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NUMERICAL MODELING OF THE COMBUSTION PROCESS IN A FIXED BED OF COAL BASED ON EXPERIMENTAL STUDIES

Abstract. This study developed a mathematical model of solid coal combustion in long-burning boilers and analyzed the influence of chemical reactions and heat transfer processes. The model is based on Reynolds-averaged Navier-Stokes equations (RANS), closed using a k-ε realizable turbulence model. The dynamics of coal particles are described using a discrete phase model (DPM). A numerical simulation of the combustion process was performed, followed by a comparison of the calculated data with experimental results. The study shows a good agreement between temperature fields and the main flow parameters obtained numerically and experimentally. The conducted validation confirms the reliability and accuracy of the developed mathematical model.

Keywords: coal combustion, numerical simulation, Computational Fluid Dynamics (CFD), Discrete Phase Model (DPM), long-burning boiler.

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Introduction. Today, coal is one of the main sources of fuel and energy on earth. It is widely used in the production of electricity and heating, as well as a raw material in the metallurgical and chemical industries. Its low cost is a key factor in its availability and frequent use [1].

However, the intensive use of solid fuels is associated with significant environmental consequences. During coal combustion, carbon (C), sulfur (S) and nitrogen (N) react with oxygen (O), leading to the formation of gaseous products, including carbon dioxide and carbon monoxide (CO_2 and CO), sulfur dioxide and sulfur trioxide (SO_2 and SO_3), as well as nitrogen oxides (NO_2 and NO) [1]. In addition to gaseous emissions, considerable amounts of solid waste containing heavy metals, such as mercury, are generated. Burning coal produces a large mass of solid waste containing heavy metals like mercury, and the formation of gaseous

substances causes acid rain and a greenhouse effect that negatively affects human health [2].

Increasing efficiency and reducing environmental damage will make it possible to use coal in further industry as the main type of source. Both experimental and numerical studies are used to develop the solution. Experimental studies require substantial material resources and complex technical implementation, whereas numerical modeling enables detailed analysis of combustion processes, prediction of flow parameters, and evaluation of the influence of various factors without additional environmental risks. Therefore, the development and application of numerical models capable of describing complex physicochemical processes of coal particle combustion and optimizing operating parameters are of particular importance [3].

Mathematical modeling based on computational fluid dynamics (CFD) is an effective tool for the detailed investigation of combustion processes and flow structures. Within this framework, several models have been developed to describe gas-solid flows:

– Two-Fluid Model (TFM)- an Euler-Euler approach in which the gas and solid phases are treated as interpenetrating continua, with closure provided by the kinetic theory of granular flow (KTGF). This method ensures high computational efficiency for large-scale systems; however, it limits the discrete representation of individual particles [4].

– CFD-DEM hybrid method- a coupled computational fluid dynamics and discrete element method that enables simulation of individual particle motion while accounting for interparticle collisions, providing high physical fidelity at the expense of significant computational costs [4].

– Dense Discrete Phase Model (DDPM)- a modified Lagrangian approach in which particle collisions are represented through model interaction forces, providing a compromise between accuracy and computational efficiency, although additional validation of this method is required [4].

– Discrete Phase Model (DPM)- the Euler-Lagrange approach used in this study [5].

In this work, coal particles were modeled as a discrete phase using the discrete phase method(DPM), which describes the movement of particles along the trajectories of individual “packages.” This approach can significantly reduce computational costs by grouping particles [5]. Despite the advantages associated with particle trajectory tracking, the DPM method remains computationally demanding when applied to large-scale systems with high dispersed-phase concentrations [6].

