Numerical modelling of agglomeration process in a granular bed containing melting particles

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Abstract. The paper considers a numerical model of a flow in a porous medium containing particles of a melting component (polymer). For this, an implicit numerical method of splitting in directions is used. Calculations are carried out for two heating methods (through the side wall, or by the input gas). The simulation results qualitatively reproduce some of the experimentally observed features of the thermal decomposition of polymer-containing mixtures. The results obtained are of interest in the study of low-grade fuels processing, often accompanied by agglomeration, as well as in the development of methods by which agglomeration can be prevented.

1. Introduction
Porous media can change their structure due to phase transitions and chemical reactions. These changes influence the coefficients of heat and mass transfer, and in some cases can lead to formation of clinkers or burnouts. These phenomena can be observed in incineration or gasification of polymer-containing fuel mixtures (such as municipal solid waste) or fuels with low-melting ash [1]. Other examples include clogging of filters or catalyst bed during hydrocarbon processing and formation of hydrate plugs during natural gas production in cold regions [2, 3]. Phase changing granular beds are used in material engineering and heat storage systems [4, 5].

Despite a large number of experimental works, the formation of agglomerates (clinkers) in packings was poorly studied theoretically. Some works [6-8] proposed CFD models of the burnout formation, taking into account the solid mechanics (spillage and compaction of particles), including using the DEM approach [9, 10]. When modeling combustion processes in porous media, as a rule, an increase in porosity is considered [11]. This phenomenon can lead to hydrodynamic instabilities at the combustion front [12]. In [13, 14], the influence of changes in porosity on free-convective flows in smoldering porous medium was studied. In [15], a stochastic approach was applied to simulate the heterogeneity of the filtration flow in a reacting porous medium, and a simple method was proposed for the relationship between the phase state of particles and the local permeability coefficient.

In this paper, a two-dimensional flow in a porous medium with variable local porosity is considered. Changes in porosity are associated with the state and content of the reactive material (polymer). To this end, a numerical model is used. Calculations are carried out for different heating conditions.

2. Mathematical model
Let us consider a section of a porous medium (granular layer) with cylindrical symmetry, through the lower boundary of which an inert gas is supplied. At the initial moment of time, the section begins to
heat up through the side wall, or by the input gas. The particles of the melting component (polymer) contained in the packing undergo a phase transition at a fixed temperature, and decompose upon further heating. The melted polymer fills the space between the solid particles, so local permeability decreases. Viscosity of the polymer is high enough to prevent its significant leakage [16]. When the polymer is thermally decomposed, the permeability is restored. The heat and mass transfer equations are written as follows:

\[
\frac{c_s \rho_s}{\partial t} \frac{\partial T_s}{\partial z} = \frac{\partial}{\partial y} \left( \lambda_s \frac{\partial T_s}{\partial y} \right) + \frac{1}{\partial t} \frac{\partial}{\partial y} \left( y \lambda_s \frac{\partial T_s}{\partial y} \right) + Q_m r_m + Q_r r_R + \alpha S \left( T^g - T^s \right),
\]

(1)

\[
\frac{c_g \rho_g}{\partial t} \frac{\partial T^g}{\partial z} + U \frac{\partial T^g}{\partial y} + V \frac{\partial T^g}{\partial y} = \frac{\partial}{\partial z} \left( \lambda_g \frac{\partial T^g}{\partial z} \right) + \frac{1}{\partial t} \frac{\partial}{\partial y} \left( y \lambda_g \frac{\partial T^g}{\partial y} \right) - \alpha S \left( T^g - T^s \right).
\]

(2)

Here \( T^s \) is the particles temperature, \( T^g \) is the gas temperature, \( c_s \) is the particles specific heat capacity, \( \rho_s \) is the density of packing material, \( t \) is the time, \( \lambda_s \) is the thermal conductivity of packing, \( z \) is the longitudinal spatial coordinate, \( y \) is the radial spatial coordinate, \( Q_m \) is the melting heat, \( r_m \) is the melting rate, \( r_R \) is the polymer decomposition rate, \( Q_R \) is the polymer decomposition heat, \( \alpha \) is the interphase heat transfer coefficient, \( S \) is the specific interphase surface, \( c_g \) is the gas specific heat capacity, \( \rho_g \) is the gas density, \( U \) is the longitudinal gas velocity, \( V \) is the radial gas velocity, and \( \lambda_g \) is the gas thermal conductivity.

