

## **NUMERICAL SIMULATION OF UTILITY BOILERS WITH ADVANCED COMBUSTION TECHNOLOGIES**

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### **ABSTRACT**

This paper presents calculations of a pulverized coal flame and a coal-fired utility boiler with advanced combustion technologies. A combustion model based on an extended Eddy Dissipation Concept (EDC) combined with finite rate chemistry is described and some applications are shown. This model can be regarded as an extension of the previously used Eddy Breakup model (EBU) where infinite fast chemistry is assumed.

It is part of a 3D-prediction code for quasi-stationary turbulent reacting flows which is based on a conservative finite-volume solution procedure. Equations are solved for the conservation of mass, momentum and scalar quantities. A domain decomposition method is used to introduce locally refined grids. Validation and comparison of both combustion models are made by comparison with measurement data of a swirled flame with air staging in a semi-industrial pulverized coal combustion facility. The application to three-dimensional combustion systems is demonstrated by the simulation of an industrial coal-fired boiler.

### **INTRODUCTION**

Prediction of utility boiler performance becomes an important tool for the development of new combustion methods. But advanced combustion modifications require more detailed modeling of turbulent combustion when, e.g., the formation and destruction processes of carbon monoxide are to be predicted in order to reduce harmful concentrations near the furnace walls. The recent development in computer hardware and numerical methods rises the possibility to use more complex combustion models in three-dimensional predictions of utility boilers. In most three-dimensional simulation codes of pulverized coal combustion for practical systems the infinite-fast-chemistry assumption is used to model the gas phase combustion. Chemical kinetics, however, have a major influence on pollutant formation, especially in combustion systems equipped with air or fuel staging. The use of a detailed description of turbulent combustion, even if available, would be extremely time and memory consuming and therefore not be applicable to practical three-dimensional calculations. Thus simplifications in the description of the turbulence behavior and the chemical reaction mechanisms are necessary. The application of a combustion model which is able to handle finite rate chemistry in turbulent combustion is presented in this paper.

## PHYSICAL MODELS

A prediction code for turbulent reacting flows has to comprise submodels for the description of flow field, combustion and heat transfer by radiation. In their entirety the different submodels form a system of strongly coupled partial differential equations. Each of these equations, except the one for radiation, can be written in form of a general transport equation:

$$\frac{\partial}{\partial x}(\rho u \Phi) = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \Phi}{\partial x} \right) + S_{\Phi} \quad (1)$$

where  $\rho$ ,  $u$ ,  $x$  and  $\Gamma$  are the density, velocity, cartesian coordinates and the diffusion coefficient. This equation describes the local change of the variable  $\Phi$  due to convection, diffusion and production under steady state conditions. Depending on  $\Phi$ , Eq. (1) represents mass, momentum, species, or energy conservation. In case of non-isothermal conditions the variables  $\Phi$  are Favre-averaged. The introduction of the concept of a standard transport equation is very useful since it allows the application of highly standardized solution algorithms.

### Fluid Mechanics and Thermal Radiation

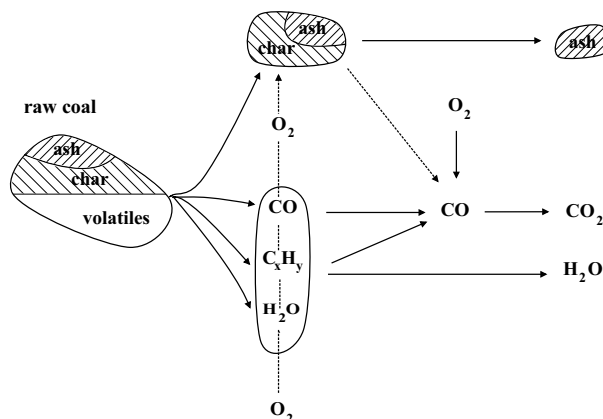
Fluid motion is described with the simple variables velocity and pressure. To evaluate the velocity field the incompressible, time-averaged Navier-Stokes equations are solved. Coupling between velocity and pressure is achieved by the SIMPLE-method. The standard  $k,\epsilon$ -model is adopted to take the turbulent state of the flow field into account. A detailed discussion on the above mentioned basic equations of numerical fluid mechanics can be found by numerous authors, e.g. in Peric [8].

Thermal radiation is an electromagnetic phenomenon and in so far not bound to molecular transport. This property is an essential difference compared with the other flow and combustion variables which are controlled by convective and diffusive transport. A variety of different models for the solution of the radiation transport equation have been developed, with individual merits and drawbacks. In the present paper we use the discrete transfer method proposed by Lockwood and Shah [5]. The basic idea is the solution of the radiation transport equation along the direction of representative rays between two wall nodes. The hemisphere surrounding a wall point is subdivided into 12 segments, each covering the same solid angle. The intensity within each segment is assumed to be constant. Since the intensity of radiation depends on absorption, emission and scattering characteristics of the medium passed through, a detailed representation of the radiative properties of a particle/gas mixture would be very complex and currently beyond the scope of a 3D-code for the simulation of industrial combustion systems. Thus, the absorption coefficient of the gas phase is assumed to have a constant value of 0.2/m. The absorption and out-scattering coefficients of the particles are evaluated according to an approach of Rizvi [9]. In-scattering is completely neglected.