Materials and methods. *Mathematical model.* The developed numerical model is based on the following governing equations.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \quad (1)$$

Equation (1) represents the conservation of mass for the gas phase. Here, ρ- is the gas density, v- is the velocity vector, and S_m denotes a volumetric mass source term associated with phase transformations and thermochemical processes such as devolatilization and char burnout of solid fuel particles [7,8]. In the present study, S_m accounts for interphase mass transfer. During coal combustion, gaseous products are generated from the solid phase, resulting in a positive contribution to

the gas-phase mass (S_m>0). The left-hand side of Equation (1) describes the transient variation of density and the convective transport of mass.

$$\frac{\partial}{\partial t}(\rho\vec{v}) + \nabla \cdot (\rho\vec{v}\vec{v}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho\vec{g} + \vec{F} \quad (2)$$

Equation (2) represents the two-dimensional Navier-Stokes equations for a viscous compressible fluid, derived from Newton's second law applied to an infinitesimal control volume. The left-hand side includes the transient and convective transport of momentum. The right-hand side accounts for pressure forces, viscous stresses, gravitational body forces, and additional external forces acting on the flow [7-9].

$$\frac{\partial}{\partial T}(\rho E) + \nabla \cdot \left(\vec{v}(\rho E + p)\right) = \nabla \cdot \left(k_{eff}\nabla T - \sum_j h_j \vec{J}_j + \left(\bar{\bar{\tau}}_{eff} \cdot \vec{v}\right)\right) + S_h \quad (3)$$

Equation (3) governs energy transport in the gas phase. It accounts for convective energy transfer, thermal conduction, species diffusion, and viscous dissipation effects. The effective thermal conductivity k_{eff} includes both molecular and turbulent contributions. The first three terms on the right-hand side represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. The source term S_h incorporates the heat released by chemical reactions as well as other volumetric heat sources [7,8].

The total specific energy is defined as:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2}$$

here: $h = \sum_j Y_j h_j$, Y_j is the mass fraction of species j, $h_j = \int_{T_{ref}}^{T} c_{p,j}\, dT$, where $T_{ref} = 298.15K$.

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho\vec{u}Y_i) = -\nabla \cdot \vec{J}_i + R_i + S_i \quad (4)$$

Equation (4) describes the conservation of species mass fractions in the gas phase. It accounts for molecular and turbulent diffusion, chemical reaction rates, and additional source terms associated with mass transfer from the dispersed phase. For a system consisting of N chemical species, only N−1 transport equations are solved, since the sum of mass fractions must equal unity [8,9].

For turbulent flows, the diffusive flux is expressed as:

$$\vec{J}_i = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc_t}\right)\nabla Y_i$$

where: $Sc_t = \frac{\mu_t}{\rho D_t} -$ turbulent Schmidt number ($\mu_t -$ the turbulent viscosity and $D_t -$ the turbulent diffusivity). The default Sc_t is 0.7 [8].

The motion of dispersed-phase particles is described in a Lagrangian framework by integrating the force balance acting on an individual particle. The governing equation accounts for aerodynamic drag, gravitational force, and additional acceleration terms resulting from particle-fluid interaction [9].

In Cartesian coordinates (x-direction), the particle force balance can be written as:

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad (5)$$

where F_x is an additional acceleration term, $F_D(u - u_p)$ is the drag force per unit particle mass, u is the fluid phase velocity, u_p is the particle velocity, ρ is the density of the continuous (gas) phase, ρ_p is the density of the particle, d_p is the particle diameter and Re is the relative Reynolds number.

Turbulent model $k - \varepsilon$ realizable. Turbulence effects are modeled using the realizable $k - \varepsilon$ model within the Reynolds-Averaged Navier-Stokes (RANS) framework [10]. Transport equations for the turbulent kinetic energy k and its dissipation rate ε are solved. Unlike the standard $k - \varepsilon$ model, the realizable formulation employs a variable model coefficient and a modified dissipation equation, ensuring realizability constraints on the Reynolds stresses and improving predictions of flow separation, recirculation, and jet-dominated flows.The turbulent viscosity is computed as a function of $k - \varepsilon$ according to the realizable formulation. All model constants are set to their default values as implemented in ANSYS Fluent [11]. The choice of the realizable k–ε turbulence model is justified by its improved numerical stability and its widespread use in industrial CFD applications, including ANSYS Fluent. Unlike the standard k–ε model, the realizable formulation employs a variable turbulent viscosity coefficient and a modified transport equation for the dissipation rate ε. This ensures compliance with the realizability constraints for the Reynolds stresses and improves the prediction of complex flows with intense turbulence, which are characteristic of combustion processes and multiphase jets.

