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Development of a gas phase combustion model suitable for low and high turbulence conditions

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HIGHLIGHTS

- The limitation of the EDC combustion model in low turbulence conditions is argued.
- A hybrid combustion model applicable over the whole Reynolds range is introduced.
- The importance of molecular diffusion at low Reynolds number is shown.
- The simulation results are in good agreement with experimental data.

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ABSTRACT

A novel hybrid gas phase combustion model suitable for low as well as high turbulent combustion conditions is proposed. In particular, in the region above the fuel bed of small-scale biomass combustion plants, gas phase mixing is highly influenced by laminar and low turbulence zones. Here, the eddy break-up combustion models are not valid because they were originally developed for highly turbulent flows. Therefore, a CFD gas phase reaction model applicable over the whole Reynolds range from laminar to turbulent flows is developed. It is a hybrid Eddy Dissipation Concept/finite rate kinetics model which calculates the effective reaction rate from laminar finite rate kinetics and the turbulent reaction rate and weights them depending on the local turbulent Reynolds number of the flow. To validate the proposed model, comparisons are made with experimental data for a series of jet flames covering laminar, transitional, and turbulent flow conditions. The simulation results show that the prediction of flame can be improved with the proposed hybrid combustion model.

1. Introduction

The production and supply of energy is one of the greatest concerns of human society. With regard to the facts that the fossil fuel resources are depleting rapidly, the necessity to find new energy resources is indispensable. During recent decades, the share of energy production by biomass combustion plants has been growing, because biomass is a CO_2 neutral source of energy in a sustainable agriculture/forestry system [1]. CFD modelling is becoming increasingly important for the development and optimisation of biomass combustion plants. Here, gas phase combustion models play a key role concerning predictions of flow, temperature, and gaseous emissions (e.g. CO).

The eddy break-up models (EBU) are the most prevalent Reynolds Averaged Navier–Stokes (RANS) based combustion models which have been successfully applied for a variety of combustion plants [2–4]. The popularity of the EBU combustion models come from their low computational costs especially for industrial applications in the context of RANS simulations. However, the empirical constants in the EBU models are not universally valid and need to be adapted depending on the application [5,6]. The EBU model first was proposed by Spalding [7] and later modified by Magnussen and Hjertager [8]. The main assumption of the EBU model is based on infinitely fast chemistry and assumes that the reaction rate is

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Nomenclature

$C_{j,r}$	molar concentration of each reactant and product species j in reaction r (kg mol m^{-3})
C_γ	EDC model constant (–)
C_{D1}	EDC model constant (–)
C_{D2}	EDC model constant (–)
C_τ	EDC model constant (–)
d	jet diameter (m)
$D_{i,m}$	diffusion coefficient for species i in the mixture (m^2 s^{-1})
D_t	turbulent diffusivity (m^2 s^{-1})
$\vec{J}_i$	diffusion flux of species i (kg m^{-1} s^{-1})
$K_{f,r}$	forward rate constant for reaction r (s^{-1})
$K_{b,r}$	backward rate constant for reaction r (s^{-1})
k	turbulent kinetic energy (m^2 s^{-2})
$M_{w,i}$	molecular weight (kg kmol^{-1})
N	number of species
N_R	number of reactions
Re	Reynolds number (–)
Re$_t$	turbulent Reynolds number (–)
R_i	net rate of production of species i by chemical reaction (kg m^{-3} s^{-1})
$\overline{R}_{i,r}$	molar rate of creation/destruction of species i in reaction r (kg mol m^{-3} s^{-1})
S_{ct}	Schmidt number (–)
T	temperature (K)
T_r	time scale ratio (–)
Y_i	mass fraction of species i (–)

Greek symbols

ε	turbulent dissipation rate (m^2 s^{-3})
γ	length fraction of EDC fine scales (–)
ν	kinematic viscosity (m^2 s^{-1})
$\nu'_{i,r}$	stoichiometric coefficient for reactant i in reaction r (–)
$\nu''_{i,r}$	stoichiometric coefficient for product i in reaction r (–)
ρ	density (kg m^{-3})
τ_{EDC}	EDC time scale (s)
$\vec{v}$	velocity vector (m s^{-1})
μ_t	turbulent viscosity (kg m^{-1} s^{-1})

