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PREDICTING CO EMISSIONS USING NOVEL NUMERICAL MODEL FOR PARTICLE IGNITION/COMBUSTION

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Abstract
This work presents development and implementation of sophisticated user defined numerical model for particle ignition/combustion. The proposed model was built in the framework of comprehensive CFD code ANSYS FLUENT. The model is based on structural sub-model for particle devolatilization and realistic mechanism for particle ignition/combustion, which allows for both homogeneous and heterogeneous particle ignition. The user model performance was compared with ANSYS FLUENT standard ignition/combustion models. Models' calculated values of CO mass fraction from semi-industrial furnace were compared against experimentally determined values. The obtained results showed that the advanced user model is superior, in predicting CO mass fractions in furnace near burner zone, compared with ANSYS FLUENT default models. It is expected that the suggested model will be utilized in calculating ignition/combustion behavior of realistic furnaces and boilers.

***Keywords**: CFD, devolatilization, ignition, combustion, emissions.*

1. INTRODUCTION

The main aim of this paper is development and implementation of advanced models for pulverized coal combustion and gasification. CFD code ANSYS FLUENT [1] has capability to model solid fuels combustion and gasification. However, significant challenges appear when standard ANSYS FLUENT models are used. Thus, sophisticated combustion/gasification user defined model was suggested. The novel model incorporates all combustion/gasification phases: ignition, devolatilization, gas phase combustion, and char combustion/gasification.

The main subject of this paper is three-dimensional CFD modeling of high-bituminous pulverized coal combustion inside 2.4 MW_t IFRF furnace [2]. Performances of totally three different combustion/gasification models were compared with experimental data. The two models are incorporated inside ANSYS FLUENT by default, and the third is user defined implemented using UDFs written in C programming language [3].

2. MATHEMATICAL MODELING

The main features of the three utilized mathematical models for combustion/gasification are presented in the paragraphs bellow. The main goal of this work was comparison between standard ANSYS FLUENT combustion/gasification models and suggested sophisticated user implemented combustion/gasification model in predicting CO and NO pollutants emissions.

2.1 Eddy dissipation combustion model (EDM)

Model is composed of the following sub-models for different combustion/gasification phases: Single kinetic rate devolatilization model [4]; Gas phase reactions: default ANSYS FLUENT global reaction mechanism composed of totally two reactions was modeled using "Eddy Dissipation" model for reaction rates modeling [5]; Char combustion reactions: single global reaction was modeled using "kinetic-diffusion limited" approach [6, 7].

2.2 Finite rate/Eddy dissipation combustion model (FR/EDM)

Model is composed of the sub-models listed below: Single kinetic rate devolatilization model [4]; Gas phase reactions: ANSYS FLUENT global reaction mechanism was used as in the previous case (EDM model) [5]; Single reaction for char combustion was modeled using "kinetic/diffusion-limited" approach [6,7].

2.3 User Defined Finite rate/Eddy dissipation combustion model (UDF FR/EDM)

Sub-models, implemented using UDFs written in C language [3], for different combustion phases are as follows: Functional group devolatilization model with distributed activation energy model – DAEM [8,9,10]. Gas phase reactions: Semi-global reaction mechanism composed of totally six global reactions was implemented based on "Finite Rate/Eddy Dissipation" model. The reactions were built in ANSYS FLUENT code using UDFs [3]. Char reactions: Totally three global reactions were implemented utilizing UDFs based on "kinetic/diffusion-limited" approach [3]. Particle ignition/combustion mechanism: Default ANSYS FLUENT mechanism, which assumes that char combustion occurs only after particle is completely devolatilized was substituted with novel, user-defined combustion/ignition mechanism. The suggested mechanism allows for all possible means for particle ignition/combustion. That is, it allows that particle combustion can take place before devolatilization is completed. Necessary condition for this to occur is that oxidation of the particle is faster than its devolatilization.

3. EXPERIMENTAL DATA

Experimental data for model validation were taken from work [2]. Measuring axes are located near burner front at distances $z = 0.25\ m$ and $z = 0.85\ m$.

Initial computational grid consisted of 52000 computational cells. This grid was gradually refined in near-burner region until the obtained solution stopped changing with the number of computational cells. Final computational mesh, adopted for all simulations in this work has totally 428000 cells.

4. RESULTS AND DISCUSSION

Logarithmic distribution of CO mass fraction along radial axis at distance $z = 0.25\ m$ is shown in Figure 1. CO distribution obtained using EDM model does not agree well with experimental data. EDM model predicts sharp decrease in CO mass fraction. Based on this, it can be concluded that EDM model is not suited even for qualitative comparison with experimental data.

Similar conclusion can be made in case of FR/EDM model predicted results in comparison with measurements. Namely, FR/EDM model severely underpredicts CO mass fraction values at radial distances up to 0.15 *m* from the burner front.

UDF FR/EDM model calculated results follow experimentally measured data. It is imported to note that the closest agreement between numerical and experimental data obtained at the close distances from the burner front, up to 0.18 *m*. Both curves, model calculated and experimentally measured, predict small increase of CO mass fraction in this zone, although experimental dependence has somewhat lower values.

CO mass fraction logarithmic distribution along radial axis at distance $z = 0.85$ *m* from the burner front is shown in Figure 2.

EDM calculated curve follows experimental trend qualitatively at small distances from the burner front, up to 0.15 *m*. However, model calculated values are significantly higher than experimentally determined. Further down from the burner front EDM calculated values drop sharply to about 10 *ppm* at the radial distance 0.28 *m*. This is in keen contrast with the experimental results.

