New Trends in Combustion Simulation

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Abstract

A review of recent developments in combustion modeling capabilities in a commercial CFD package is given. The range of available combustion models is presented with a particular focus on new reaction models for finite rate chemistry. The recently implemented models are illustrated by two sample applications, like the development of a NO_x postprocessor based on the Eddy Dissipation Concept (EDC) model utilizing the ISAT algorithm.

Keywords: CFD, combustion models, finite rate chemistry, NO_x

1. Introduction

When early commercial CFD packages became available more than 20 years ago, simulating the complex physics inside combustion chambers was already one of the target applications. Of course, projects were often limited by computer resources these days. Therefore in most cases reaction was taken into account using relatively simple approaches such as the Eddy Dissipation model.
Today, with increasing maturity of CFD technique and computing power, one focus in numerical simulation of combustion is in the area of non-equilibrium chemistry and multiphase flow. New fields of application, such as the formation of pollutants in technical flames or the optimization of combustion processes, can be tackled that way.

2. Numerical Algorithm

Numerical flow simulation, or more common Computational Fluid Dynamics (CFD), relies on solving conservation or transport equations for mass, momentum, energy and participating species. If the flow is turbulent, model equations for specific turbulent quantities have to be solved in addition. Since even with today's super computers resolving turbulent length scales directly results in tremendous effort, Reynolds averaged equations are applied to include the physics of turbulence. To discretize and solve the governing flow equations the Finite Volume method is employed by the majority of commercial CFD codes.

Table 1: Models for gaseous combustion available in FLUENT [1]

	Premixed flames	Diffusion flames	Partially premixed flames
Equilibrium chemistry	Zimont model (Reaction progress variable)	Mixture fraction model	Zimont-/ Mixture fraction approach
	Eddy Dissipation model (Magnussen and Hjertager)		
Detailed chemistry		Flamelet model	
	Finite Rate model Eddy-Dissipation-Concept model PDF Transport model		

The Reynolds averaged transport equation for the mass fraction $\overline{Y}_k$ of the kth species in differential notation can be written as follows:

$$\left\{\frac{\partial}{\partial t}\left(\overline{\rho}\overline{Y}_k\right)+\right\} \frac{\partial}{\partial x_i}\left(\overline{\rho u_i}\overline{Y}_k\right) + \frac{\partial}{\partial x_i}\left(\overline{\rho u''_i Y''_k}\right) = \frac{\partial}{\partial x_i}\left(\overline{\rho D_k \frac{\partial \overline{Y}_k}{\partial x_i}}\right) + \overline{R}_k \qquad (1)$$

For the gaseous phase the source term $\overline{R}_k$ is the key to combustion modelling.

Depending on the speed of the reactions to be modelled as well as on the current state of mixing between fuel and oxidiser different approaches are applied.

Early combustion models have been derived on the assumption of chemical equilibrium. Taking into account detailed kinetics of reactions usually results in much higher computational effort.

Table 1 provides an overview of models for gaseous combustion available in the commercial CFD code FLUENT.

3. Combustion Models for Processes governed by Kinetics

With increasing power of computers and workstations the interest in combustion models for detailed kinetics has been growing continuously in recent years.
With laminar flame processes ruled by kinetics can be described using the Finite Rate model. Like other models suited for non-equilibrium chemistry the Finite Rate approach relies on a reaction mechanism including Arrhenius parameters to define the reactions to be simulated.
Moreover, with turbulent flames three different models are available to do simulations with detailed kinetics of reactions:

Flamelet Model
One means to combine turbulent flow and detailed kinetics of reactions assuring acceptable computational effort is the so called Flamelet model. It takes advantage of assuming the turbulent diffusion flame to consist of a large number of single laminar crosscurrent diffusion flames, so called flamelets, on a suited microscale. As with the Mixture Fraction model computational efficiency results from decoupling the solution reaction and flow. The approach is suited to tackle moderate non-equilibrium phenomena resulting from aerodynamic strain.