Numerical simulation. Numerical simulation was used to reproduce the combustion of solid coal in a frontal furnace chamber whose design corresponds to the laboratory setup. Coal particles were treated as reacting (burning) particles within a Lagrangian framework. Two inlet channels are located on the side walls of the chamber: the upper inlet supplies air, while the lower inlet is used for coal particle injection. The incoming primary air initiates ignition and sustains the oxidation reaction in the region above the coal bed, forming a stable vertical flame. The geometric features of the side part of the chamber, including the stepped inlets, replicate the actual conditions of interaction between the air jet and coal particles and provide an adequate numerical representation of the aerodynamics and heat transfer. The main objective of the problem is to track the propagation of thermal effects, which depend directly on the oxidizer, namely air.

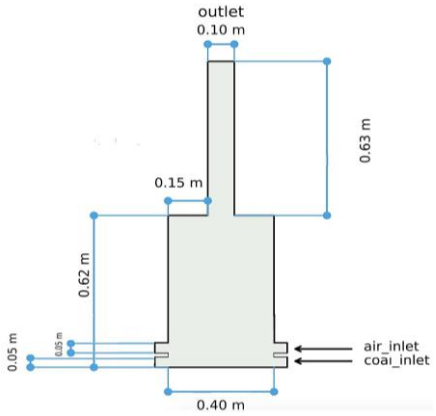

Fig. 1. Geometry of the computational domain.

Figure 1 shows the geometry of the computational setup. Coal, in the form of particles, was introduced through the lower side steps (size 0.5 m), whereas the two upper side inlets were assigned for the air flow (0.05 m each). The spatial step was 0.0035 m, resulting in a total of 25530 computational mesh elements. The coupling between the pressure and velocity fields was handled using the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm, which is widely applied for incompressible and weakly compressible flows [12].

At the air inlet (air_inlet), Dirichlet boundary conditions were specified for velocity, temperature, and species composition. The velocity vector was directed normal to the boundary with a magnitude of 0.5 m/s , and the inlet air temperature was set to 300 K . The component mass fractions were prescribed as $Y_{O_2} = 0.23$ and $Y_{N_2} = 0.77$, while the initial concentrations of all other gaseous species were taken as zero.

Coal was supplied through the coal_inlet boundary. For the gas phase, Dirichlet conditions with zero velocity and a temperature of 300 K were imposed. Coal particles were injected using the discrete phase model (DPM) with an initial temperature of $T_p = 500\,K$.

At the outlet, a pressure outlet condition was applied with a specified gauge pressure of $p = 0$. For velocity, temperature, and species mass fractions, Neumann boundary conditions with zero normal gradients were used, ensuring free outflow from the computational domain.

All remaining boundaries were treated as stationary walls. A Dirichlet condition was imposed for velocity, corresponding to the no-slip condition. Thermal interaction with the walls was described by the adiabatic Neumann boundary condition(∂T/∂n=0). No mass transfer through the walls was allowed, which was represented by zero normal gradients of the species mass fractions.

Research results and discussion. The following figure shows the temperature fields at various times showing the development and stabilization of the flame during coal combustion. At the initial stage of the combustion process, a region of elevated temperature is observed near the ignition zone. As time increases, the high temperature region expands and a stable flare structure forms. Over time, the temperature field stabilizes, which indicates that the process has reached quasi-steady state.

The table 1 presents a comparison between experimental and numerical results for concentration and temperature.

Table 1

Comparison of experimental and numerical results for concentration and temperature.

Parameter	Experiment	CFD
$C0_2$ (%)	9.08-14.15%	13.94%
CO, mg/m^3	903-1233 mg/m^3	980 mg/m^3
Temperature, K	1173,5 K	1627 K

