

Marangwanda, Garikai T.; Madyira, Daniel M.; Babarinde, Taiwo O.

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Combustion models for biomass: A review

Garikai T. Marangwanda^{a,b}, Daniel M. Madyira^{a,*}, Taiwo O. Babarinde^{a,c}

^a Department of Mechanical Engineering Science, University of Johannesburg, Johannesburg, South Africa

^b Department of Fuels and Energy Engineering, School of Engineering Sciences and Technologies, Chinhoyi University of Technology, Chinhoyi, Zimbabwe

^c Mechanical Engineering Department, Covenant University Ota., Ogun State, Nigeria

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Abstract

The present work seeks to review the current biomass combustion models in use for industrial applications. Combustion efficiency of coal fired boilers is a major concern for engineers and policy makers especially with the effect emissions have on the climate. Biomass, a renewable fuel, offers an alternative source of energy even when used in collaboration with coal. However, switching of fuel from coal to biomass on an industrial scale is an expensive task if taken up on an experimental basis. This leaves Computational Fluid Dynamics as a viable option for investigating the fuel switching at lower cost. This requires understanding of the numerical combustion models available. The combustion models presented are divided into particle drying models, devolatilization models, heterogeneous combustion and homogenous combustion. Other supporting models that are investigated are based on the particle tracking models, heat transfer models as well as turbulent models. The work is concluded with a summary of the industrial and laboratory applications that have used the models presented. As the models are numerous, trends can be drawn for the most common models as well as the reasons why they are used. Biomass combustion modelling is mainly influenced by the particle shape and the particle surface area under consideration during the combustion process.

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Keywords: Biomass; Combustion; Computational Fluid Dynamics

1. Introduction

In existing coal-fired boilers, co-firing using biomass or organic waste provides an attractive approach to pollution control and efficient use of both the fossil fuel and biomass waste. This is because biomass fuels are considered Carbon Dioxide (CO₂) neutral fuels as they use the same carbon dioxide during their growth [1,2]. The utilization of sawdust in co-firing is an active research area, particularly in Scandinavian countries and Latin American countries that generate significant amounts of waste biomass residue [3]. Biomass is an organic substance that can be classified as woody biomass, non-woody biomass, process waste and processed fuel. Biomass comes in different sizes and properties as given in Table 1 [4].

* Corresponding author.

E-mail address: dmadyira@uj.ac.za (D.M. Madyira).

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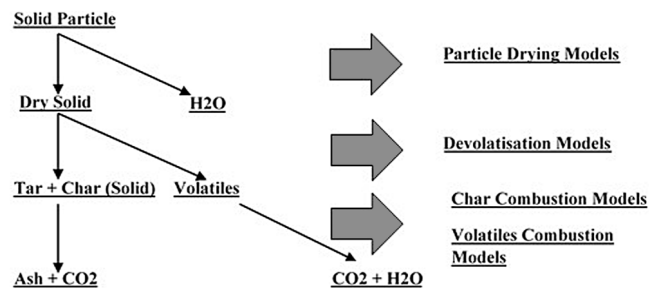
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Table 1. Thermo-chemical properties of biomass [4].

Moisture content (w-%)	Net calorific value (J/kg)	Ash content (%)	C, % (on dry basis)	H (%)	N (%)	O (%)	S (%)	Cl; K; Ca
5–60	18.5–20	0.4–0.5	48–52	6.2–6.4	0.1–0.5	38–42	<0.05	Trace

Legislations have also been put forward in countries like Chile to discourage use of fossil fuels towards carbon neutral fuels [5]. Sawdust being a waste, poses a great risk to the environment and infrastructure as it can burn for almost a year once set on fire. In addition, waste disposal is causing a challenge especially for developing countries as evidenced by the amount of waste sawdust found in Manicaland, Zimbabwe [6]. Generally, when biomass is used at the expense of coal, practical results have shown a decrease in SO_x and NO_x emissions though at the expense of increase in slagging and fouling within the boilers [7]. In as much as western countries have successfully used biomass to produce electricity on a large scale, the African countries are lagging behind in terms of research and implementation of biomass on a large scale [2].

