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MATHEMATICAL SIMULATION OF COAL PARTICLES COMBUSTION
NUMERICKÉ MODELOVÁNÍ SPALOVÁNÍ UHELNÝCH ČÁSTIC

Abstract

In this paper example of mathematical modeling of mixture coal ignition using plasm jet is presented. At the beginning the computation was simplified so that coal mixture is ignited by air about 5700 K instead of plasm. Task is defined as turbulent flow of air and coal particles with heat transfer and chemical reaction. In software Fluent 6.3 flow can be solved by turbulent models, heat transfer then by radiation models. Mathematical model of continuous discrete phase was created, which characterizes adrift of coal particle. Model was solved by method of finite volume.

Abstrakt

V článku je prezentován příklad matematického modelování zapálení uhelné směsi plazmovým hořákem. Na začátek byl výpočet zjednodušen na příklad, kde se uhelná směs zapálí místo plazmy vzduchem o teplotě 5700 K. Úloha je definována jako turbulentní proudění vzduchu a uhelných částic v práškovodu s přenosem tepla a chemickou reakcí. V softwaru Fluent 6.3 lze proudění řešit tzv. *modely turbulence*, přenos tepla pak tzv. *radiačními modely.* Byl vytvořen matematický model turbulentního proudění spojité fáze a diskrétní fáze, což charakterizuje unášení uhelných částic a spalování. Model byl řešen metodou konečných objemů.

1 Mathematical model of turbulence for compressible flow

1.1 Reynolds equation, continuity and energy equation, species transport equation

In mathematical model there are used following equations [1]:

- Continuity equation

$$\frac{\partial \rho}{\partial t}+\frac{\partial\left(\rho \overline{u_j}\right)}{\partial x_j}=0 . \tag{1.1}$$

- Momentum equation

$$\frac{\partial\left(\rho \overline{u}_i\right)}{\partial t}+\frac{\partial\left(\rho \overline{u_i} \overline{u_j}\right)}{\partial x_j}=-\frac{\partial p}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu_t \frac{\partial \overline{u_i}}{\partial x_j}\right)+\rho \delta_{i3} g+\rho f_c \varepsilon_{ij3} \overline{u_j}+\rho f_i \tag{1.2}$$

- Heat transfer equation

$$\frac{\partial}{\partial t}\left(\rho \overline{h}\right)+\frac{\partial}{\partial x_j}\left(\rho \overline{u_j} \overline{h}\right)=\frac{\partial}{\partial x_j}\left(\lambda_t \frac{\partial \overline{T}}{\partial x_j}\right)+\frac{d \overline{p}}{dt}+\frac{\partial\left(\overline{\tau_{jl}} \overline{u_j}\right)}{\partial x_l}, \tag{1.3}$$

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- Species transport equation [3]

$$\frac{\partial}{\partial t}\left(\rho \overline{Y_i}\right)+\frac{\partial}{\partial x_j}\left(\rho \overline{u_j}\,\overline{Y_i}\right)=\frac{\partial}{\partial x_j}\overline{J_i}+R_i+S_i\ , \qquad (1.4)$$

where :
t ...... is time,
x_i..... is coordinate,
ρ..... is density,
$\overline{Y_i}$ .. is mass fraction of product species i,
$\overline{u_i}$ .. is velocity component,
$\overline{p}$ ... is pressure,
λ_t .. is turbulent thermal conductivity,
R_i .... is net rate of production of species i,
$\overline{J_i}$ .. is diffused flux of species i.
S_i..... is the rate of creation by addition from the dispersed phase
μ_t .. is turbulent viscosity

2 Models of combustion in Fluent 6.3

2.1 Discrete Phase Model (DPM) [3]

This model plays an important role in particle combustion. With the aid of discrete phase model (DPM) and species transport model it is possible to define chemical reactions on user defined particles. It could be used by modelling of coal combustion. Disadvantage of this modelling is difficulty of data definition. All reactions, species and material properties must be set up separately in comparison with predefined models in Fluent. Advantage of this type of modelling is more accuracy of results.