### Coal combustion scheme

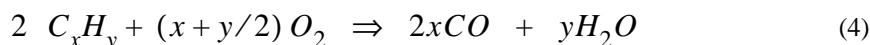
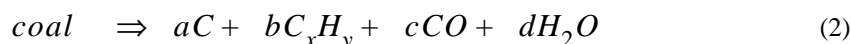
Coal combustion is a very complex process and not all physical aspects are well understood. The principle steps of the reaction progress which have to be consid-

ered are the thermal decomposition of the raw coal and the subsequent burnout of the char and the volatile matter, as outlined in Fig. 1.



**Figure 1.** Reaction model of pulverized coal combustion

Physical constraints and hardware limitations necessitate strong simplifications to allow the simulation of coal combustion processes. In this paper we use the reduced four-step reaction scheme according to Eq. (2) to (5)



with a, b, c, d as coal dependant parameters. The reaction scheme comprises nine different species, with ash and nitrogen as inert components. A strong simplification is made by assuming a no-slip condition between the particles (coal, char, ash) and the surrounding fluid. This is done to ensure the applicability to practical three-dimensional problems. Thus the motion of the solids can be described with the Eulerian approach and the general transport equation is applicable to all species of the reaction scheme. This is a very effective way to calculate the distribution of the solid mass fractions.

The source terms of the species transport equations are evaluated from the reaction rates of the four chemical reactions which are subject to different control mechanisms. If the typical time scale of the reaction progress is larger than the time scale of turbulent mixing, the reaction is assumed to be chemically limited. The chemical limitation dominates pyrolysis, Eq. (2), and char burnout, Eq. (3). A detailed discussion of the reaction model can be found in Schnell [11]. A simple one-step pyrolysis model is used. The amount and composition of the volatiles are taken from experimental data. At the moment all tars and hydrocarbons are summarized to one 'average' composition  $C_xH_y$ .

### Gas phase reaction rates

In practical combustion systems of engineering interest, turbulent flow conditions prevail. In order to calculate such combustion systems it is necessary to consider the

interaction between the various physical and chemical processes. This includes modelling of turbulence, the interaction between turbulence and chemistry, the chemical reactions, heat and mass transfer, etc. Libby and Williams [4] and Bray [1] had shown that intermittency is a common feature of turbulent combustion. This is another important issue which a combustion model must be able to describe.

To calculate some basic quantities (like temperature or oxygen concentration) for many cases of interest, the chemical kinetics can be considered to be much faster than the turbulent mixing process. But in some important processes such as combustion in advanced systems equipped with air or fuel staging, pollutant formation and extinction of flames, the chemical kinetics have a dominating influence. To calculate these problems, a combustion model must be developed which is able to handle finite rate chemistry in turbulent combustion.

An adequate way to describe the statistical character of species concentrations and temperature in reacting turbulent flows is a joint probability density function (PDF) of all these variables [4]. Once the PDF is known, chemical kinetics could be easily added to calculate combustion rates in turbulent flows by integrating over all variables. But the direct calculation of a joint PDF causes many uncertainties about fluctuations, shapes of PDF's and correlations of fluctuations. Also the combustion model has to describe many details of the turbulent combustion process, it must be applicable to three-dimensional problems and elliptic flows on available computers. Therefore PDF methods for modeling the turbulent combustion in utility boilers need very strong simplifications and assumptions and are not examined in the present work.

**Eddy Breakup Model (EBU).** Another popular way to calculate turbulent gas combustion is the use of an Eddy Breakup model. This model, first proposed by Spalding [13] and modified by Magnussen [7], is based on the turbulence decay and assumes infinite-fast-chemistry. The reaction progress, written as source term of a reacting gaseous fuel, is calculated from

$$S_{fuel} = C_r \bar{\rho} \frac{\varepsilon}{k} \min \left( m_{fuel}, \frac{m_{oxidant}}{r_{fuel}}, \frac{m_{products}}{2r_{fuel}} \right) \quad (6)$$

with  $C_r=4$ . The Eddy Breakup model originally assumes a single-step irreversible reaction, but it has been extended to a two-step mechanism for the combustion of hydrocarbons with CO as intermediate species by many authors. The hydrocarbon reaction rate is calculated from Eq. (6). The CO reaction rate is the slower of the mixing rate, see Eq. (6), and a kinetic rate without influence of turbulence. This two-step application is called EBU model in the present paper. Details of the model can be found in Schnell [11].