Subscript

b,r	backward reaction
EDC	Eddy Dissipation Concept
FRK	finite rate kinetics
f, r	forward reaction
i	species index
r	reaction
t	turbulent

controlled by turbulent mixing [8]. The Eddy Dissipation Concept (EDC) is an extended version of EBU model developed by Magnussen [9] which can incorporate detailed chemistry calculations in turbulent combustion. However, in the region above the fuel bed and in small-scale biomass combustion applications (size-range < 500 kWth), the gas phase mixing and reaction progress is highly influenced by laminar and low turbulence zones. Here, the EBU gas phase combustion models, which are originally developed for highly turbulent flows, are not valid, leading to wrong predictions of the reaction progress and wrong concentrations of gas species (CO, NO_x species, etc.).

The EDC, which enables the consideration of the complex interaction of turbulence and detailed reaction kinetics, was taken as a basis for the development of a general gas phase combustion model applicable for the entire Reynolds-number range of flows. However, gas phase combustion models like the EDC are originally developed for high-Reynolds-number conditions. The EDC is based on the turbulent energy cascade, which means that larger eddies break up into smaller eddies, and the reactions take place in the so-called fine structures, where the fluid is mixed on a micro-scale.

In biomass grate furnaces, in particular above the fuel bed, the flow is in the low Re range. Here, the flue gas varies from 0.5 to 2 (m/s). Moreover, in small-scale combustion plants (up to 100 kW), even the exit Reynolds number of the secondary air jets may be in the laminar to transition region. Therefore, the prediction of the flue gas species and temperature strongly depends on the CFD gas phase combustion model applied. In the EDC, the prediction mainly depends on the turbulent quantities k and ε, where a large error on the predictions is imposed when the flow approaches low Reynolds conditions. Here, it is important to simulate the combustion progress by the pure finite rate kinetics model.

Therefore, an advanced gas phase reaction model has to be developed which is sensitive regarding local flow conditions. The model should reliably distinguish between the mixing or kinetically dominated zones. Hence, a novel hybrid gas phase combustion model which utilizes combined finite rate kinetics and EDC combustion models is presented in this work. The hybrid model was implemented in ANSYS® FLUENT®.

The model development was done based on the simulation of measured jet flames by Barlow and Frank [10] (Sandia flame D as well as flame A with a jet Re number of 1100 and flame B with a jet Re number of 8200). Since it is well-known that k–ε models over-predict the spreading rate of round jets, the model constants were modified in order to minimize additional effects influencing gas phase combustion modelling. Furthermore, at low-turbulent combustion regimes the description of the reaction kinetics is of high relevance since it has a considerable influence on the simulation results.

During typical biomass combustion conditions with air staging the most relevant components released are H_2O, CO_2, CO, H_2, and CH_4 [11–13]. All these species are also relevant during Methane combustion [14,15]. Moreover, the combustion model developed can be applied together with any reaction mechanisms, which of course has to be validated for the target application. Currently, the Skeletal Kilpinen97 mechanism [16] which has extensively been validated for biomass combustion conditions is being applied [17] for biomass grate furnaces. Hence, the reduced DRM-22 reaction mechanism [15] was selected based on the simulation of Sandia flame D.

At low-Re conditions the influence of molecular diffusion on mixing becomes comparable to the influence of turbulent diffusion. Therefore, the diffusion of each gas species in the mixture was taken into account and compared with the conventional approach (constant value for the diffusion of the species in the mixture) for the simulation of flame A (Re = 1100) and B (Re = 8200). While the EDC together with the differential-diffusion (diff-diff) approach gave a good agreement with measurements for flame B with moderate turbulence, it failed to predict the laminar flame A. With finite rate kinetics (FRK) good results could be achieved for flame A. Since it could be shown that the EDC is not valid below turbulent Reynolds number of 64 [18], a hybrid EDC/FRK model is introduced. The model calculates the reaction rates with the FRK