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Calculation of coal-water fuel combustion technology based on mathematical modeling

Calculation of technology of burning of coal-water fuel (CWF) on the basis of mathematical modeling is presented. Numerical simulation of the process of burning coal-water fuel was carried out in the software package ANSYS Fluent. It is based on the laws of conservation of mass, energy and momentum in a multicomponent medium and the solution of the Navier-Stokes equations, continuity and heat transfer. A mathematical model of the combustion of CWF consists of three phases. For modeling the combustion of pulverized coalwater fuel, using the model of breakup of eddies (Eddy-Dissipation Model) and the parameters of injection of droplets into the furnace were set using the «Discrete Phase Model» function. In ANSYS Fluent, a threedimensional formulation of the problem is given and the Navier-Stokes and Reynolds-averaged energy equations are solved. To account for turbulence, a two-parameter model «k-ɛ»is chosen.In the course of numerical simulation, the distribution field patterns of velocity vectors were obtained. When conducting a thorough analysis of the furnace temperature regime, we realized that the optimal combustion temperature of CWF is 700–1200 °C. The relation of the particle residence time in the combustion chamber of the furnace on its diameter is obtained.

Keywords: hydrocarbon fuel, numerical simulation, ANSYS Fluent, the Navier-Stokes equations, the process of burning.

Introduction

The process of fuel combustion in technical devices is a difficult and expensive process, which involves high cost of each experiment and equipment, this is a very complicated process of pre-mathematical studies. To facilitate the process of preliminary research, numerical modeling is currently used [1].

The numerical simulation of the process of burning coal-water fuel was carried out in the software package ANSYS Fluent. It is based on the laws of conservation of mass, energy and momentum in a multicomponent medium and the solution of the Navier-Stokes equations, continuity and heat transfer. The combustion mixture depends on the speed of the reaction and can occur in laminar flow and turbulent flow. The process of burning CWF is the turbulent combustion regime. Chemical reactions and turbulence have a mutual influence, in consequence of which the flame can increase turbulence by accelerating the flow and changing the viscosity, and turbulence in turn changes the structure of the flame intensifying mixing and reaction rates

The process of burning CWF is the combustion of a mixture that consists of water-carbon droplets and coal particles [2]. To describe the combustion of this mixture takes the approach of Euler and Lagrange. According to this approach, the Eulerian component is responsible for the equations of motion, heat transfer and combustion in the gas medium, and the Lagrange approach is responsible for the description of the motion and heat and mass transfer of a single particle. A two-parameter turbulence model «k- ϵ » is used to account for gas turbulence, which also takes into account the influence of individual particles.

A mathematical model of the combustion of CWF consists of three phases. The first phase is the gas phase, it is described by the following equations:

1. The equation of continuity

$$\frac{\partial p}{\partial t} + \frac{\partial (pU_i)}{\partial x_i} = J_{evap} + J_{vap} + J_{char}.$$
(1)

2. Mass balance equation of gas components:

$$\frac{\partial \rho C_{N_2}}{\partial t} + \frac{\partial \rho C_{N_2} U_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_i}{Sc_i} \frac{\partial C_{N_2}}{\partial x_i} \right).$$
(2)

3. Equations of mass change of gas components:

$$\frac{\partial \rho C_{O_2}}{\partial t} + \frac{\partial \rho C_{O_2} U_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Sc_t} \frac{\partial C_{O_2}}{\partial x_i} \right) - \beta_{vol} J_{vol} - \beta_{CO} J_{CO} - J_{char}^{O_2};$$
(3)

$$\frac{\partial \rho C_{vol}}{\partial t} + \frac{\partial \rho C_{vol} U_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Sc_t} \frac{\partial C_{vol}}{\partial x_i} \right) + \alpha_{vap} J_{vap} - J_{vol};$$
(4)

$$\frac{\partial \rho C_{CO}}{\partial t} + \frac{\partial \rho C_{CO} U_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_i}{Sc_i} \frac{\partial C_{CO}}{\partial x_i} \right) + J_{char}^{CO} - J_{CO}; \qquad (5)$$

$$\frac{\partial \rho C_{H_2O}}{\partial t} + \frac{\partial \rho C_{H_2O}U_i}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Sc_t} \frac{\partial C_{H_2O}}{\partial x_i} \right) + J_{evap} \,. \tag{6}$$

4. The equation of motion

$$\frac{\partial \rho U_j}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_i} = -\frac{\partial p}{\partial x_j} + \rho g_j + F_j + \frac{\partial}{\partial x_i} \left[(\mu + \mu_T) \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left[\rho k + (\mu + \mu_T) \frac{\partial U_k}{\partial x_k} \right] \right], \quad (7)$$

where j = 1, 2, 3.