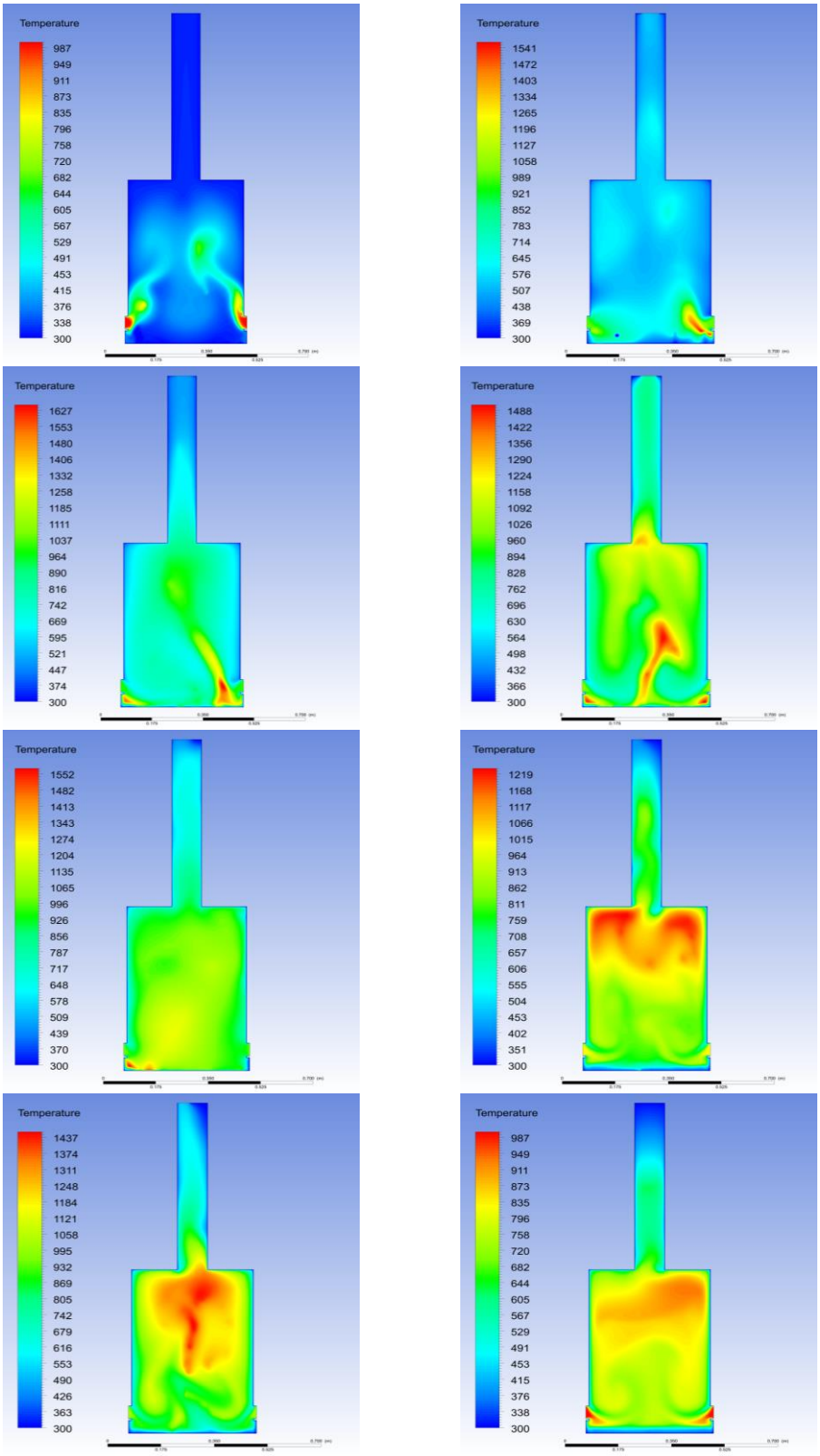

Fig. 2. Temperature contours in the computational geometry at different time points (t = 2, 3, 4, 5,6,7,8,9 and 10 seconds, respectively) for an initial coal combustion temperature T = 500K and an initial air velocity 0.25 m/s

The observed discrepancy between the experimental and numerical temperature values may be attributed to several factors. In the experiment, temperature measurements were performed at a specific location within the installation, whereas the numerical model considers a temperature value of 1627 K at computational coordinates that may not fully coincide with the position of the measurement sensor. In addition, the boundary conditions used in the model are idealized, which affects the inflated temperature values.

At the same time, the obtained values the main gaseous component concentrations are consistent with the results of experiments, without going beyond the measurement error. This confirms the accurate representation of the mathematical model and the correctness of the description of the chemical combustion process. Thus, the observed temperature discrepancy is quantitatively limited, does not contradict the overall physical trends of the process, and does not reduce the reliability of the developed model.