Fluent provides the following options of discrete phase modelling:

- Calculation of the discrete phase trajectory using Lagrangian formulation that includes the discrete phase inertia, hydrodynamic drag and force of gravity, for both steady and unsteady flows.
- Turbulence prediction on particles dispersion due to turbulent eddies present in the continuous phase.
- Warming-up and cooling down of the discrete phase.
- Particles burning.
- Break-up of drops.
- Evaporation and boiling of drops.

The main limitation of this model is that volume fraction must be lower then 10-12%. It is impossible to simulate periodical flow in this model.

2.2 Model of premixed combustion

Fuel and oxidizer are mixed before they enter into the combustion device, see Fig.2.1.

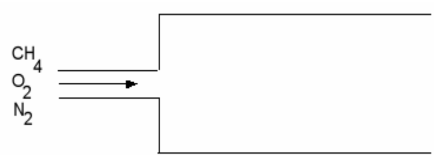

Fig. 2.1 Model of premixed combustion

Reaction takes place in combustion area, with unburnt reactant and burnt product separation. For example there are engines with internal combustion, lean premixed gas turbine and gas-leak explosion. Premixed combustion is characterised by unstability and it occurs as a thin flame propagation, which is controlled by turbulence. For subsonic flows, the overall rate of the flame propagation is determined by both the laminar flame speed and the speed of turbulent eddies. The flame front propagation is modelled by solving a transport equation for the density-weighted mean reaction progress variable, denoted by c [2]:

$$\frac{\partial}{\partial t}(\rho c)+\frac{\partial}{\partial x_j}\left(\rho \overline{u_j} c\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Sc_t}\frac{\partial c}{\partial x_j}\right)+\rho S_c\ , \qquad (2.5)$$

where:
c...... is mean reaction progress variable,
Sc_t... is turbulent Schmidt number,
S_c .... is reaction progress source term (s^{-1}).

$$c=\frac{\sum_{i=1}^{n}\overline{Y_i}}{\sum_{i=1}^{n}\overline{Y_{i,eq}}}\ , \qquad (2.6)$$

where
n ....is number of products,
$\overline{Y_i}$ ....is mass fraction of product species i,
$\overline{Y_{i,eq}}$ ....is equilibrium mass fraction of product species i .

Limitations

Limitations of the premixed combustion model:

- It is necessary to use pressure-based solver. The premixed combustion model is not available with density-based solvers.
- The premixed combustion model is valid only for turbulent, subsonic flows. These types of flames are called deflagrations. Explosions, also called detonations, where the combustible mixture is ignited by the heat behind a shock wave, can be modelled with the finite – rate model using the density – based solver.
- The premixed combustion model cannot be used in conjunction with the pollutant (soot, NO_x) models. However, a perfectly premixed system can be modelled with the partially premixed model, which can be used with the pollutant models.
- The premixed combustion model cannot be used to simulate reacting discrete-phase particles, because these should be solved in a partially premixed system. Only inert particles can be used with the premixed combustion model.

2.3 Model of non-premixe combustion

Non-premixed model is predefined in Fluent. Combustion fuel and oxidizer enter the reaction zone in distinct streams in non-premixed model. Examples of non-premixed combustion include pulverised coal furnaces, and diesel internal combustion engines.