5. The equation of energy

$$\frac{\partial \rho T}{\partial t} + \frac{\partial \rho U_i cT}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\left[\frac{\mu}{\Pr} + \frac{\mu_T}{\Pr_T} \right] c \frac{\partial T}{\partial x_i} \right) + Q_{vol} J_{vol} + Q_{CO} J_{CO} - \frac{\partial q_i^{rad}}{\partial x_i} + \Theta .$$
(8)

6. The equation of state

$$\rho = \frac{p}{R_0 T \left[\frac{C_{O_2}}{M_{O_2}} + \frac{C_{N_2}}{M_{N_2}} + \frac{C_{vol}}{M_{vol}} + \frac{C_{CO}}{M_{CO}} + \frac{C_{CO_2}}{M_{CO_2}} + \frac{C_{H_2O}}{M_{H_2O}} \right]},$$
(9)

where U_i — components of the velocity vector of gas; T, p — the temperature and pressure of the gas; ρ, α — reduced density and volume fraction of gas; $J_{evap}, J_{vap}, J_{char}$ — the rate of evaporation of the volatiles and combustion of coke oven sludge; μ, μ_i — molecular and turbulent viscosity of gas; F_j, Θ — components of the force and heat exchange of interfacial interaction; $J_{vol}, J_{CO}, Q_{vol}, Q_{CO}$ — the intensity and the thermal effect of gas-phase combustion of volatiles and carbon monoxide.

The second is the disperse phase. It describes the movements of particles. According to the Lagrangian approach, the entire spectrum of CWF particles can be divided into different fractions, the nature of which motion is determined by a single marker particle and transferred to all such fraction particles. The nature of the particle motion is described by the following equations:

1. Equations of motion of a particle of the 1-st group

$$\frac{dU_{j}^{i}}{dt} = \gamma_{i} \left(U_{j} - U_{j}^{i} \right) + g_{j}, \qquad (10)$$
where $j = 1, 2, 3, \ \gamma_{i} = \frac{3c_{D_{i}} \left| \vec{W} - \vec{W}^{i} \right| \rho}{4d_{i} \rho_{p} \alpha_{g}} \text{ and } c_{D_{i}} = \begin{cases} \frac{24}{\text{Re}_{i}} \left(1 + 0.15 \,\text{Re}_{i}^{0.687} \right) \,\text{Re}_{i} \leq 1000 \\ 0.44 \, \text{Re}_{i} > 1000 \end{cases};$

$$\text{Re}_{i} = \frac{\rho \left| \vec{W} - \vec{W}^{i} \right| d_{i}}{\mu}, \qquad (11)$$

 U_j^i — components of the velocity of particles; ρ_p — density of particles; d_i — diameter of particles of *i*-groups.

2. Equations of heat and mass transfer and combustion particles

$$\frac{dm_i}{dt} = -\dot{M}_i^{evap} - \dot{M}_i^{vap} - \dot{M}_i^{char}; \qquad (12)$$

$$m_i c_p \frac{dT_i}{dt} = Q_{char} \dot{M}_i^{char} + \pi d_i^2 \Big[\alpha_{conv} \left(T - T_i \right) + \varepsilon_p \left(H - 4\sigma T_i^4 \right) \Big] - Q_{vap} \dot{M}_i^{vap} - L_{vap} \dot{M}_i^{evap} , \qquad (13)$$

where m_i — mass of a single particle; c_p — heat capacity of a particle; Q_{char} — calorific value of coke; Q_{vap} — the heat required for the release of volatile; L_{vap} — latent heat of vaporization; ε_p — the degree of blackness of the particles; α_{conv} — the coefficient of convective heat transfer of a single particle.