Eddy Dissipation Concept Model
The Eddy Dissipation Concept (EDC) model takes advantage of assuming part of the fluid to be thoroughly mixed within a particular cell as well as to be the main driver for chemical reaction. These well mixed portions of a subvolume, the so called "fine scales", are regarded to resemble a constant pressure reactor. That way the governing equations loose part of their complexity. Using the simplified equations for species conservation the corresponding source terms are derived from an Arrhenius-type reaction mechanism. To solve for the fine scales the ISAT algorithm (in-situ adaptive tabulation) [2] is applied to the resulting transient system of equations.
For detailed reaction mechanisms made up by dozens of species and several hundred reactions, it is hardly feasible to completely solve for kinetics before entering the flow calculation. Therefore the ISAT algorithm employs a reference table where reaction data is collected as the flow simulation proceeds. Each time a new composition vector ϕ^1 made up from species content, temperature and pressure has to be determined in a new time step dt for a given composition vector ϕ^0, the algorithm checks the reference table for entries calculated already. In case a set of values ϕ^0 is found within acceptable tolerance, the new set is defined by just interpolating from existing entries. When suited values have not been found, direct integration serves to derive the new vector ϕ^1 also completing the table.
Having solved for species distributions and related life time of fine scales, the EDC model is applied to determine source terms for the Reynolds averaged species equations.
Using that approach, even very slow reactions in turbulent flow, e.g. CO burnout in quenched flames and NO_x reduction in SNCR systems, can be analyzed.

EDC Application: Simulation of NO_x formation in a biomass grate furnace
CFD was successfully applied to optimize the design of biomass furnaces with respect to flue gas burnout and temperature distribution by several research groups. However, the simulation of NO_x
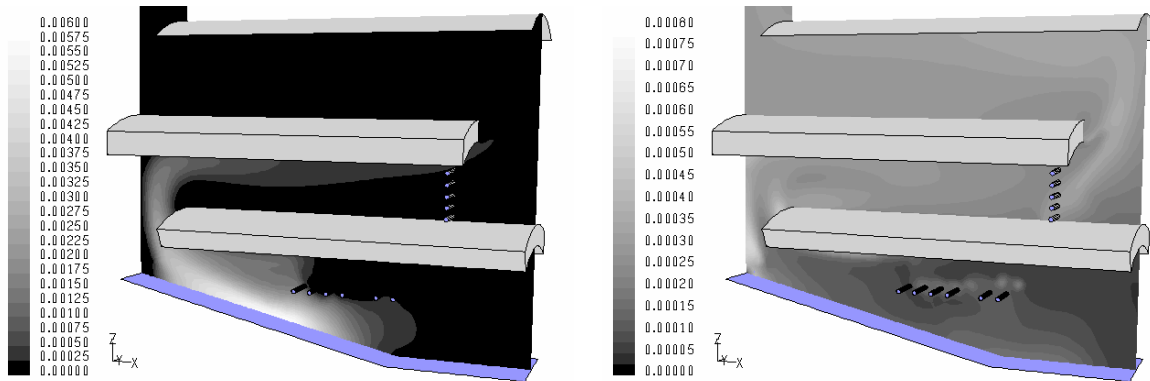
Figure 1: Calculated mole fraction profiles of NH$_3$ and NO in a 440 kW pilot-scale biomass grate furnace (left hand picture…profile of mole fraction X$_{NH3}$ [-] in the vertical symmetry plane of the furnace; right hand picture…profile of mole fraction X$_{NO}$ [-] in the vertical symmetry plane of the furnace)

formation was limited by the necessity to include far more complex chemistry than for combustion simulation which leads to computation times that are by far too long for engineering applications. BIOS BIOENERGIESYSTEME GmbH in cooperation with the Institute for Resource Efficient and Sustainable Systems, Graz University of Technology, developed a CFD NO$_x$ formation model for biomass grate furnaces which covers the release of NO$_x$ precursors from the fuel bed and the subsequent CFD simulation of NO$_x$ formation with detailed chemistry in the combustion chamber [3].

An own-developed empirical model was used for the combustion of solid biomass on the grate. This model supplies velocities, species concentrations (CH$_4$, CO, CO$_2$, H$_2$, H$_2$O, O$_2$, NO, NH$_3$, HCN) and temperatures of flue gas above the surface of the fuel layer as boundary conditions for subsequent CFD simulation of turbulent reactive flow in the furnace. Under the assumption that NO$_x$ formation reactions do not significantly influence the flow pattern in the furnace, a time saving 2-step approach was applied for CFD simulations. The Realizable k-ε turbulence model, the Eddy Dissipation / Finite Rates Kinetics combustion model in combination with a global methane 3-step mechanism (CH$_4$, CO, CO$_2$, H$_2$, H$_2$O) and the Discrete Ordinates radiation model where used for basic gas phase combustion simulation in the present case. The models were validated for combustion simulation in biomass furnaces with lab-scale test cases as well as FT-IR in-situ measurements of species concentrations (CH$_4$, CO, CO$_2$, H$_2$O) and temperature measurements at a pilot-scale 440 kW$_{th}$ biomass grate furnace with air staging technology [4,5,6]. The CFD simulation of gas phase fuel NO$_x$ formation in a postprocessor mode was performed with the Eddy Dissipation Concept in combination with a detailed reaction mechanism with 50 species and 253 reactions (Kilpinen 92) which was developed under consideration of NO$_x$ kinetics in biomass combustion systems. This method allows for a detailed consideration of both flow and chemistry.

