Complex modeling of installation for thermal processing of organic compounds

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Abstract. This paper presents the results of a numerical study of an installation for the thermal decomposition of organic substances by pyrolysis. Unlike with combustion, pyrolysis allows the processing of toxic and infected substances with high environmental safety. However, at the pre-project phase, difficulties often arise due to the lack of preliminary data relating to the decomposition process, the combustion of pyrolysis products, the intensity of heat exchange in the reactor and the combustion chamber. A possible solution to the problem may be pre-project computer simulation. In this paper, the ANSYS Fluent software program was used to simulate the installation of pyrolysis of moistened plastic, in which heat is supplied to the material through a heating wall. To maintain the process, the heat of combustion of its decomposition products is used. An approach of reducing the two-phase problem to a single-phase one is proposed, which allows minimizing the calculation time and increasing the convergence of the solution. Based on calculation results, the distribution of velocity fields, temperatures, heat fluxes and concentrations of substances in the installation was obtained. Calculation results allow to optimize the installation design and predict its capacity.

1. Introduction
Thermal processing of organic substances (including waste) by pyrolysis is a proven and reputable technology of their safe disposal. The most promising application of waste pyrolysis plants is their arrangement in regions of the country distant from gas pipe-lines, where they can become a source of heat and electricity for small settlements. In addition, these installations are characterized by a high environmental safety.

Pyrolysis is a thermal decomposition of organic substances at temperatures of 450°C and higher and nearly absence of oxygen with the formation of non-condensable gas, tar, pyrogenic water and semi-coke residue. Due to the lack of forced supply of oxygen, the formation of toxic compounds based on chlorine during pyrolysis is significantly less than during combustion [1]. Gaseous pyrolysis products can be efficiently combusted and the released heat can be used for maintaining the process and generating energy for the consumer.

While developing the technology, it is necessary to obtain preliminary information about the working features of the experimental test bench (hereinafter installation) under various operating conditions. For example, it is very important to get information related to heat transfer parameters, the rates of pyrolysis and combustion of their gaseous products, the velocities and temperatures of substances, etc. The most reasonable in this case is the use of computational fluid dynamics means, for
example, the widely used ANSYS software package [2]. Computer simulation using this software package can help to estimate the effectiveness and reliability of previously made design solutions, as well as predict the maximum capacity of the projected installation.

2. Description of study object
In this investigation, the stationary operating mode of an installation intended for the utilization of mixtures of organic substances of different elemental composition was studied in the ANSYS Fluent program. The basic scheme of the installation is shown in figure 1a.

![Diagram of the installation](image)

**Figure 1.** Installation for thermal processing of organic compounds.

1 — pyrolysis reactor; 2 — mixer; 3 — reactor cover cap; 4 — combustion chamber; 5 — heating wall; 6 — gaseous pyrolysis products outlet; 7 — burner.

Reactor 1 is a cylindrical vessel with a diameter of 0.25 m and a height of 0.35 m with a cover cap 3 placed in the upper part of the combustion chamber 4. The heat required for the pyrolysis process is generated in the combustion chamber and through the heating wall of the reactor 5 is transferred to the material. Volatile substances (vapor and gas products of thermal decomposition of organic substances), formed during pyrolysis, are pumped out by means of an injection burner 7 from the reactor via the outlet pipe of the gaseous products 6 to the combustion chamber. Also the air is supplied to the burner for combustion. Combustion of volatile pyrolysis products provides autothermal process in the reactor, and the excess heat of the combustion products is disposed of.

The installation is meant to work with a continuous feed of material into the reactor, which is loaded using a screw. Automatic unloading of solid residue in this design is not provided, therefore, a periodic shutdown of the installation and manual unloading of accumulated semi-coke from the reactor is necessary. The expected capacity of the installation is 5-10 kg/h, depending on the type of material being processed, the capacity of the installation can vary widely.

3. Research method
The complex operation of the pyrolysis installation on wet plastic was investigated in this work. Such a combination is typical, for example, for medical waste. Since composition of gaseous pyrolysis products is very diverse [3] it was decided to replace all of its combustible components with one equivalent substance - methane CH₄. The entire non-combustible gas residue was assumed as carbon dioxide CO₂. The amount of equivalent methane was calculated from the condition of preservation of the available heat of combustion of the gaseous pyrolysis products. Since the yield of semi-coke
during the pyrolysis of plastic amounts to 1-2%, it was neglected in the numerical model. The initial conditions for the calculation are presented in table 1

| Parameter                              | Value | Dimension |
|----------------------------------------|-------|-----------|
| Wet plastic mass-flow rate             | 5     | kg/h      |
| Heat value of dry plastic              | 44    | MJ/kg     |
| Moisture/Plastic ratio                 | 0.25/0.75 | -        |
| Heat of pyrolysis                      | 1     | MJ/kg     |
| Heat power of pyrolysis products       | 46.87 | kW        |
| Mass-flow rate of equivalent CH₄       | 3.375 | kg/h      |

Table 1. Initial conditions for calculations.

At the first stage of the study, a finite-difference mesh of the model was created in the ANSYS Iceem program. Due to the different nature of the processes occurring in the installation elements, the mesh is made composite and is connected via several interfaces (Figure 2). In the model, there were made separate estimated volumes for the pyrolysis reactor, the metal wall of the reactor, and the combustion chamber with a burner. The estimated volume of the heating wall is set as a solid material, the thermal and physical characteristics of which are assumed by the corresponding with stainless steel: density 7900 kg/m³, heat capacity 580 J/(kg K), thermal conductivity coefficient 25 W/(m K). The thickness of the reactor shell is 3 mm, the thickness of the reactor bottom is 4 mm. The finite-difference mesh is made of tetrahedrals and consists of 1.8 million cells.