The ability of Computational Fluid Dynamics (CFD) to capture combustion parameters makes it an indispensable and affordable tool in optimization of combustion processes. However, a mathematical description of combustion is complex as fluid mechanics, mass transfer, chemical kinetics and thermodynamics issues all come into play. The fluid mechanic and thermodynamic conservation equations (mass, momentum and energy) need to be satisfied to have a valid model [8]. Solid fuel combustion, for example between biomass and air, is a multiphase process as solid and gaseous phases are included. CFD codes utilize a Discrete Phase Model (DPM) to capture the multiphase nature of the combustion of solid fuels. A Discrete Phase Model considers how a continuum phase (gaseous substance) interacts with discrete phase (solid particles) in a process [9]. The processes that a solid fuel undergoes during combustion can be summarized in Fig. 1. This paper will give insight on the current methods of practice in Computational fluid dynamics with respect to combustion of biomass only.

**Fig. 1.** Solid fuel combustion process [10].

2. Biomass drying models

The first stage during biomass fuel combustion, particle drying, involves the removal of H₂O from the solid fuel particle. Biomass particles generally increase temperature at a rates between 100 K/s to 1000 K/s depending on several factors when injected into the furnace, hence the time taken to complete the drying process is very small [11]. Using experimental data, Yin et al. [8] demonstrated why combusting untreated biomass is an energy intensive process which was further supported by Ma et al. [12]. To model particle drying in CFD, logic arguments are employed to come up with testing laws. Water vaporization is a property dependent on local pressure and temperature hence biomass particles start to give off moisture at a relatively low temperature of 25 °C with a very low water vaporization rate [12,13]. It is usually assumed that the vaporization temperature of the biomass volatiles is much greater than that of water. The energy equation that is modelled in CFD will be trying to solve Eq. (1) which represents the conduction, convection, radiation heat transfer and enthalpy of vaporization during the drying process.

$$m_p c_{p,p} \frac{dT_p}{dt} = h A_p (T_\infty - T_p) + \varepsilon_p A_p \sigma (\theta_R^4 - T_p^4) - Q_v \quad (1)$$

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 , σ , θ_R and I are the continuous phase local temperature, convective heat transfer coefficient, Stefan-Boltzmann constant (5.67×10^{-8} W/m² K⁴), radiation temperature, heat transfer due to vaporization respectively and radiation intensity respectively. Ranz and Marshall [10] proposed a correlation adaptable for CFD to determine the convective heat transfer coefficient. Since the water vapour has to be carried away from the particle surface during the drying process, the diffusion equation has to be modelled as well. For CFD applications, Ma et al. [12] simplified the vapour molar flux equation so as to determine the diffusion coefficient. Particle drying is based mainly on heating and transfer of the H₂O molecules from the particle surface. As a result, little thought has been placed on this process in terms of variations in models [10].

3. Biomass devolatilization models

Devolatilization occurs just as the particle reaches the particle vaporization temperature in the absence of oxygen, signifying the release of volatiles from the biomass particle. It is common practice to have the particle vaporization temperature represent the onset of volatile release rather than water vapour release so as to avoid ambiguity with the equations [10]. A lot of thought has gone into formulating different models to capture the devolatilization process as emphasis is on the volatile yield rate and composition. It is argued that devolatilization commences during the particle drying processes as some light volatiles will begin leaving the fuel particle [12]. This makes it difficult to accurately quantify the volatile yield rate in terms of particle mass and corresponding constituents. This leaves room for development of CFD models that can capture devolatilization that begins whilst the particle is drying. Unfortunately, the only way to offset devolatilization in CFD modelling is to fix a vaporization temperature which is usually high to enable moisture evaporation but in turn causes distortion of volatile yield rate [14]. When the particle temperature equals vaporization temperature, the energy equation almost similar to Eq. (1) is modelled with the addition of latent heat of vaporization during the devolatilization process.

A number of approaches have been used to model the complex devolatilization processes. The simplest are empirical and employ global kinetics, where Arrhenius expressions are used to correlate rates of weight loss with temperature. The simple models can accurately predict the volatile yield rates depending on the input parameters whilst the more complex network models are good at predicting the composition of volatiles [15]. The simplest model which assumes volatiles are released at a constant rate independent of the volatiles already released is called The Constant Rate Model. The other devolatilization models available are:

3.1. Single-rate kinetic model

This is the most used model for various industrial boilers because of its simplicity. The model assumes that devolatilization is a first-order reaction with respect to the amount of volatiles remaining in the particle [8]. Eq. (2) represents the model equation used to represent the devolatilization process [16].

$$-\frac{dm_p}{dt} = k(m_p - (1 - f_{v0})(1 - f_{w0})m_{p0}) \quad (2)$$

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

The parameters k , f_{w0} , E , A_1 , T represent kinetic rate, mass fraction of evaporating/boiling material activation energy, pre-exponential factor and activation temperature respectively. Different exponents have been proposed by researchers to improve on the accuracy of this model in predicting devolatilization [8]. However Di Blasi [17] managed to propose the pre-exponential factor and activation energy for biomass in a generalized manner. According to Tabet [18], the constant rate and single kinetic rate model have a limitation of not being able to predict the composition of volatiles. However, they offer a compromise between computational power and accuracy thus their wide use in industry [19,20].

