Modelling of porous biomass pyrolysis in screw reactor

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Abstract. This paper is concerned with the development of a model of wood pyrolysis in a screw reactor as the first stage of the multistage gasification process. To prevent clinkering of particles and thermal inhomogeneities, screw-type transportation is used to transport fuel. In order to describe kinetics of pyrolysis and transport of volatiles within the wood particles and their transition to the gas phase we carried out the studies using a complex of synchronous thermal analysis. A detailed numerical modeling of pyrolyzer was performed with the Comsol Multiphysics software which makes it possible to optimize the design and operating parameters of the pyrolysis process in a screw reactor.

1. Introduction
One-stage processes of fuel gasification have been developed and thoroughly studied in Russia and other countries throughout the 20th century. They remain the basis for the creation and design of modern gasification equipment. Numerous studies showed that the one-stage gasification processes had already achieved the limit of perfection beyond which a considerable improvement in their operating characteristics turned out to be impossible or unprofitable.

The gasification technology meeting the contemporary level of technology development should correspond to the following criteria:
1) the gasifier should operate in automatic, mainly unmanned mode;
2) the gasifier operation should be stable and provide insignificant variations in gas composition and flow rate that randomly occur over time;
3) it should produce the minimum amount of liquid and solid waste;
4) the conversion process should be, if possible, little sensitive to changes in the properties of fuel biomass, i.e. moisture content and size of particles;
5) the efficiency of converting fuel chemical energy into gas chemical energy should reach 80-85%.

The staged gasification technology meets the current technical requirements most completely. In the first stage of the process the allothermal pyrolysis of biomass is organized using producer gas heat and exhaust gases of an engine unit. In this stage the volatiles (gas and tar) are produced from the fuel. In the second stage tar is decomposed under the action of heated air and steam outside the fuel bed. Further, the formed steam-gas mixture reacts with the charcoal in the third stage of the process.

In the last years there has been continuous evolution of the calculation models of pyrolysis plants. The research presented in [1] shows a mathematical description of the pyrolysis process. The authors devised a calculation model for the plant designed by them. The model consists of a set of stages of drying, thermal decomposition, interphase transitions and cooling. Thus, the total duration of the wood feedstock decomposition \( \tau_{m} \) process was represented by a set of stages: heating \( \tau_{h} \), drying \( \tau_{d} \), thermal decomposition \( \tau_{td} \), and cooling of char coal \( \tau_{c} \). This method allowed the common model to be
decomposed into sub models suitable for practical implementation that have different degrees of detail and respective form of equations (ordinary differential or in partial differential). A distinctive feature of this problem statement is the use of a one-dimension representation of distribution of parameters in the space of pyrolyzer chamber.

In the same way the authors of [1] describe all the above enumerated stages. The only assumption in their model was the absence of non-uniform distribution of parameters in the cross section. To verify their model the authors of [1] made an experimental bench since in their case, as in many other studies, verification of the constructed mathematical models is based on the unique experimental data. This complicates a comparative analysis of the proposed approaches to the selection of the best description of the processes that occur in similar plants.

A more thorough study on partial gasification, on the basis of a numerical modeling and application of thermogravimetical analysis is presented in the recent publications [2, 3]. For example in the research [4] the authors applied a 3-D representation of the calculated region, which made it possible to more accurately determine variation in temperature profiles and gas motion velocities along the modeled furnace. Thus, a good correspondence was achieved between the calculated data and the experimentally measured process of fuel conversion. The analysis of the numerical modeling results that was carried out by the authors allowed them to make a conclusion on the effect of heat generated in the gasification process on 3d temperature fields and gas velocities inside the furnace. Thus, the detailed three-dimensional representation of an object in the numerical models is a necessary condition for the successful description of complex adjoining processes that occur in the course of gasification.

![Figure 1.](image.png)

A diagram of the screw reactor for multistage gasification.

Thus, the analysis of the existing studies shows the necessity to consider the detailed modeling of spatially distributed processes of heat-mass exchange, including the equations of kinetics of chemical reactions, considering natural constraints that follow from the laws of conservation. The most promising seems to be representation of heat-mass exchange equations in a 3d form. In this case the problem of a correct consideration of closing relationships in such a statement is not an exceptional characteristic of such detailed descriptions due to insufficient information on multi-parameter models that describe pyrolysis process. Thus, each new mathematical model requires verification involving results of multi-factor experimental studies.