Although the Eddy Breakup model has turned out to give results of reasonable accuracy when applied to various practical combustion systems (e.g. [11],[14]), its applicability is limited. The model cannot properly describe cases in which the coupling between turbulence and multistep chemistry is strong.

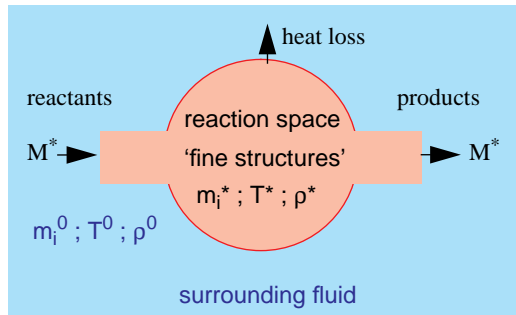
**Eddy Dissipation Concept (EDC).** As proposed by Magnussen [6], the EDC is a general concept for treating the interaction between turbulence and chemistry in flames. The method is based on a detailed description of the dissipation of turbulent eddies and can be considered as an extension of the Eddy

Breakup model. In the EDC the total space is subdivided into a reaction space, called the 'fine structures' and the 'surrounding fluid'. All reactions of the gas phase components are assumed to take place within this reaction space. Thus in order to be able to treat the reactions within the fine structures, the volume fraction of the reaction space and the mass transfer rate between the fine structures and the surrounding fluid have to be determined. Both quantities are derived from the turbulence behaviour of the fluid. According to Magnussen [6], the mean net mass transfer rate of a species  $i$  between the fine structures and the surrounding fluid can be expressed as

$$R_i = \frac{\bar{\rho} M \chi}{1 - \gamma^* \chi} (m_i - m_i^*) \quad \left[ \frac{\text{kg}}{\text{m}^3 \text{ s}} \right] \quad (7)$$

where  $\bar{\rho}$  is the local mean density of the gas,  $m_i$  is the local mean value of the mass fraction of species  $i$ , and  $m_i^*$  is its value in the fine structures. The correction factor  $\chi$  designates the fraction of the fine structures which is sufficiently heated and may react. A formula for  $\chi$  can be found in [6].

Based on simple geometrical assumptions, the flow rate  $M$  per unit time can be derived from a consideration of the decay rate of turbulence, according to Eq. (8) with the turbulent kinetic energy  $k$ , the dissipation of turbulent kinetic energy  $\varepsilon$  and the kinematic viscosity  $\nu$ . The mass fraction  $\gamma^*$  occupied by the fine structures is also obtained from the local turbulence, see Eq. (9).



**Figure 2.** Homogeneous stirred reactor

$$M = 23.6 \left( \nu \varepsilon / k^2 \right)^{\frac{1}{4}} \frac{\varepsilon}{k} \quad (8)$$

$$\gamma^* = 9.7 \left( \nu \varepsilon / k^2 \right)^{\frac{3}{4}} \quad (9)$$

By treating the reacting fine structures locally as a homogeneous stirred reactor (Fig. 2), which transfers mass and energy only to the surrounding fluid, every chemical kinetic mechanism can be linked with this concept. The reaction rates of all species are calculated on a mass and enthalpy balance for the fine structure reactor. The net mean transfer rate of a certain species  $i$  from the surrounding fluid into the fine structures equals the mean consumption (or production) rate of the same species within the fine structures.

Denoting quantities in the fine structures with an asterisk, the chemical reactions and the mass transport can be described by the following algebraic equations for species conservation and total enthalpy  $h$  [kJ/kg].  $q^*$  is the net energy rate per volume which is transferred between the fine structures and the surroundings by other mechanisms like radiation, and  $W_i$  is the molecular weight [kg/kmol]. In this balance the flow rate  $M^*$  must be related per unit volume of the fine structures.

$$\frac{M^*}{1 - \gamma^* \chi} (m_i^* - m_i) = \frac{\omega_i^* W_i}{\rho^*} \quad \text{with} \quad \omega_i^* = f(T^*, m_i^*) \quad (10)$$

$$\frac{\rho^* M^*}{1 - \gamma^* \chi} (h^* - h) = q^* \quad \text{with} \quad M^* = 2.43 \left( \frac{\varepsilon}{\nu} \right)^{0.5} \quad (11)$$

From Eq. (10) and (11) it is possible to calculate the mass fractions  $m_i^*$  and temperature  $T^*$  in the fine structures as a function of the known quantities  $T$  and  $m_i$  (mean temperature and mean mass fractions respectively). The mean reaction rates of all species can then be calculated by either using the mass transfer rate expressed by Eq. (7) or by the chemical reaction rate  $\omega_i^*$  inside the fine structures. One should keep in mind that the reaction takes place only in a fraction of the total space which is defined by Eq. (9). Since the chemical reaction rates  $\omega_i^*$  in the fine structures are generally functions of all mass fractions and the temperature, a set of non-linear, coupled, algebraic equations must be solved.