First 3D CFD simulations were performed for the above mentioned furnace under different operating conditions. Fibre board was used as fuel with a high nitrogen content. Fig. 1 shows calculated mole fraction profiles of NH$_3$ and NO in the vertical symmetry plane of the furnace. Considering all uncertainties in comparing measurements with simulations of grate fired furnaces which underlie fluctuations in operating conditions and flow, the qualitative and quantitative agreement with experiments and kinetic simulations was good. Previous calculations with various NO$_x$ postprocessors which could not even give qualitatively correct results, were outperformed. No HCN emissions where calculated at the furnace outlet which is in accordance with literature and experience. The average conversion rate of NH$_3$ (which showed to be the predominant NO$_x$ precursor) in the furnace was in qualitative agreement with detailed kinetic investigations with an ideal reactor network. Furthermore, the NH$_3$ conversions rates could be verified with FT-IR in-situ measurements near the secondary air nozzles which showed NH$_3$ concentrations below the detection limit. The calculated NO emissions at the furnace outlet where about an order of magnitude higher as the corresponding NO$_2$ emissions, which is in compliance with literature data and measurements (conventional flue gas analysis). For all test cases the simulated NO$_x$ emissions (NO and NO$_2$) where about 10% higher than the measured ones at the boiler outlet.

The developed CFD NO$_x$ postprocessor in combination with detailed reaction kinetics could be successfully tested for 3D furnaces simulations. More tests and comparisons with measurements at

various biomass furnaces (pilot-scale and industrial scale) are necessary and ongoing in order to validate the CFD model. First calculations needed about 2 weeks on a single PC processor for a grid size of 275,000 cells, but a considerable speed up can be achieved with parallel processing. The newly developed NO_x postprocessor allows to investigate in detail NO_x reduction measures in biomass grate furnaces and, therefore, is a powerful tool for the optimisation of furnace designs and process control. However, a reduced NO_x reaction mechanism is currently being developed in order to allow for a reduction of calculation time and to make this time-consuming method more attractive for industrial applications. Furthermore, a coupled simulation of both combustion and NO_x formation reactions with the EDC and this reduced mechanism is planned in order to overcome weaknesses of basic combustion simulation with the EDM and global combustion chemistry.

PDF Transport Model
Compared to alternative methods like the concept of "Presumed PDFs", solving PDF transport equations is the most general means to determine a probability density function P. Transport equations describing the evolution of PDFs in time and space can be derived from the Navier-Stokes equations. The PDF transport equation solved in FLUENT reads as follows:

$$\frac{\partial(\overline{\rho}P)}{\partial t} + \frac{\partial(\overline{\rho}\overline{V_i}P)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\overline{\rho u_i'' \mid \psi}P\right) + \frac{\partial}{\partial \psi_k}\left(\overline{\rho\left(\frac{1}{\rho}\frac{\partial J_{i,k}}{\partial x_i}\bigg|\psi\right)}P\right) + \frac{\partial}{\partial \psi_k}\left(\overline{\rho}\,S_k\,P\right) \quad (2)$$

The probability density function may be interpreted as the probability for a fluid portion to be of a certain composition, temperature and pressure. With this type of PDF, a so called composition PDF, some standard turbulence model is needed in addition.
 The main advantage of this approach lies in the fact that the highly non-linear source term is well defined and does not call for additional modeling of turbulent fluctuations of species and temperature. In contrast turbulent convection and molecular diffusion (first terms on the right hand side of eq. (2)) need to be modeled.
As common a gradient diffusion approach serves to account for turbulent convection. For turbulent diffusion of species and energy the Modified Curl model [7] or the IEM [8] model can be chosen.
Since the PDF is high dimensional, the transport equation is solved by a stochastic method, the Monte-Carlo algorithm. This method approximates the probability density function by many discrete values referred to as stochastic particles each representing a single state of the reacting flow.