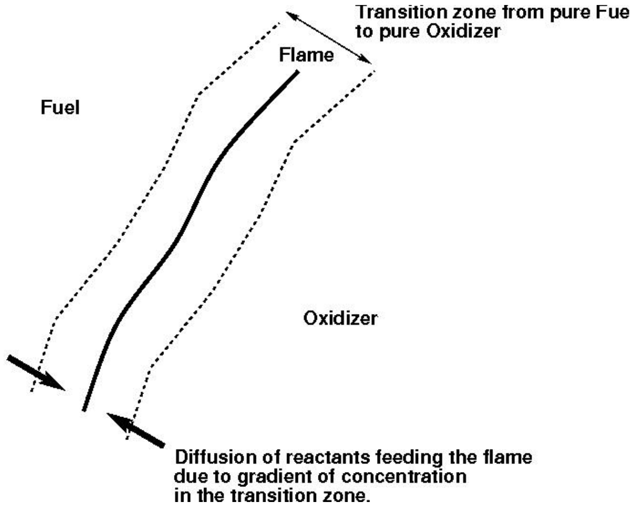

Fig.2.2 Principle of non-premixed combustions

In certain presumptions, the thermo-chemistry can by reduced to a single parameter: the mixture fraction. The mixture fraction, denoted as f, is the mass fraction, which is originated in the fuel stream. In other words, it is the local mass fraction of burnt and unburnt fuel stream elements (C, H, respectively S, N) in all species CO_2, H_2O. The mixture fraction is a conserved scalar value, and therefore its governing transport equation does not have a source term.

The Favre mean (density averaged) mixture fraction equation is

$$\frac{\partial}{\partial t}\left(\rho \overline{f}\right)+\frac{\partial}{\partial x_j}\left(\rho \overline{u_j}\,\overline{f}\right)=\frac{\partial}{\partial x_i}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \overline{f}}{\partial x_i}\right)+S_m+S_{user}\,, \tag{2.7}$$

where

$\overline{f}$ ...is mixture fraction,

S_m .....is due solely to transfer of mass into the gas phase form liquid fuel droplets or reacting particles,

S_{user} ..is any user-defined source term.

Once mixed, the chemistry can by modelled as being in chemical equilibrium with the Equilibrium model, being near chemical equilibrium with the Steady Laminar Flamelet model, or significantly departing from chemical equilibrium with the Unsteady Laminar Flamelet model. Non premixed modelling involves the solution of transport equations for one or two conserved scalars. Equations for individual species are not solved. The non-premixed modelling approach has been specifically developed for the simulation of turbulent diffusion flames with fast chemistry.

3 Problem-solving

As described above, it is possible to define coal combustion by several models in Fluent: non-premixed, premixed and discrete + species models. Results were compared with the same problem solved by CFX software.

3.1 Problem description

Assignment modelled ignition mixture of coal particles and air through plasm burner. At the beginning the computation was simplified so that coal mixture is ignited by air about 5700 K instead of plasm. Above defined assignment was solved step by step in Fluent (non-premixed, premixed model and then user-defined chemical reaction by means of species model with coal discrete phase). [4]

3.2 Geometry of area

Problem was solved in area, which is created of one outlet and two inlets, see Fig 3.1.

Computational grid:

In Gambit created grid has 78000 cells and region is bounded by two inlets, one outlet and wall, see Fig 3.2.

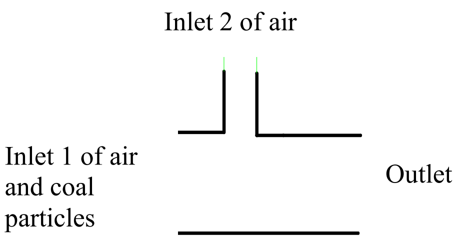

Fig. 3.1. Geometry of area

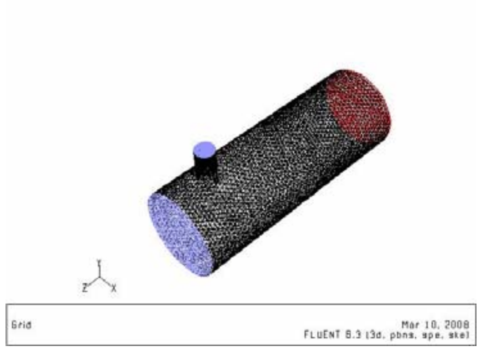

Fig. 3.2. Computational grid

3.3 Physical properties

For solution were used air and coal particles of these properties.

air
ρ = 1,225 kg/m^3
c_p=1006,43 J/kgK
λ = 0,0242 W/mK
μ = 1,7894*10^{-5} kg/ms

coal
ρ = volume – weighted – mixing law
c_p= mixing law
λ =volume – weighted – mixing law

3.4 Boundary conditions

Flowing medium is air. The velocity of air on inlet 1 is 11 ms^{-1} and temperature is 343 K. By this inlet coal particles enter too, they are defined through injections by mass flow 0,01kgs^{-1}. By inlet 2 the air enters too. This air supplies plasm about temperature 5700K and mass flow 0,03kgs^{-1}. Outlet boundary condition is defined as pressure outlet.