**Application of the EDC to the coal combustion model.** The EDC is used to model the gas phase combustion of the pyrolysis products and the CO arising from char burnout. Two irreversible global reactions represent the combustion of the volatiles (Eq. (4) and (5)). For the reaction of the 'average' hydrocarbon (Eq. (4)) the overall rate, proposed by Zimont and Trushin [15] has been increased by an order of magnitude as a result of detailed comparisons with experimental data

$$\omega_{hc} = - \frac{2}{x} A_{hc} m_{hc} m_{o_2} e^{-\frac{E_{hc}}{RT}} T^{-3/2} \quad \left[ \frac{kmol}{m^3 s} \right] \quad (12)$$

with  $A_{hc} = 3.39 \cdot 10^{14} \text{ m}^3/(\text{kmol s})$  and  $E_{hc} = 1.67 \cdot 10^5 \text{ kJ}/(\text{kmol K})$ .  $x$  refers to the formula of the 'average' hydrocarbon  $C_x H_y$ , and  $R$  is the universal gas constant. The reaction rate of carbon monoxide (Eq. (5)) is calculated from the global expression reported by Howard et al. [3]

$$\omega_{co} = - A_{co} \rho^2 \frac{m_{co}}{W_{co}} \left( \frac{m_{o_2} m_{H_2O}}{W_{o_2} W_{H_2O}} \right)^{1/2} e^{-\frac{E_{co}}{RT}} \quad \left[ \frac{kmol}{m^3 s} \right] \quad (13)$$

with  $A_{co} = 1.3 \cdot 10^{11} \text{ m}^3/(\text{kmol s})$  and  $E_{co} = 1.26 \cdot 10^5 \text{ kJ}/(\text{kmol K})$ . With the reaction rates  $\omega_{hc}$  and  $\omega_{co}$  formulated for the conditions of the fine structure reactor and the stoichiometry derived from the reaction scheme (Eq. (4) and (5)), the following equation system to calculate the mass fractions in the fine structures is obtained.

$$\frac{\rho^* M^*}{1 - \gamma^* \chi} (m_{hc}^* - m_{hc}) = \omega_{hc} W_{hc} \quad (14)$$

$$\frac{\rho^* M^*}{1 - \gamma^* \chi} (m_{co}^* - m_{co}) = \omega_{co} W_{co} - x \omega_{hc} W_{co} \quad (15)$$

$$\frac{\rho^* M^*}{1 - \gamma^* \chi} (m_{o_2}^* - m_{o_2}) = 0.5 \omega_{co} W_{o_2} + \left( \frac{x}{2} + \frac{y}{4} \right) \omega_{hc} W_{o_2} \quad (16)$$

$$\frac{\rho^* M^*}{1 - \gamma^* \chi} (c_p T^* - c_p T) = - \omega_{co} W_{co} H_{co} - \omega_{hc} W_{hc} H_{hc} + q^* \quad (17)$$

$H$  denotes the heat of reaction [ $\text{kJ}/\text{kg}_{\text{fuel}}$ ] and  $c_p$  the specific heat [ $\text{kJ}/(\text{kg K})$ ]. Here  $q^*$  is the net energy rate which is transferred from the fine structures by radiation. As a simplification the mean value of the  $\text{H}_2\text{O}$  concentration is used in Eq. (13), because there is no consumption of  $\text{H}_2\text{O}$  in the reaction mechanism.

Generally it is necessary to solve the coupled system Eq. (10) and (11) to assure numerical stability. But in the present case with only two global reaction rates, experience showed the possibility to decouple Eq. (14) to (17) and incorporate the iteration procedure of this algebraic equation system into the iteration process of the numerical solver. For that purpose, the oxygen concentration and temperature of the fine structures are taken from the 'previous' iteration. Then all 'new' quantities of the fine structure reactor can be calculated analytically. In some applications, under-relaxation of these properties may be necessary.