3.2. Chemical Percolation Devolatilization (CPD) model

The model's strength is on its ability to predict the volatile compositions unlike the previous models. This is because the CPD model is based on the physical and chemical transformations that take place within the fuel structure. The chemical transformations are based on considering multiple reaction mechanisms which include bridge breaking and rearranging, side-chain cracking and gas release, tar distillation, and cross-linking [18].

3.3. Functional Group Devolatilization (FGD) model (1979)

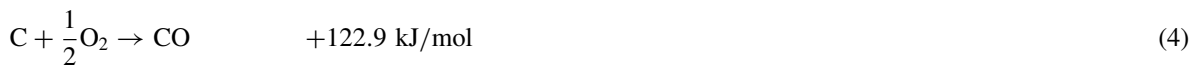
As proposed by Solomon and Colket [21] the FGD model is based on the elemental and functional groups of the species that make up the biomass. Unlike the CPD model, this model is not based on all the reaction mechanisms during devolatilization but on only the functional species thus requiring less computational power. This favours the FGD model for most industrial applications which require the composition of volatile species. The FGD model allows a detailed prediction of the composition of volatile species (gas yield, tar yield and tar functional group and elemental composition) and of char (elemental and functional group) as validated by Ma et al. [22] for a 0.5 MW Pulverized Furnace Test Facility [18].

3.4. Other devolatilization models

Due to continued research, several models continue to be derived. The Universal Devolatilization Process Model is a derived process from the Chemical Percolation Model and the Competing Two step model so that it can predict the volatile composition at lesser computational power [23]. The Distributed Activation Energy Devolatilization Model (DAEM) is also a derived model which uses a lot of equations making it an expensive model to use [24].

4. Biomass heterogenous char reaction models

The char that is left after devolatilization undergoes surface chemical reactions so as to consume the combustible char, mainly carbon fraction of the particle. Char oxidation occurs at higher temperatures thus the particle temperature must be higher than the vaporization temperature to activate this reaction. The simple global surface reactions represented in Eqs. (3) to (5) try to explain the chemical reactions that take place close to the char surface during heterogenous combustion. The Carbon Monoxide that is formed will then react with Oxygen under homogenous reactions which will be explained under homogenous reaction models [25,26].



Heterogenous char combustion is a surface process which makes the effect of particle shape pronounced at this stage. This is because biomass particles come in different shapes and sizes which are non-spherical. Biomass nonspherical particles tend to have a larger surface as well as a significant amount of porosity which increases the oxygen flux [18]. The heterogenous char combustion models include:

4.1. Diffusion-limited rate model (1971)

This model assumes that the surface reaction proceeds at a rate determined by the diffusion of the gaseous oxidant to the surface of the particle [10]. Baum and Street [27] refined the equations so that they can be compatible with CFD without causing a lot of closure problems approach for CFD. To capture the nonspherical nature of biomass particles, Yin et al. [8] proposed to introduce a factor, enhancement factor, into the usual CFD diffusion equation so as to capture the biomass properties as given by Eq. (6):

$$\frac{dm_p}{dt} = -4\pi d_p D_{i,m} \frac{D_0 T_\infty \rho}{S_b(T_p + T_\infty)} \phi_{eh} \quad (6)$$

where $D_{i,m}$, Y_{ox} and ϕ_{eh} represent the diffusion coefficient for the oxidant in the bulk gas, local mass fraction of the oxidant in the bulk gas respectively and the enhancement factor due to particle surface area. Since biomass has an irregular shape, the shape factor seizes to be 1 thus the enhancement factor automatically is greater than one [8]. However, this model assumes a constant particle diameter throughout char combustion which is not the actual case in reality. Consequently, the char particle increases its porosity whilst the density is decreasing [18]. As a result, the experimental results deviate from modelled results for large particles making the model suitable for pulverized biomass.