For modelling the standard turbulent k-ε model is used.

3.5 Results

Temperature, flow velocity and pressure drop are evaluated in comparison of three used models in Chart 1.

Types of model	Δp [Pa]	T [K]	v [m/s]
Discrete model	99,4	343 – 5270	12,1
Non-premixed model	385,33	334 - 3250	63,4
Premixed model	167,63	343 - 5270	94,7

Chart 1

In line with contemplation discrete model is most exact in comparison with CFX modelling. There is an illustration of velocity magnitude, see Fig 3.3. Static temperature of during reaction is image, see Fig 3.4.

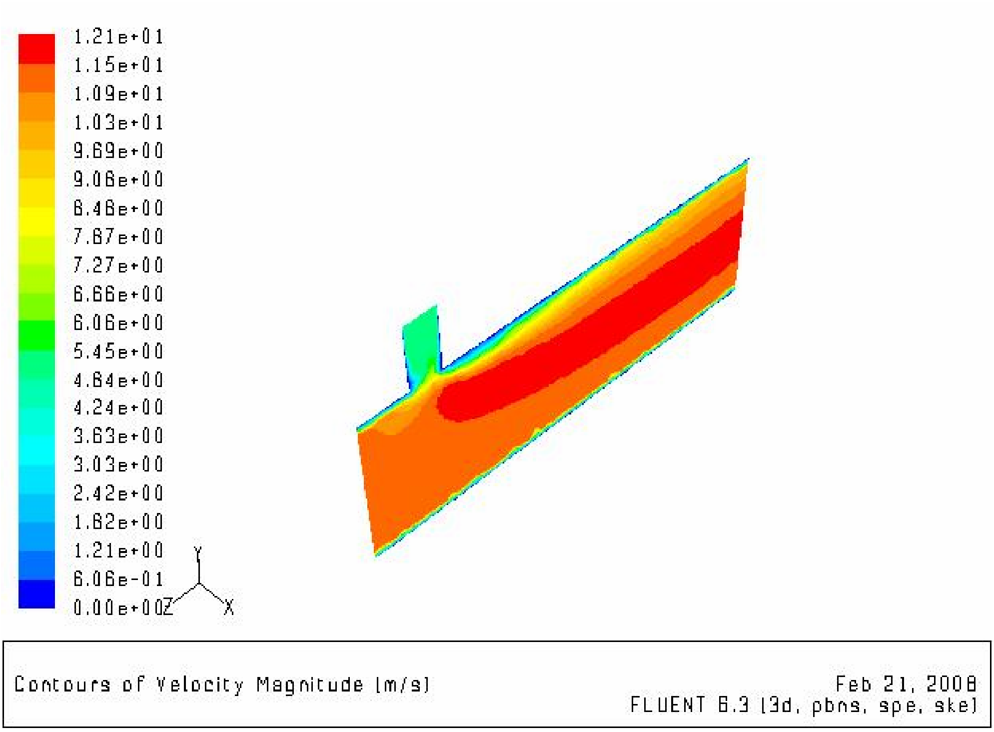

Fig. 3.3 Velocity Magnitude

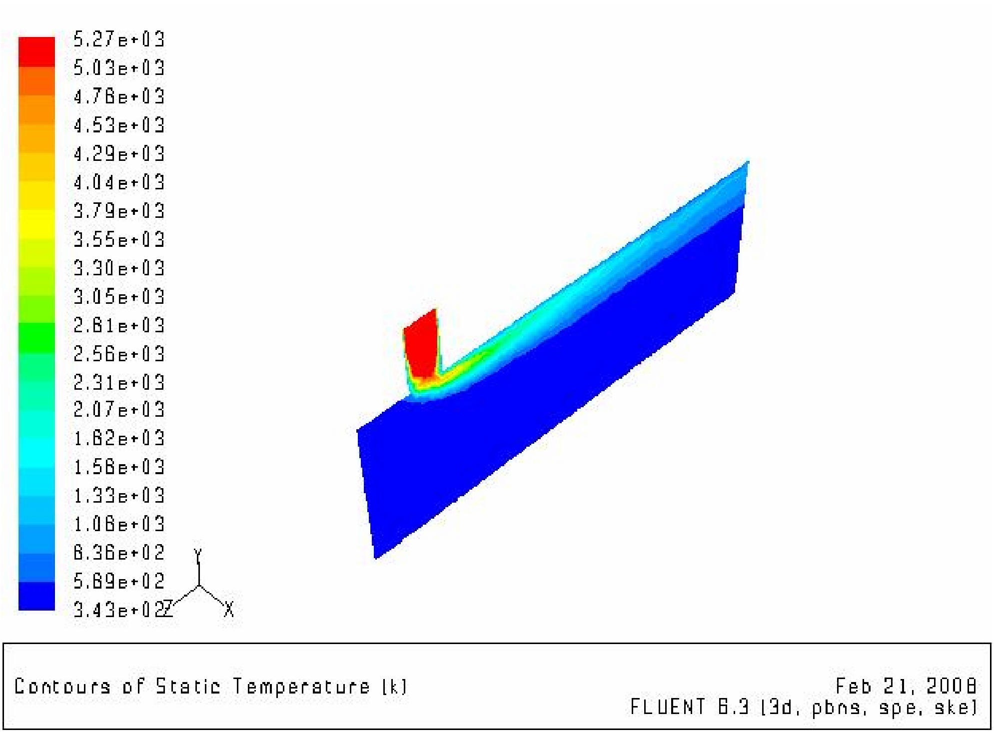

Fig 3.4 Static temperature

4 Conclusion

The paper deals with modelling and evaluating of coal particle combustion using three combustion models in software Fluent that means non-premixed model, premixed model and model of discrete particles. After comparison of all models, we can say, that for our example non-premixed model is unsuitable, because it does not enable to exceed adiabatic temperature, and constants in Fluent are defined for gas fuel only (methane). Premixed model can display velocity magnitude and temperature. For our example it is unsuitable as well because of no possibility to display mass fraction, which is important