## NUMERICAL SOLUTION

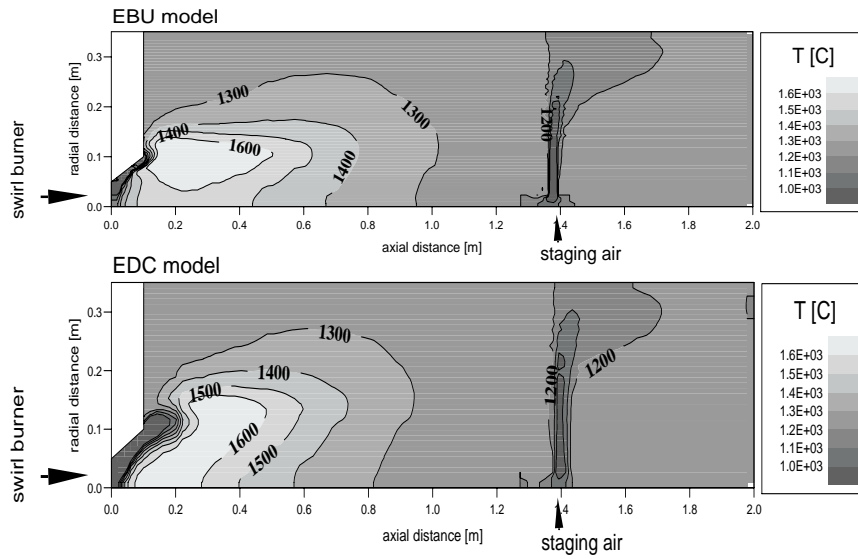
Numerical methods have to be adopted for the solution of the system of differential equations formed by the physical models. The coupling between the equations necessitates an iterative solution procedure consisting of a loop comprising all sub-models. The transport equations are discretized using a non-staggered finite volume method. A disadvantage of the method is the decoupling of the velocity and pressure field, resulting in non-physical solutions. To overcome this problem, a pressure-weighted interpolation method (PWIM) is used.

To reduce numerical diffusion the monotonized linear-upwind scheme (MLU) is used for the calculation of the convective fluxes. The scheme is implemented as a source term correction to the UPWIND scheme. The system of highly coupled non-linear partial differential equations is solved numerically using a Gauss-Seidel algorithm. In order to accelerate the convergence rate, the pressure correction equation is solved using the Strongly Implicit Procedure.

A domain decomposition method is applied in order to achieve both a very fine discretization where a high resolution is needed and a coarse discretization where low resolution is sufficient. The application of this method allows the splitting of the computational domain into an arbitrary number of orthogonal subdomains with arbitrary grid spacings. Thus memory requirements and computational expenditure are reduced without affecting the accuracy of the results. The transfer of data between different domains is achieved by applying the principle that physical quantities like mass, momentum and energy have to be conserved through the transfer. This approach leads to a negligible influence of the domain decomposition technique on the stability of the overall solution procedure. A detailed description of the method is given by Schneider et al. [10].

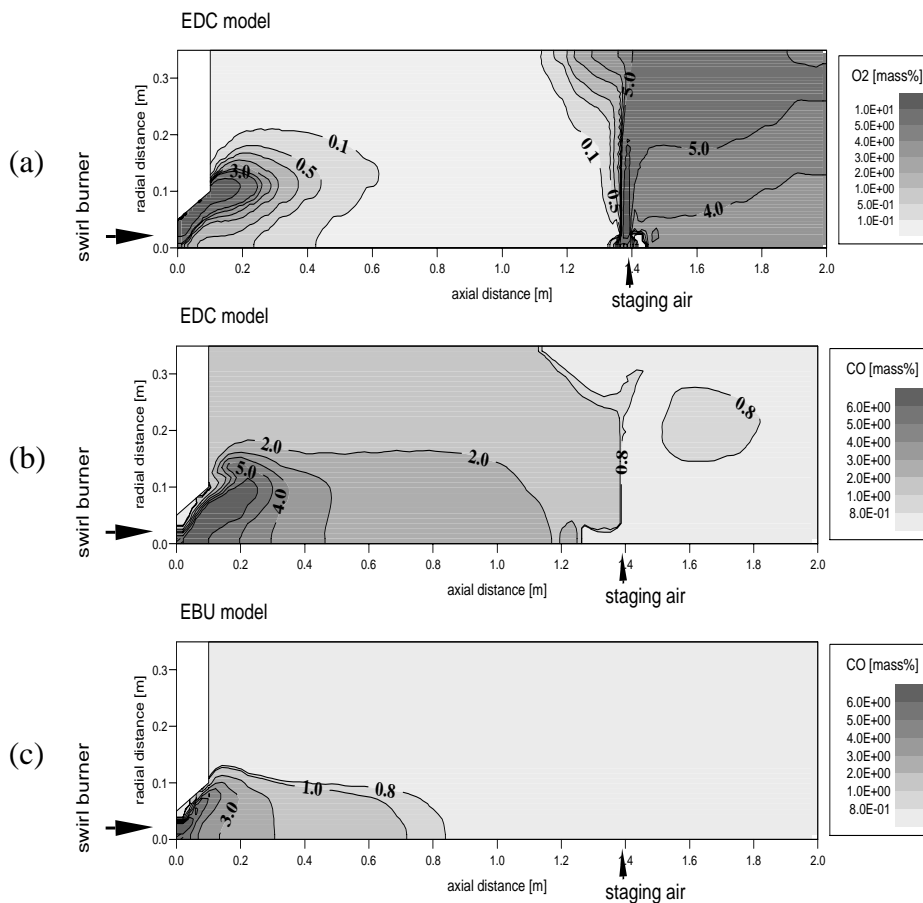
## SWIRLING FLAME CALCULATIONS

To validate the proposed mathematical model of pulverized coal combustion, data obtained at our semi-industrial coal combustion facility with a thermal power of 350 kW are used. The diameter and length of the vertical, cylindrical combustion chamber are 0.75m and 7m respectively. The swirl burner is located at the top of the chamber and the swirl has an angle of about  $25^\circ$  and a length of 0.1 m. This