Conclusion. This study presents a comprehensive investigation of coal combustion in a furnace chamber through a combination of experimental measurements and numerical simulations. The primary objective was the development and validation of a mathematical model capable of accurately reproducing the physical and chemical processes occurring during solid fuel combustion.

The experimental campaign included measurements of flue gas temperature and the concentrations of major combustion products (CO_2 and CO) under different operating conditions. These data were used to verify the numerical model implemented in ANSYS Fluent. The model incorporates a Lagrangian discrete phase approach (DPM) to describe coal particle heating, devolatilization, and heterogeneous char combustion, coupled with a turbulent gas-phase flow modeled using the realizable k–ε formulation within the RANS framework.

A comparison between numerical predictions and experimental results demonstrated good agreement, particularly for CO and CO_2 concentrations. This confirms the reliability and predictive capability of the developed model. Although minor discrepancies were observed in temperature distributions, these differences can be attributed to idealized boundary conditions in the numerical setup and spatial variations between measurement and sampling locations. Overall, the model adequately captures the dominant thermo-physical and chemical phenomena governing the combustion process.

Parametric numerical analyses revealed a significant influence of inlet air velocity and initial coal temperature on temperature fields and species concentration distributions. Variations in air velocity affect mixing conditions and heat transfer intensity, while the initial fuel temperature influences devolatilization rates and heat release characteristics during the early combustion stages.

The developed numerical framework can be applied to further investigations of coal combustion processes, emission prediction, and optimization of furnace operating regimes. Future work will focus on extended parametric studies, refinement of reaction kinetics schemes, and the implementation of optimization strategies aimed at minimizing NOx and CO emissions while maintaining high thermal efficiency.

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ЭКСПЕРИМЕНТТІК ЗЕРТТЕУЛЕР НЕГІЗІНДЕ КӨМІРДІҢ ҚОЗҒАЛМАЙТЫН ҚАБАТЫНДА ЖАНУ ПРОЦЕСІН САНДЫҚ МОДЕЛЬДЕУ

Аңдатпа. Бұл зерттеуде ұзақ жанатын қазандықтарда қатты көмірдің жану математикалық моделі жасалды және химиялық реакциялар мен жылу алмасу процестерінің әсері талданды. Модель Рейнольдс-орташаланған Навье-Стокс теңдеулеріне (RANS) негізделген және k-realizable турбуленттік моделі арқылы жабылған. Көмір бөлшектерінің динамикасы дискретті фаза моделі (DPM) арқылы сипатталады. Жану процесінің сандық модельдеуі жүргізілді, одан кейін есептік деректер эксперименттік нәтижелермен салыстырылды. Зерттеу сандық және эксперименттік жолмен алынған температура өрістері мен негізгі ағын параметрлері арасындағы жақсы сәйкестікті көрсетеді. Жүргізілген валидация жасалған математикалық модельдің сенімділігі мен дәлдігін растайды.

Тірек сөздер: көмір жағу, сандық модельдеу, есептеуіш гидродинамика(CFD), дискретті фазалық модель(DPM), ұзақ жанатын қазандық.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ПРОЦЕССА СЖИГАНИЯ В НЕПОДВИЖНОМ СЛОЕ УГЛЯ НА ОСНОВЕ ЭКСПЕРИМЕНТАЛЬНЫХ ИССЛЕДОВАНИЙ

Аннотация. В данном исследовании разработана математическая модель горения твердого угля в котлах длительного горения и проанализировано влияние химических реакций и процессов теплопередачи. Основу модели составляют осредненные по Рейнольдсу уравнения Навье-Стокса (RANS), замкнутые с использованием k-ε realizable модели турбулентности. Динамика угольных частиц описывается с применением дискретной фазовой модели (DPM). В работе выполнено численное моделирование процесса горения с последующим сопоставлением полученных расчетных данных с экспериментальными результатами. В рамках исследования показано хорошее совпадение температурных полей и основных параметров течения, полученных численным и экспериментальным путем. Проведенная валидация подтверждает надежность и точность разработанной математической модели.

Ключевые слова: сжигание угля, численное моделирование, вычислительная гидродинамика (CFD), дискретная фазовая модель (DPM), котел длительного горения.