in terms of emission standards. In our case the best way of solution is using of discrete model, which allows display temperature, velocity and mass fraction species. It enables to exceed the adiabatic temperature and it is usable for various fuels. By using this model we can obtain more accurately results, but computation takes a longer time. DPM model is consistent with results gained from CFX software in values of velocity, pressure, temperature and concentration of species and reaction products.

5 Literature

[1] KOZUBKOVÁ, M., DRÁBKOVÁ, S. *Numerické modelování proudění – FLUENT I.* [Online]. c2003. Ostrava: VŠB – TUO, 116 s, poslední revize 9.1.2006 [cit. 2006-01-09]. Dostupné z: <URL: http://www.338.vsb.cz/seznam.htm>.

[2] Ansys, Inc. *ANSYS Documentation Overview*. [Online]. c2006. poslední revize 9.1.2006 [cit. 2006-01-09]. Dostupné z: < http://www.ansys.com/services/ss-documentation-manuals.asp>.

[3] FLUENT: Fluent 6.3.26 - User's guide. Fluent Inc. 2006. VŠB-TU Ostrava <URL:http://spc.vsb.cz/DOC/Fluent_6.3/html/ug/main_pre.htm

[4] Tomáš Blejchař, Rostislav Malý: Model spalování uhlí v CFD programu Ansys/CFDMezinárodní konfrence "Energetika a životní prostředí 2007, 26-27.9.2007, Sborník ISBN 978-80-248-1586-2, str.19-31.

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