**Figure 3.** Comparison of temperature distribution predicted with EBU and EDC model

geometry represents a typical example of a burner flow into a low confinement. The pulverized coal (35 kg/h) is transported with air (56 m<sub>n</sub><sup>3</sup>/h, 60°C) through the primary inlet of the burner. One part of the combustion air (141 m<sub>n</sub><sup>3</sup>/h, 280°C) enters the furnace through the secondary inlet of the top burner with a swirl num-

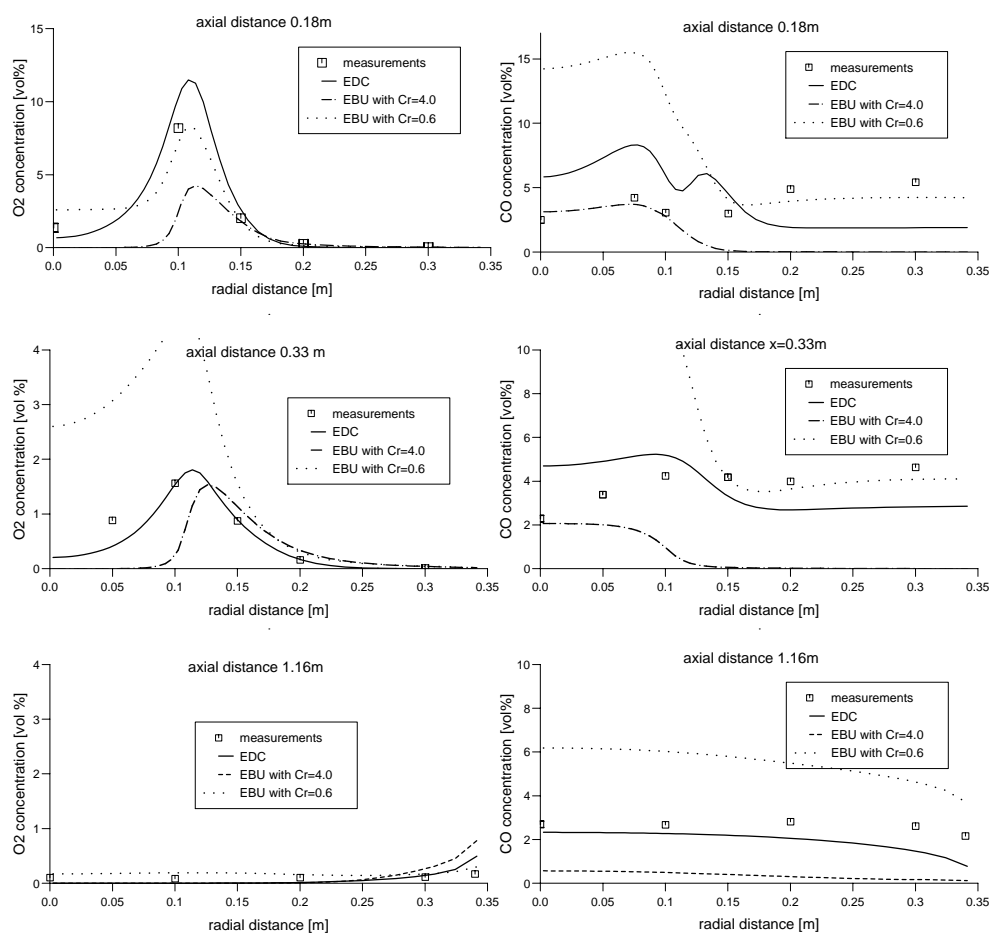


**Figure 4.** Predicted oxygen and CO concentrations

ber of 0.5, the other part ( $140 \text{ m}_n^3/\text{h}$ ,  $280^\circ\text{C}$ ) through a lance at an axial distance of 1.35 m from the burner. A 2-dimensional axisymmetric numerical grid with  $120 \times 50$  nodes was found to give adequate results.

The predicted temperature distribution (Fig. 3) shows only minor differences between the two combustion models under investigation. Some influence may be found at the ignition zone near the quarl, but in the present case this is not important for the general shape of the flame. Unfortunately there are no measurement data available to validate the models in this region. The calculated oxygen and carbon monoxide concentrations (Fig. 4) demonstrate the behavior of this air-staged flame. The swirl burner with a stoichiometric ratio of 0.7 in the primary zone produces a short flame with internal recirculation zone. A large reduction zone with low oxygen concentration is located between the burner and the staging air inlet. In this region the CO concentration is quite high.