Mass rate of vaporization of the drop: $\dot{M}_i^{evap} = \pi d_i^2 k_c \left[\left(\rho C_{H_2O} \right)_{surf} - \left(\rho C_{H_2O} \right) \right] \right]$, where $k_c = \frac{D_{H_2O}}{d_i} \left(2 + 0.6 \operatorname{Re}_1^{0.5} Sc^{0.33} \right)$ — mass transfer coefficient; D_{H_2O} — the diffusion coefficient of vapor, $\left(\rho C_{H_2O} \right)_{surf}$ — density and concentration of vapor on the surface of a drop or particle.

The mass rate of flow of volatiles (Law of Arrhenius): $\dot{M}_i^{vap} = k_{vap} \exp\left(-\frac{E_{vap}}{R_0 T_i}\right) \cdot f_{vo} \cdot m_{oi}$, where m_{oi} — the initial mass of dry particle; f_{vo} — mass fraction of volatiles in dry coal; E_{vap} — energy of activation.

The burning rate of the coke residue is described by the following equation:

$$\dot{M}_{i}^{char} = \pi d_{pi}^{2} \rho C_{O_{2}} \frac{K_{k} K_{D}}{K_{k} + K_{D}};$$
(14)

$$K_{k} = k_{char} \exp\left(-\frac{E_{char}}{R_{0}T_{i}}\right), \tag{15}$$

where K_D is described by the following dependency

$$K_D = \frac{D_{O_2}}{dp_i} \left(2.0 + 0.16 \,\mathrm{Re}_i^{0.667} \right). \tag{16}$$

And the final phase is the effect of the dispersed phase on the gas phase. The control volume method is used to account for the influence of particles on the gas phase. To do this, the entire computational domain is divided into a finite number of elements within which the values of the desired functions can be considered homogeneous. And for each such element the proper values are calculated J_{evap} , J_{vap} , J_{char} , F_j , Θ .

To calculate the parameters of the CWF in the ANSYS Fluent package complex, the first step is to build a vortex furnace model by means of CAD programs. Then, using the Gambit package, which is a Fluent preprocessor, a finite difference grid is constructed based on the resulting model (Fig. 1). This model includes: nozzle (1), outlet (2), lower blast system (3), boiler furnace (4). The finite-difference grid is constructed on the basis of tetrahedral elements with uniform distribution throughout the volume, the number of which is equal to 300000 cells.



l — nozzle; *2* — outlet; *3* — lower blast system; *4* — boiler furnace

Figure 1. Finite difference grid

In ANSYS Fluent, a three-dimensional formulation of the problem is given and the Navier-Stokes and Reynolds-averaged energy equations are solved [3–5]. To account for turbulence, a two-parameter model $(k-\varepsilon)$ is chosen. The equations are solved taking into account the implicit scheme of the 2nd order of accuracy in space for the convective terms of the equations. Thermo-physical properties of air are calculated by polynomial dependence on temperature. For modeling the combustion of pulverized coal-water fuel, using the model of breakup of eddies (Eddy-Dissipation Model) and the parameters of injection of drops in the furnace was set using «Discrete Phase Model».

To initialize the numerical simulation, the following parameters were specified:

1) Source data — heat output of the furnace — 0.3 Gcal/h; the flow rate of the CWF through the atomizer — 200–300 kg/h; mass fraction of solid phase — 42–58 %; ash content of coal in CWF — 7 %; the particle size– 0–100 μ m; velocity of the fuel particles is 30–60 m/s; air pressure — 0.2–0.5 MPa; the pressure of combustion air — 0.001–0.002 MPa; the excess air ratio is 1.1 to 1.4.

2) Boundary conditions on the air supply through the nozzle: velocity of gas — 50 m/s; temperature — 300 K; turbulent energy — 0.1 k; energy dissipation rate — 0.1 E.

3) Boundary conditions for the supply of air through the lower blast system-hole width — 3mm; gas velocity — 30 m/s; temperature — 300 K; turbulent energy — 0.1 K; energy dissipation rate — 0.1 E.

In the course of numerical simulation, the distribution field patterns of velocity vectors were obtained (Fig. 2).



Velocity Vectors Colored By Velocity Magnitude (m/s)

Figure 2. Distribution field of velocity vector

In Figure 2 it is seen that in the upper region of the furnace and on the left border of the nozzle are formed areas of high speeds. It can also be observed that when the fuel is fed through the nozzle, it is picked up by the air flow coming through the lower ducting system, and twists, as a result of which the speed increases to reach the upper boundary of the furnace.