4.2. Kinetics/diffusion-limited model

As a step further from the previously mentioned model, this model is based on the works of Baum and Street [27] as well as Field [28] for CFD adoption. Simply put, the char surface reaction rate must be controlled partly by the diffusion rate (physical control) and partly by reaction kinetics (chemical control). The chemical control is due to the intrinsic chemical reaction kinetics which might also include pore diffusion. The equations which capture both diffusion and chemical kinetics are given by Eq. (7) [5,18]:

$$\frac{dm_p}{dt} = -A_p P_{ox} \frac{D_0 R}{D_0 + R} \phi_{eh} \quad (7)$$

where A_p , P_{ox} , D_0 and R represent the particle surface area, partial pressure of the oxidant species in the gas surrounding the combusting particle, diffusion rate coefficient and kinetic rate. Mitchell et al. [29] proposed correlations to determine the kinetic parameters from the biomass ultimate analysis. Biomass derived char particles have higher volatile matter and porosity which tends to increase the diffusion rate hence char combustion as well [30]. Fortunately, the Kinetics/Diffusion-limited Model has extensions for specific applications which are the Field Char Oxidation Model and the Gibb Char Oxidation Model. The Gibb Char Oxidation Model is more adapted for biomass particles because it includes parameters that capture the char particle void fraction, volume/internal surface area ratio, effective internal diffusion coefficient of oxygen within the pores and the product ratio of the carbon atoms/oxygen molecules involved in the oxidation processes [10].

4.3. Smith intrinsic char reaction model (1982)

This model is derived from the previous Kinetics/Diffusion-limited Model, but the main difference is in the chemical rate which is expressed in intrinsic chemical and pore diffusion rates. This improves the accuracy of the Smith Intrinsic Char Reaction Model. For Biomass, Ma et al. [22] also managed to modify the intrinsic model so it includes the enhancement factor due to particle shape for biomass char particles.

4.4. Multiple surface reaction model

Focus is put more on the chemical reactions with this model and acknowledgement is also put on the fact that the char particle depletes during combustion thus the surface changes. Reactions represented from Eqs. (3) to (5) are modelled using kinetics/diffusion limited rate model and combined into one equation as represented in Eq. (8). However, the model has limitations in alternating between non-premixed, premixed and partially premixed combustion [31].

$$\frac{dm_p}{dt} = + \frac{P_{g,CO_2}}{\frac{1}{R_{S,CO_2}} + \frac{1}{D_{S,CO_2}}} + \frac{P_{g,O_2}}{\frac{1}{R_{S,O_2}} + \frac{1}{D_{S,O_2}}} + \frac{P_{g,H_2O}}{\frac{1}{R_{S,H_2O}} + \frac{1}{D_{S,H_2O}}} \quad (8)$$

where P_g , R_s and D_s are the partial pressures of the gas, kinetic reaction rate and diffusion coefficient for the three reactions represented from Eqs. (3) to (5).

4.5. Multistep semi global kinetics char combustion model

As a continued approach from the Multiple Surface Reaction Model, more focus is put on the chemical reactions during char combustion. The reaction kinetics parameters (activation temperature, energy and ratio between CO and CO₂) are more pronounced in this model though it makes an important assumption that other intermediate reactions are more important than others such as the O₂ mechanism [32,33].

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 [34]. As a step further, Burke and Shumann [35] 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 [35] developed the continuous film model which considers oxidation of C and CO within the boundary layer to CO₂ which comes at the expense of computational power and complexity. This in turn makes the continuous film model unattractive for engineering modelling applications.

5. Homogenous volatile matter combustion models

The volatiles released during devolatilization create a source for gaseous combustion. Volatiles carry most of the energy for biomass combustion with the volatiles consisting mostly of CO, CO₂, H₂O, with CH₄, H₂ and other inorganic products. However, in CFD simulations, the volatile gases are lumped into one single “artificial” species, CH_yO_x or a few artificial species. Since volatiles are gases, the models used for homogenous combustion are generally applicable for both coal and biomass combustion. Uncertainty is associated with determining the composition of high temperature volatiles. For homogenous volatile matter combustion models to be employed, knowledge of the chemical reaction mechanisms to be used need to be taken into account as well. The simplest of these mechanisms is the Global one step reaction mechanism which forms a simple equation without any intermediate species [12,30]. Using the general lumped form of volatiles, the Eq. (9) can be used to represent the mechanism.



For a more accurate approach, the global two step reaction mechanism is employed, taking carbon monoxide as the intermediate species. However, another mechanism was proposed by Jones and Lindstedt [36] which is a 4-step mechanism to improve on the accuracy of volatile combustion. The four reactions are considered to be enough to give enough detail during the volatile combustion process [18]. The common volatile combustion models include:

5.1. Eddy-dissipation model

In the context of combustion, the eddy dissipation model acknowledges that the chemical kinetic rate (chemical reaction) is faster than the rate of turbulent mixing. The model further assumes that the chemical kinetic rate is directly proportional to the time required to mix reactants at a 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].