As expected, the major influence of the included chemical kinetics into the Eddy Dissipation Concept can be seen most obviously for the intermediate combustion species, which is the CO concentration in the present case. Figure 4c shows the CO prediction using the EBU model. Here, the reaction rate of CO oxidation is too fast and the CO concentration in the reduction zone is underpredicted.



**Figure 5.** Radial profiles of  $\text{O}_2$  and CO concentrations at various axial distances

In Fig. 5, predicted  $O_2$  and CO concentration profiles are compared with measurement data at several axial distances from the burner. Obviously, the predicted CO concentration can be influenced by adjusting the EBU constant  $C_r$  of the CO reaction rate in Eq. (6). Visser [14] reported good prediction results of swirling pulverized coal flames using an EBU constant  $C_r=0.6$ . In the present case this modification leads to an overprediction of the CO concentration. It may be deduced from Fig. 5 that the predictions using EDC agree better with the experimental data than the EBU model calculations, although some discrepancies near the burner exist. Adjusting the constant  $C_r$  to improve the EBU calculations is not a general concept to calculate various combustion cases.

When discussing these results of pulverized coal combustion, it must be considered that the species concentrations are not only affected by the gas phase combustion model. The coal pyrolysis and char burnout model may also cause some shortcomings. No measurements of the char burnout are available to examine the presented flame calculation. Another known source of error is the applied simple chemical mechanism without inclusion of reverse reactions. To explore these phenomena in more detail, the EDC should be applied to gas flames.

The overall performance of the complete pulverized coal model is further demonstrated by the predicted axial and tangential velocity profiles shown in Fig. 6. Although a simple  $k,\epsilon$ -turbulence model is used, reasonable agreement with LDV data is found which is a necessary prerequisite to validate combustion models. The assumed no-slip condition of the particles seems to cause no significant error, see e.g. [2], [12].

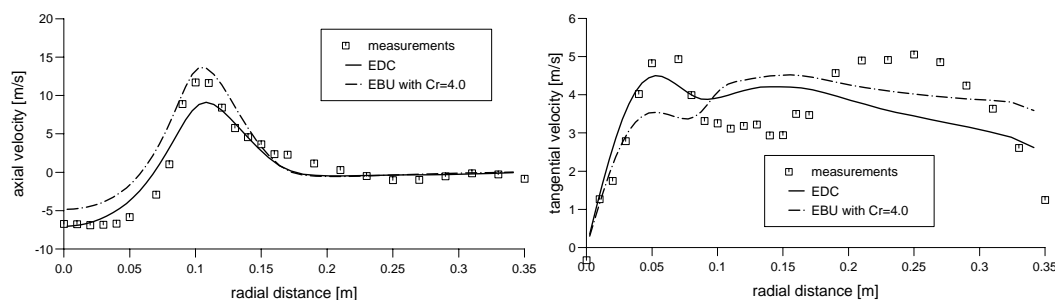


Figure 6. Axial and tangential velocity profiles at axial distance 0.18m

## Utility Boiler Simulation

The three-dimensional predictions are carried out for a coal-fired utility boiler. The boiler has a height of 28m and a cross-section of approximately 8m square. Six swirl burners are located on the front wall. They are distributed on three burner levels and equipped with air staging through several adjacent nozzles. The boiler is discretized with a multi domain grid with one fine domain for each of the three burner levels. The numerical grid depicted in figure 7 has  $50 \times 27 \times 84$  nodes in the main domain and  $50 \times 22 \times 22$  in each subdomain. All boundary conditions, input data and coal parameters were provided by the boiler manufacturer.

Figure 7 shows the predicted CO concentration in a horizontal slice on the lowest burner level for the EBU and the EDC model. As in the above investigation,