FR/EDM model, similarly to EDM model, does not show satisfying performance in determining CO mass fraction. Although FR/EDM calculated curve has similar behavior to experimental, FR/EDM values are much higher than experimentally measured. UDF FR/EDM model exhibits significantly better performance in predicting CO mass fraction values compared with two previously described models, EDM and FR/EDM. UDF FR/EDM calculated curve follows trend of experimentally measured data.

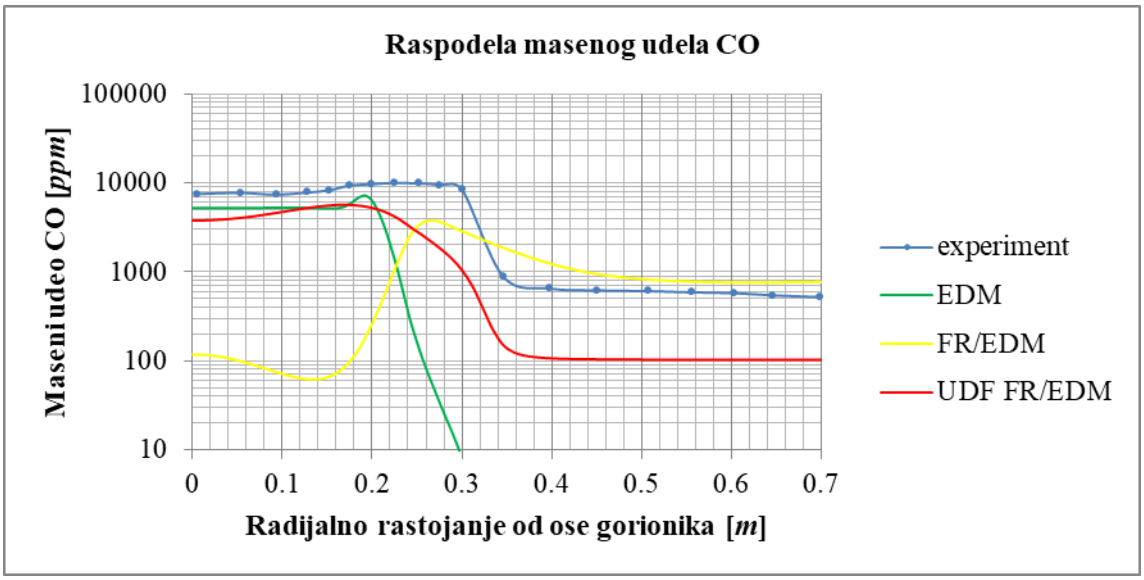

Figure 1. CO mass fraction logarithmic distribution along radial axis at distance z = 0.25 m from the burner front

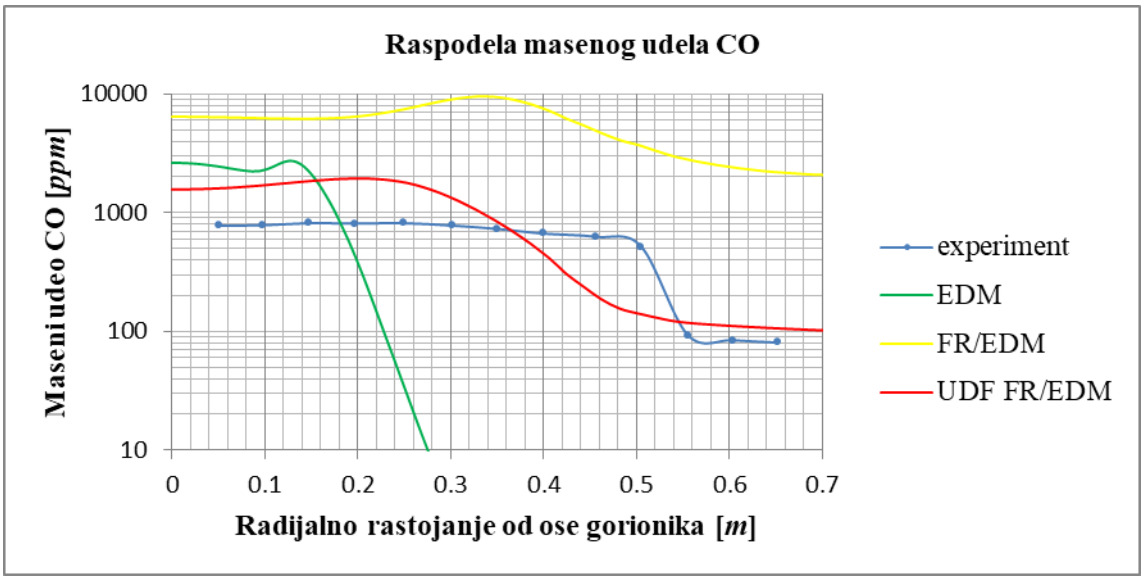

Figure 2. CO mass fraction logarithmic distribution along radial axis at distance z = 0.85 m from the burner front

5. CONCLUSIONS

The following conclusions were drawn based on the performed work: Novel combustion model for particle ignition/combustion was suggested; The proposed model was developed and built in ANSYS FLUENT framework using UDFs; Model performance was tested against experimental data available in scientific literature; It was shown that the user model outperforms standard ANSYS FLUENT ignition/combustion models in predicting CO emissions from experimental furnace; The novel model showed high accuracy in predicting CO emissions in near burner zone; Model accuracy is largely based on built in structural devolatilization and ignition/combustion sub-models; The next step is model utilization is in numerical calculations of combustion in real scale furnaces and boilers.

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ABBREVIATIONS

CFD	Computational Fluid Dynamics
DAEM	Distributed Activation Energy Model
EDM	Eddy Dissipation Model
FG	Functional Group
FR	Finite Rate
IFRF	International Flame Research Foundation
UDF	User Defined Function