2. Mathematical model

The geometry used for modeling a screw pyrolyzer is presented in Fig.1. The interior space is filled with a solid mass by 40%, which should provide easy circulation of the produced gases around screw. The screw represents a spiral with a wall, 3 mm thick, which is wound on a hollow shaft. The interior space of the pyrolyzer with solid fuel and formed products is separated from heating gases by a wall, 5 mm thick. The screw represents a geometrically complex structure. There are 11 complete spiral turns with a pitch of 139 mm on the hollow steel shaft. An external diameter of the spiral made up 139 mm, the shaft diameter was 38.6 mm. In the calculation we took into account the body of the screw, shaft and external coating. All the objects are constructed from cylinders. The construction of all these objects caused the emergence of surfaces and regions of small size at the point of their intersection. The total number of components in the calculation mesh equals N. Optimal distribution and sizes of mesh cells were calculated with the Comsol Multiphysics Software on the basis of corresponding
algorithms that ensure good convergence for the differential equations applied. The calculation mesh includes different number of cells:

For gas part it includes hot gas from internal combustion engine and gas inside the screw above the porous medium.

For a surface of solid elements it includes all solid surfaces.

For the others it includes solid volumetric parts such as screw, spiral, coating, etc.

The Comsol Multiphysics Software is used as a simulation environment. Heat exchange in the process of pyrolysis is simulated considering physical properties (porosity, permeability, etc.) of the medium [5]. The equation of a diffusion barrier for the plane separating the porous solid body from the gas space in the pyrolyzer is set as follows:

$$-nD_{ij} \nabla c_{li,u} = \frac{D_{si}}{d_s} (c_{li,u} - c_{li,d})$$

$$-nD_{ij} \nabla c_{li,d} = \frac{D_{si}}{d_s} (c_{li,u} - c_{li,d})$$

(1)

where $d_s$ – barrier thickness, mm; $D_{si}$ – diffusion coefficient, m$^2$/s. In the calculations we assumed a bed thickness of 5 mm and a diffusion coefficient of $10^{-6}$ m$^2$/s.

The boundary conditions chosen to solve the problem are:

An inlet temperature of fuel is 20°C;

An inlet temperature of heating gases is 600÷800°C;

A velocity of fuel flow in pyrolyzer is 0.001 m/s;

An inlet velocity of heating gases is 0.1÷1 m/s.

3. Results and discussion

The calculated fields of the gas phase velocity $u$ in the longitudinal cross section of the screw reactor are presented in Fig. 2. The highest values of $u$ are observed over the surface of filled low-grade solid fuel.

Markedly distinct velocity fields and as a consequence the diffusion coefficients characterizing transfer of the gas phase from the porous mass to the free space can be formed for different operating conditions. Figure 3 presents instantaneous values of gas flow velocities through the surface of the filled solid fuel mass. The effect of heating gas temperature on the diffusion processes of formed gas yield was analyzed. The calculations show a negligible effect of the boundary conditions on motion of the media in the region modeled by the diffusion thin bed. This fact suggests feasibility of using the constant coefficients to describe gas transition from the porous medium to the space free for gas flow in the screw reactor. The maximum change in the velocity was equal to ~1% at the change of the heating gas temperature by 140 K at the pyrolyzer inlet. Thereby, the general distribution type of values in the velocity field did not change.

The applied approach to determination of the fields of concentrations of substances formed in the course of substance reaction demonstrated satisfactory results of the calculation example. The highest
concentration of steams formed during drying is observed in the zone of intensive heating – in the initial part of the screw reactor, and as they flow along the reactor the concentrations level off in the sections. As was mentioned in the work [21], the direct application of the Arrhenius modified models leads to the similar effects. The correct analysis of physical constraints requires more strict descriptions of the laws of concentration distribution which are based not only on the values of gas temperatures and velocities. One of the methods to solve this problem is to specify the initial concentration of associated water.

4. Conclusions
The model of heat transfer and aerodynamics of the pyrolyzer was developed for express optimization calculations. The temperature distribution in the pyrolyzer reactor was obtained in a wide range of operating conditions. Moreover, it is confirmed that in the considered thermal conditions the process of fuel conversion proceeds to completion. Inclusion of the kinetic block in the model of heat transfer made it possible to determine the concentration fields of the formed substances (steam, etc.).

Acknowledgments
The research was performed at Melentiev Energy Systems Institute SB RAS under the support of Russian Science Foundation (Grant № 16-19-10227) on the equipment of the multi-access scientific center “High temperature circuit”.

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Figure 3. The fields of gas flow velocity on the surface.