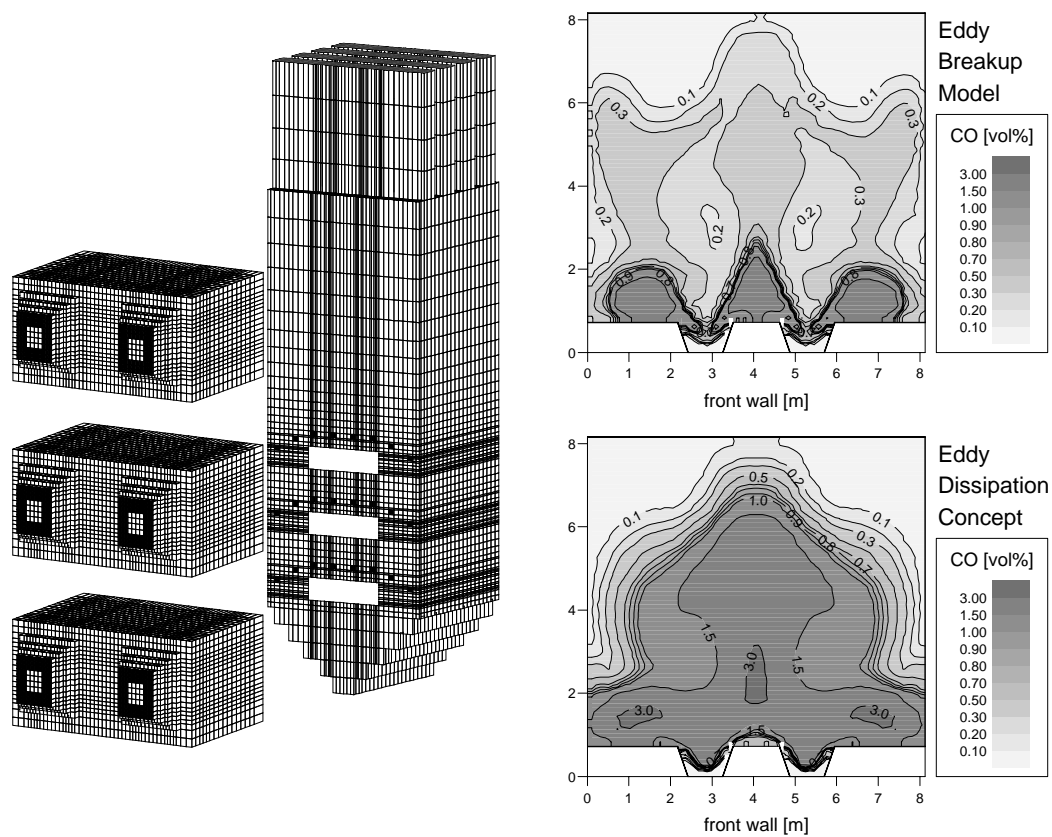


Figure 7. Multi domain grid and predicted CO concentration on the lowest burner level

the inclusion of chemical reaction rates leads to a substantial increase of the calculated carbon monoxide concentrations.

The comparison of the three-dimensional boiler simulation with measured concentration profiles must be done very carefully. Uncertainties about the steadiness of boiler operation during the measurement campaign and difficulties with suction probes in large boilers make it difficult to obtain reliable data. On the other hand, the correct prediction of the flow field cannot be assured because of the coarse numerical grid, problems associated with turbulence modelling, potential effects of false diffusion and some uncertainties in the boundary conditions.

Measurements of two CO concentration profiles were made on the lowest burner level, one along the burner axis and one parallel to the front wall at a dis-

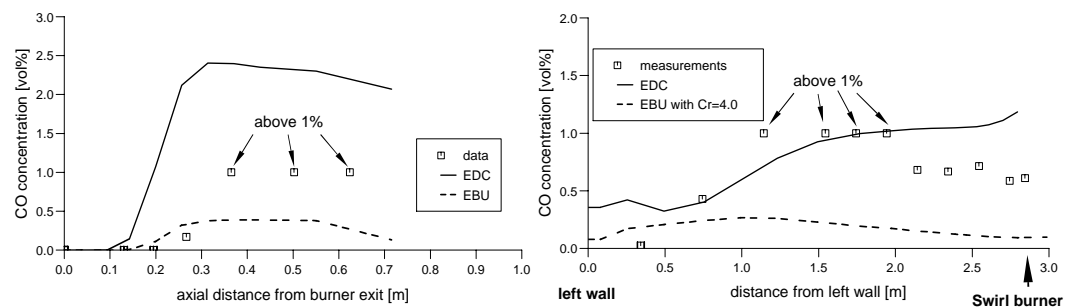


Figure 8. CO profiles on the lowest burner level: along burner axis (left) and at 2m wall distance

tance of 2m. The magnitude of the measured CO concentration can adequately be predicted only with the EDC model (Fig. 8), although in some regions, e.g. near the wall, the discrepancies are yet unsatisfactory.

## CONCLUSIONS

A combustion model able to handle finite rate chemistry in turbulent combustion has been described. The model is based on an extended Eddy Dissipation Concept combined with a simple two-step reaction mechanism for the gas phase reactions.

Predictions of pulverized coal combustion systems with air staging have been presented. It has been shown that the inclusion of chemical kinetics in the combustion model can achieve significant improvement in comparison to a combustion model which assumes infinite fast chemistry. The EDC combined with finite rate chemistry is a promising concept to calculate the near burner field of swirled flames. The quality of the EDC in far flame regions cannot be assured from the presented calculations and the available measurement data. More work should be done to examine these regions. Further investigations focusing on gas flame simulations computed with the EDC using detailed chemical reaction mechanisms should ensure the quality of the model.

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