Rate of melting is determined by heat transfer and melting temperature [17], and decomposition rate depends on temperature according to Arrhenius law [18]:

\[
r_m \left( T^s \right) = \begin{cases} 0, & T^s < T_m \\ \frac{c_s \rho_s}{Q_m} \frac{\partial T^s}{\partial t}, & T^s \geq T_m, \rho_p > 0 \\ \end{cases}
\]

(3)

\[
r_R \left( T^s \right) = k_R \rho_p \exp \left( - \frac{E_L}{R_s T^s} \right) \rho_m.
\]

(4)

Here \( T_m \) is the melting temperature, and \( \rho_m \) is the melted polymer mass fraction. Gas velocity is found using Darci approximation:

\[
U = -\frac{k_F \partial P}{\mu \partial z}, \quad V = -\frac{k_F \partial P}{\mu \partial y}.
\]

(5)

Here \( P \) is the gas pressure, \( \mu \) is the gas viscosity, and \( k_F \) is the permeability coefficient. Density and pressure are connected by ideal gas state equation. Heat and mass balance gives a relative fraction of melted polymer:

\[
X_m = \frac{\rho_m}{\rho_p}.
\]

(6)

This variable determines local porosity II, which, in its turn, determines local permeability. Simple variant of Kozeni-Karman formula is used in calculations:
\[ k_p = \frac{\Pi d_p^2}{150(1 - \Pi)}, \quad \Pi = \Pi^{\min} X_m + \Pi^{\max} (1 - X_m). \] (7)

The gas has a constant temperature at the inlet boundary, the packing material does not transfer heat through the gas-permeable boundaries, the temperature is constant on the wall, and the radial gradients on the symmetry axis are zero. The pressure drop is kept constant: the gas flow rate through the upper boundary is determined by the permeability of the packing and can change both with a change in viscosity and with a change in porosity [14, 19]. A specially developed computational code is used for the numerical solution. The solver is based on an implicit method for the linearized transfer equations on a two-dimensional uniform spatial grid. Equations (1-3) are split in the longitudinal and radial directions, after which they are reduced to a discrete form [20]. Description of the numerical method and examples of its usage may be found in [15].

In papers [13, 14, 21, 22], a monotonic increase in porosity during physic-chemical processes is considered. In contrast to previous works, in the presented calculations, the porosity changes non-monotonically, since it is proportional to the mass fraction of the intermediate product.

Fig. 1 shows the results of calculations with different sizes of the spatial grid step (the time step is chosen according to the CFL criterion). As porous medium is heated, the output gas flow decreases due to the agglomeration of particles. With a grid step size of approx. 2.5 mm or less, the dynamics of agglomeration changes only slightly; therefore, further calculations were carried out for this size.

![Figure 1](image)

**Figure 1.** Dependences of gas flow on time with different grid step sizes:
(1) – 7.5 mm; (2) – 4 mm; (3) – 2.5 mm; (4) – 2 mm.

3. **Results of calculations**

Maximum heating temperature in calculations is 900 K. Packing height is 14 cm and diameter is 7 cm, polymer fraction is 50%. As expected, agglomeration starts near the heating source. When heated through the side wall, the area occupied by the agglomerate begins to grow from the wall to the center (Fig. 2). However, when the temperature becomes high enough, the agglomerate decomposes and the wall region again becomes permeable to gas. The input gas cools the wall, and the heat flux in the radial direction decreases, so the agglomerate decomposition slows down. The agglomerate gradually decreases, but remains fairly stable.
Figure 2. Isotherms and agglomeration area when the packing is heated through the side wall (heating rate is 1 K/s).

When packing is heated with input hot gas, the agglomeration area grows from the lower boundary upwards. This process is slow because the growing agglomerate blocks the supply of the heating medium (Fig. 3). Therefore, the growth and decomposition of the agglomerate occurs in the thermal conductivity mode, and the change in the pressure drop insignificantly affects the rate of heat transfer.

The side wall cannot be heated instantly. Hence, we conducted additional calculations with the wall temperature increasing linearly to the maximum value (after which it does not change). In the course of heating, the polymer melts and decomposes; therefore, the fraction of the melted polymer passes through a maximum in all cases. The results show that the slower the heating rate of the wall, the more polymer mass in the packing has time to melt before decomposition begins (Fig. 4).

Figure 3. Isotherms and agglomeration area when the packing is heated by input gas (gas flow is about of 1 m/s).
Figure 4. Dependence of the maximum fraction of molten polymer on the wall heating rate.

The regions with a sharply inhomogeneous gas flow over the cross-packing section observed in the calculations can be considered as burnouts, which are often formed during fixed-bed combustion. The formation of burnouts during fixed-bed combustion was studied using numerical simulation in [6, 7] for initial conditions with inhomogeneous porosity. In this work, burnout develops even with a uniform initial porosity: flow inhomogeneity appears when a heating source interacts with a packing. Note that the qualitatively performed calculations are confirmed by experimental data [23, 24], where burnouts are also observed at the interface between the particle layer and the heating wall.

Conclusions
The modes of granular packing agglomeration have been studied using mathematical modeling. The state of the particles affects the local permeability, which decreases when the phase transition temperature is reached and is restored during the thermal decomposition of molten particles. The calculations show that different heating conditions lead to different scenarios for the growth and decomposition of agglomerate. When heated through the side wall, the agglomeration area fills most of the packing section (at low heating rates, almost the entire packing). When heated by hot input gas, the agglomeration area spreads from the lower boundary, and the growth of the agglomerate occurs much more slowly due to the blockage of the heating agent flow.

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