional Group Devolatilization Model, Universal Devolatilization Process Model the FLASHCHAIN Model. These phenomenological models can not only predict the volatile compositions but are able to treat different coal species in one go without the need to constantly change the modelling parameters. However, this comes at the expense of a lot of pre modelling experiments and computational power requirements. Of all the coal combustion processes, devolatilization causes the most problems. All the devolatilization models reviewed find it difficult to perform an adequate analysis of the process at low temperatures. This is mainly due to the fact that as soon as a coal particle is heated during particle drying, light volatiles will start escaping the particle.

Of the heterogenous char combustion models reviewed, an almost equal distribution on the use of the models is deduced. In terms of accuracy, the Smith's Intrinsic Char Reaction offers more accurate results because it acknowledges the porous nature of char. However, because the coal particles are pulverised in the models reviewed, the effect of the char pores is rendered secondary as the particles are already minute.

The homogenous volatile combustion is considered generic as all fuels pass through the gaseous phase. The Eddy Dissipation Model finds use in most of the coal combustion applications alongside the 2-step reaction mechanism. This can be attributed to the fact that too much focus is put on the devolatilization process. The Weighted Sum of Gray Gases Model holds an advantage over other radiation models because it focuses on the radiation emitted by the main products CO_2 and H_2O. The other models have limitations which affect the combustion modelling accuracy to a greater extent. These limitations result in lack of conservation of radiation energy. Because coal is considered spherical for most of these industrial applications, a general drag model is sufficient and the classic Schiller-Naumann Model can be employed for most of the applications. However, because of advancement in fluid mechanics, the Morsi and Alexander Model has found use in more and more applications. Lastly the turbulence models used are centred around the k-ε model as it offers compromise between computational power and accuracy. In case swirling takes a huge role in the application, other models such as of the realizable k-ε and k-ω need to be considered for the sake of increasing accuracy.

Overall, combustion processes are treated as distinct processes during modelling (e.g. devolatisation starts after drying, char combustion starts after devolatilization and so on), though they actually run in parallel in practise. This affects the parameters of each model as the devolatilization model does not necessarily have to wait for particle drying to end but can occur simultaneously. In conclusion, due to the fact that large industrial power plants have little wiggle room to perform experiments on their equipment due to cost limitations, CFD offers alternatives that can be employed to improve plant efficiency.

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