Figure 3 shows the dependence of the particle residence time in the combustion chamber of the furnace on its diameter. It can be seen that the larger the diameter, the longer the particles will burn, also from the previous figures it can be concluded that the particles entering the combustion chamber will move along a spiral trajectory.



Figure 3. The residence time of the droplets of particles in the boiler furnace

The data of the numerical experiment are well approximated by the linear dependence: t = 0.0149d + 0.4745.

Due to the device of the vortex furnace, it helps to increase the retention time of burning particles in the furnace space, which has a beneficial effect on the reduction of ash residue and volatiles. When conducting a thorough analysis of the temperature regime of the furnace, we realized that the optimal combustion temperature of CWF is 700–1200 °C.

We observed that after prolonged fuel flow in the vortex furnace, the temperature levels off and reach 1143 °C, which provides isothermality, the stability of combustion and small under burning of fuel.

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Математикалық модельдеу негізінде сулы-көмірлі отынның жағу технологиясын есептеу

Математикалық модельдеу негізінде сулы-көмірлі отынды (СКО) жағу технологиясын есептеу ұсынылған. Сулы-көмірлі отынның жану үдерісін сандық модельдеу ANSYS Fluent бағдарламалар пакетінде жүргізілді. Ол көп компонентті ортада массаны, энергияны және импульсті сақтау заңдарына және Навье-Стокс теңдеулерін шешуге, жылудың үзілмеуіне және тасымалдануына негізделген. СКО жану сипаттамасының математикалық моделі үш фазадан тұрады. Шашыраңқы сулы-көмірлі отынның жануын модельдеу үшін құйынның ыдырау моделі (Eddy-Dissipation Model) пайдаланылды, ал оттыққа тамшы инжекциясының параметрлері «Discrete Phase Model» функциясын пайдалану арқылы қойылды. ANSYS Fluent-те есептің үш өлшемді тұжырымын анықтайды және Навье-Стокс теңдеулері және Рейнольдс бойынша орташаланған энергия шешіледі. Турбуленттілікті есепке алу үшін екі параметрлік «k-є» үлгісі таңдалды. Сандық модельдеу барысында жылдамдық векторларын бөлу өрісінің суреттері алынды. Оттықтың температуралық режиміне мұқият талдау жүргізу кезінде СКО жануының оңтайлы температурасы 700–1200 °С екенін дәлелденді. Сонымен қатар оттықты жағу камерасындағы бөлшектердің болу уақытының оның диаметріне тәуелділігі алынды.

Кілт сөздер: сулы-көмірлі отын, сандық модельдеу, ANSYS Fluent бағдарламасы, Навье-Стокс теңдеулері, жану процесі.

Н.К. Танашева, Л.Л. Миньков, А.Ж. Тлеубергенова, К.К. Саденова

Расчет технологии сжигания водоугольного топлива на основе математического моделирования

Представлен расчет технологии сжигания водоугольного топлива (ВУТ) на основе математического моделирования. Численное моделирование процесса сжигания водоугольного топлива проводилось в пакете программ ANSYS Fluent. Оно основано на законах сохранения массы, энергии и импульса в многокомпонентной среде и решения уравнений Навье-Стокса, неразрывности и переноса тепла. Математическая модель описания горения ВУТ состоит из трех фаз. Для моделирования горения распыленного водоугольного топлива использовалась модель распада вихрей (Eddy-DissipationModel), а па-

раметры инжекции капель в топку задавались с использованием функции «DiscretePhaseModel». В ANSYS Fluent задается трехмерная постановка задачи и решаются уравнения Навье-Стокса и энергии, осредненные по Рейнольдсу. Для учета турбулентности выбирается двухпараметрическая модель «k-ɛ». В ходе численного моделирования были получены картины поля распределения векторов скорости. При проведении тщательного анализа температурного режима топки доказано, что оптимальная температура сжигания ВУТ составляет 700–1200 °С. Кроме того, получена зависимость времени пребывания частицы в камере сжигания топки от ее диаметра.

Ключевые слова: водоугольное топливо, численное моделирование, программа ANSYS Fluent, уравнения Навье-Стокса, процесс горения.

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