In this paper, an approach is proposed, which consists of reducing a multi-phase problem with the application of the Euler model to the equivalent single-phase one. An applied single phase included a mixture of gaseous substances, moisture, and organic plastic. Species Transport model was used to describe this phase. Solid materials were modeled as parts of a total mixture with their densities ρₛ=850 kg/m³, viscosity μₛ=0.001 kg/(m∙s) and thermal conductivity coefficients (moisture λₘ= 0.6 W/(m²·K), plastic λₚ= 0.2 W/(m²·K)).

Turbulence in the numerical model was taken into account - the k-ε Standard model with the Standard Wall Function. Laminar and turbulent diffusion were also taken into account in the transport equations for the components of the gas mixture: the diffusion coefficient was assumed as D = 2.8·10⁻⁵
m²/s, and the Schmidt number Sc = 0.7. However, in the pyrolysis reactor, due to the specifics of the occurring processes, the laminar flow regime was set, and diffusion was completely turned off.

In the numerical model, four reactions were included: the reaction of CH₄ oxidation to CO, the reaction of CO oxidation to CO₂, moisture evaporation (was assumed as equivalent chemical reaction) and the reaction of pyrolysis. The first two reactions are exothermic, the last two are endothermic. The heat of evaporation reaction is set equal to Q_{ev} = 2.44 MJ/kg, the heat of plastic pyrolysis Q_{pyr} = 1 MJ/kg. The kinetic characteristics of the evaporation process were assumed to be similar for municipal solid waste [4] (k₀=14 s⁻¹, Eₐ=26 kJ/mol, n = 1.531), and for the plastic decomposition reaction a thermogravimetric studies were carried out using the synchronous thermal analysis instrument NETZSCH STA 449 F3 Jupiter at a heating rate of 10 °C/min (k₀=2.8·10¹⁸ s⁻¹, Eₐ=287 kJ/mol, n=1). For first two chemical reactions the Finite-Rate/Eddy-Dissipation model was used.

The boundary conditions at the inlet are given by mass-flow rates (Mass-flow-inlet). Air consumption is set from the condition of achieving air excess in the combustion chamber equal to \( \alpha = 1.7 \) (with full decomposition of organic matter in reactor). The gas mixture outlet is set by zero static pressure (Pressure-outlet). The boundary conditions at all walls of the model except the reactor wall are set adiabatic (zero heat flux). The calculation process was carried out sequentially in two stages:

- calculation when the Eddy-Dissipation model is working (Finite-Rate model is disabled), the mixing constants for evaporation and pyrolysis reactions are predeterminedly large to get complete processing of material regardless of the heating of the reactor;
- inclusion of the Finite-Rate model and obtaining the final solution.

4. Simulation results

Figures 3-5 show the visualization of the simulation, the main results of the calculation are summarized in table 2. Analyzing the obtained data allows to make a conclusion that operation of the installation is characterized by extremely high temperatures despite the high air excess \( \alpha = 1.7 \). Due to the higher heating the temperature of the combustible mixture at the outlet of the reactor is 883 °C, and as a result, the combustion starts in the burner channel.

![Figure 3](image_url)

**Figure 3.** Characteristics of gases in the central longitudinal cross-section of the installation.

a) temperature fields, °C; b) velocity vector field, m/s.

Another consequence of higher heating is the rapid decomposition of the material - as shown by figure 4b, plastic takes up a small volume of the reactor. The temperatures on the heating wall are on average 1050-1150°C on the outside and 1000-1050°C on the inside surfaces. At the bottom of the reactor the temperature reaches 1280 °C.
Figure 4. Mass fractions of combustible substances in the installation model
a) fraction of methane in the longitudinal cross-section of the installation; b) fraction of the original plastic in the central lateral cross section.

Figure 5. Thermal characteristics of the reactor wall
a) on the outer surface of the wall; b) on the inner surface of the wall.

The calculation showed that the installation operation is characterized by intense heat transfer (figure 5), the values of the heat transfer coefficients are on average 40-50 W/(m²-K).

| Parameter                                      | Value   | Dimension |
|------------------------------------------------|---------|-----------|
| Maximum gas temperature in combustion chamber | 1806    | ºC        |
| Average gas temperature in combustion chamber | 1206    | ºC        |
| Average gas temperature at the combustion chamber outlet | 1138 | ºC |
| Gas mixture temperature at the reactor outlet | 883     | ºC        |
| Total heat absorption on the reactor wall      | 6.7     | kW        |
| Radiation heat absorption on the reactor wall  | 5.7     | kW        |

Conclusions
An approach is proposed for solving a three-dimensional steady problem of a plastic pyrolysis by heating wall. The simulation results showed that plastic decomposition in a reactor with heating wall is
possible but completeness of decomposition is not a limiter, process is limited by high temperatures in the combustion chamber and on the wall of the reactor (maximum flame temperature is 1800 °C, average temperature of gases in reactor is 1200°C). Despite the small volume of the combustion chamber radiation heat transfer amounts significant value - about 85% of total heat absorption. Thus for high-caloric organic compounds decomposition it is necessary to arrange additional cooling of the combustion chamber or to feed only part of the pyrolysis products to the burner and to direct excess pyrolysis products to condensation or to a third-party source of heat and electricity. This approach can be used to model the pyrolysis of any organic compounds.

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