5.2. Finite rate chemistry model

This model is based on computing the chemistry reaction rates of the different species during the combustion process. 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 are not factored leaving the chemistry mechanisms contributing much of the information [10]. 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 [37].

5.3. Eddy Dissipation Concept (EDC) model

The Eddy Dissipation Concept (EDC) is an extension of Eddy Dissipation Model (EDM) so as to consider details of chemical reaction mechanisms. 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. 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 [38,39].

5.4. Other homogenous combustion models

Other models in practice include the Equilibrium Approach model and Mixed is reacted model. These models work best for applications with high Damköhler numbers ($Da \gg 1$), meaning turbulence occurs very quickly compared to the actual reaction [34].

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 energy transfer 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 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 and radiation intensity source term. Because modelling is associated with reducing an equation whilst capturing the essential physics, radiation models formed to solve the Radiative Transfer Equation can be grouped into two categories. One group of models solves for the radiative direction whilst the other group solves for the radiation level of energy on the electromagnetic spectrum [26]. 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. Spectral Models include the Weighted Sum of Gray Gases Model, Gray Model and the Multiband Model [40].

8. Particle tracking models

From Newton's 2nd Law of motion, particle motion is due to forces acting on the particle. 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) [5]. The multiphase flow (Solid and Gas) uses the Lagrangian Particle Tracking Model also known as the Particle Transport model. Since force is a function of mass, the description of the particle volume, surface or diameter is of paramount importance. Particle Diameter model can be based on the following distributions: Specified Diameter, Uniform in Diameter by Number, Uniform in Diameter by Mass, Rosin Rammler, Nukiyama Tanasawa, Discrete Diameter and Particle Diameter Change Due to Swelling [10]. For biomass whose shape is less spherical, particle shape factors need to be employed [16,18].

Drag force models used in CFD are mainly centred on determining the particle drag coefficient which has been studied under experimental conditions for quite a long time. The oldest and simplest model employed in CFD codes is the Schiller–Naumann model [41] which has its strength with spherical particles and less computational space requirements. Morsi and Alexander [42] also proposed their own model which is sensitive to the velocity at which the particles are travelling in the combustion chamber. A more common approach with irregular shaped particles like biomass in determining particle drag coefficients was proposed by Haider and Levenspiel [43]. This model uses particle shape factor coefficients to take into account the deviation from the usual spherical shape. As alluded to before, particle motion is greatly affected by the shape of the particle. A more recent particle drag model was proposed by Hölzer and Sommerfeld [44] which includes shape factors for both elongated and transverse positions. This model adapts the shape of the particle to be more spherical by use of coefficients unlike the previous models.

9. Conclusions

The models reviewed in this paper reflect how easy it is to get lost in the interpretation and choice of the best model for a certain application. From the models reviewed, emphasis is on the particle motion and particle surface area. The biomass particle models have to be altered to incorporate the enhancement factor as proposed by Yin et al. [8]. The enhancement does have shortcomings in the way it generalizes the cylindrical and prism shape with regards to biomass particles. The single rate devolatilization model is used for most applications with the need to determine the volatile yield rate. This model offers a compromise on the computational power but lacks the accuracy that is offered by the FG-DVC model with regards to determining both the compositions and yield rate. The FG-DVC finds its use mostly when the biomass species changes properties throughout its application. The kinetic/diffusion surface reaction model has found more use in industry as the assumption that char from biomass can be assumed to be non-porous which is not necessarily the case. Using the Smith's intrinsic char model is however recommended because char is known to be porous. The eddy dissipation model is sufficient for modelling the homogenous volatile combustion for most industrial applications. However, this process is very sensitive to the parameters that would have been chosen in the devolatilization process simply because the volatile composition affects how the volatile combustion takes place. The drag coefficients used in industry vary but the Hölzer and Sommerfeld [44] is recommended because it is more recent and can capture well the shape orientation of the biomass particle during combustion. Lastly the turbulence and radiation models are generalized around the $k-\epsilon$ model and the P1 model.

To conclude, when one is tasked with a modelling problem involving combustion, knowledge of the different approaches is of paramount importance. ANSYS Fluent offers default settings and constants which need to be modified by User Defined Functions to cater for the specific industrial applications under consideration. Justification and development of these models should be based on the overall use.

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