PDF Transport Application: Flame D
The well documented flame D serves to validate the PDF transport model. Due to differences in flow velocity and species concentration this partially premixed flame resembles to a diffusion flame.
For numerical analysis standard k-ε turbulence model and skeletal reaction mechanism have been applied on an axisymmetric mesh made up from 2352 cells. A comparison of measured and computed results for the mass fraction of CO along the normalized radius of the flame shows good agreement (Fig.2).
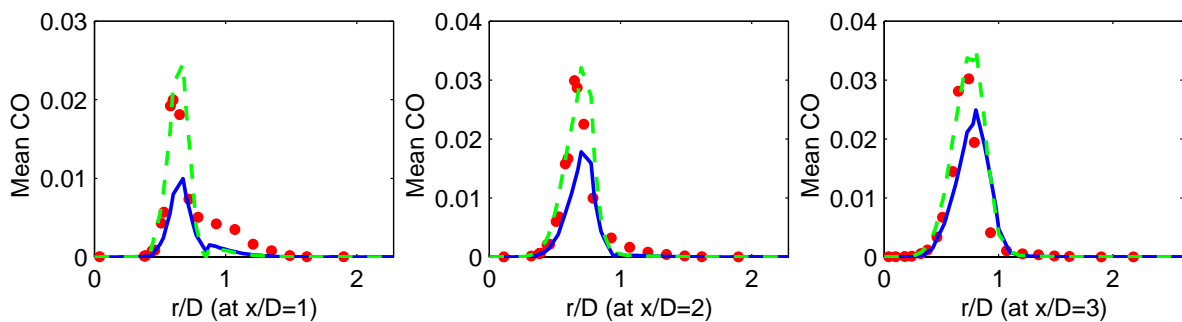

Figure 2: Mass fraction of CO along normalized radius of flame (• measured, Modified Curl and IEM)

4. Summary

Taking a look at combustion modelling in commercial CFD codes has shown a clear tendency towards more complex approaches accounting for detailed kinetics of reactions. In this context the implementation of the PDF transport model and the ISAT algorithm deserves special attention. At the moment the PDF transport model is the most general approach to solve the closure problem arising from turbulence-species interaction. As a consequence of the usage of the ISAT technology the EDC model has evolved to a valuable finite rate model for industrial scale applications. The most recent class of new combustion models just now allows for analyzing complex phenomena like formation and destruction of pollutants in modern combustors.

5. References

[1]   FLUENT 6.1 User's Guide Volume 2, Fluent In., February 2003.
[2]   POPE, S. B., "Computationally efficient implementation of combustion chemistry using in-situ adaptive tabulation", Combustion Theory and Modeling, 1:41-63, 1997.
[3]   OBERNBERGER, I., WIDMANN, E., SCHARLER, R., Entwicklung eines Abbrandmodells und eines NOx-Postprozessors zur Verbesserung der CFD-Simulation von Biomasse-Festbettfeuerungen, Endbericht des gleichnamigen Forschungsprojektes des Bundesministeriums für Verkehr, Innovation und Technologie (GZ 73.182/2-V/3/2001), Institute for Ressource Efficient and Sustainable Systems (ed.), Graz University of Technology, 2003.
[4]   SCHARLER R., Entwicklung und Optimierung von Biomasse-Rostfeuerungen durch CFD-Analyse, Dissertation, Technische Universität Graz, Austria, 2001.
[5]   SCHARLER, R., FLECKL, T., OBERNBERGER, I., „Modifikation der Magnussen-Parameter für Biomasse-Rostfeuerungen mittels Heißgas in-situ FT-IR Absorptionsspektroskopie", in: Tagungsband der Konferenz "20. Deutscher Flammentag", September 2001, Essen, VDI-GET (Ed.), VDI Berichte Nr. 1629, pp. 509-514, ISBN 3-18-091629-X, 2001.
[6]   SCHARLER, R., FLECKL, T., OBERNBERGER, I., „Modification of a Magnussen Constant of the Eddy Dissipation Model for biomass grate furnaces by means of hot gas in-situ FT-IR absorption spectroscopy", Progress in Computational Fluid Dynamics, Vol. 3, Nos. 2-4, pp. 102 – 111, 2003.
[7]   JANICKA, J., KOLBE, W., KOLLMANN, W J., "Closure of the transport equation for the pdf of turbulent scalar fields", Journal Non-Equilibrium Thermodynamics, 4:47, 1978.
[8]   DOPAZO, C., O'BRIEN, E. E., "Functional formulation of nonisothermal turbulent reactive flows", Phys. Fluids, 17:1968, 1975.