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SIMULATING THE HYDROCARBON WASTE PYROLYSIS IN REACTORS OF VARIOUS DESIGNS

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Abstract

The study presents a simulation of pyrolysis reactors of various designs performed in the COMSOL Multiphysics software package. The non-isothermal flow (k–ε turbulent flow) module is used. The advantages this technique has over other commonly used ones are shown. The results indicate that under the same conditions, heating in sectional reactors is more intense. To achieve optimal results, the coolant flow rate in new reactors maybe by an order of magnitude less compared to the conventional design. The use of sectional reactors for multi-flow processing of hydrocarbon waste is advisable.

Keywords:

Sectional reactor;
Pyrolysis;
Hydrocarbon waste;
Heat transfer;
Turbulent flow.

Introduction

Designing the complex technical systems requires optimal costs for the development, manufacture, and testing of experimental and process equipment [1]. Simulation has become widespread in the practice of designing complex technical systems. This is due to several advantages. The technique allows speeding up the equipment development by reducing time to create and test expensive experimental process facilities and models. A simulation computational model allows studying the system operation features under different conditions and implementing conditions in 2D and 3D modes, thereby significantly reducing the time for full-scale engineering development. Simulation allows implementing complex systems and evaluation characteristics, which are not applicable in the laboratory or field experiments, or analytical techniques [2].

The paper describes simulation models of thermodynamic processes of the hydrocarbon waste pyrolysis. Pyrolysis is a controlled thermal decomposition of organic substances (oil sludge, plastics, waste oils, etc.) [3, 4]. This way of hydrocarbon waste disposal minimizes the harmful effects on the environment.

The paper demonstrates the results of studying the dependencies of the raw material (waste) heating intensity on the coolant flow rate in various design reactors; the heat flow patterns in the pyrolysis reactors of a new design [5, 6] developed in the laboratory of the Oil and Gas Institute at Siberian Federal University have been determined.

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Types of turbulence models

At the initial stage of simulating any heat exchanger, more accurate results shall be achieved with determining the optimal turbulence model. Today in modern physics, the turbulent flow simulation is among the issues that have not been completely solved in one way or another. However, this task remains extremely urgent, since turbulent flows of various media are observed in many natural and technological processes.

There are many approaches to the calculation of turbulent flows. Some of them are only being developed and used mainly for scientific research, while others are being widely used in engineering CFD calculations.

Turbulent flows are characterized by the velocity field fluctuations. The flow parameters can be determined using different turbulence models. The main criterion for choosing turbulence models should be the possibility to reflect the flow pattern with flow separation and the formation of a discrete flow type [7].

Currently, there are various turbulence models: DNS, LES, DES, etc. These techniques require significant computational efforts. The Reynolds-averaged Navier-Stokes equation models are the most widely used ones. The *k-ω*, SST, and *v*2-*f* models have a higher degree of convergence. However, in calculations based on these models, good convergence is difficult to achieve without a perfect initial approximation [8].

The Baldwin-Lomax model is described by a single equation and is solved directly for the eddy viscosity modified. It poorly describes the laminar-turbulent transition and intense separations [9].

The Spalart-Allmaras model does not accurately describe shear and separated flows and the turbulence decay [10].

The *k-ω* model is too sensitive to the initial conditions [11].

Among the generally recognized models, the *k-ϵ* (standard, low Reynolds, and square) models can be particularly specified as the most applicable ones [12].

The *k-ϵ* model is popular in industrial applications. This model is well suitable to simulate flows with an adverse pressure gradient and those in a zone with strongly skewed geometry [13].

To build the *k-ϵ* viscosity model, two parameters should be determined:

1. The specific turbulent kinetic energy [14]:

$$k = \frac{1}{2}\overline{\overline{v}' \cdot \overline{v}'} \tag{1}$$

where v is coefficient of eddy viscosity, m^2s^{-1}.

2. The turbulent energy viscous dissipation rate:

$$\varepsilon = 2\nu tr\overline{\left(grad\overline{v}' \cdot \left(grad\overline{v}'\right)^T\right)} \tag{2}$$

where: r is particle radius, m; T is temperature, °C; t is time, s.

Equations (1) and (2) have been built under the following assumption: turbulence is characterized by a time scale proportional to that of the averaged flow.

The *k-ϵ* model benefits are:

- relatively high accuracy in the calculation of free shear flows in the near-wall zones,
- the universality of use,
- setting any additional parameters is not required.
- the mathematical *k-ϵ* model has no peak hypervelocity concentration areas, and the flow pattern looks more correct.

Today, there are two powerful software systems for finite element analysis: Ansys Fluent and Comsol Multiphysics. Each of these systems has its benefits and drawbacks. The main difference of Comsol from Ansys is the explicit intelligibility of the process describing equations and the boundary conditions to end-users. In Ansys, on the contrary, the mathematical formulation is hidden from the user, which makes this system more suitable for engineers rather than physicists and mathematicians. In our opinion, in this research, the Comsol Multiphysics software package has the benefits such as a simpler interface, a realistic *k-ϵ* turbulence model, and the availability of materials required for the study in the library. This software package is used by researchers to solve various industrial problems [15].

Metodology for performing simulation

To achieve the goals set, SolidWorks and COMSOL Multiphysics software packages have been used. Various pyrolysis reactor modifications have been used as the study objects: single-section (conventional) (fig.1) [16], two-section (fig.2) [5], and multi-section (fig.3) [6] ones.

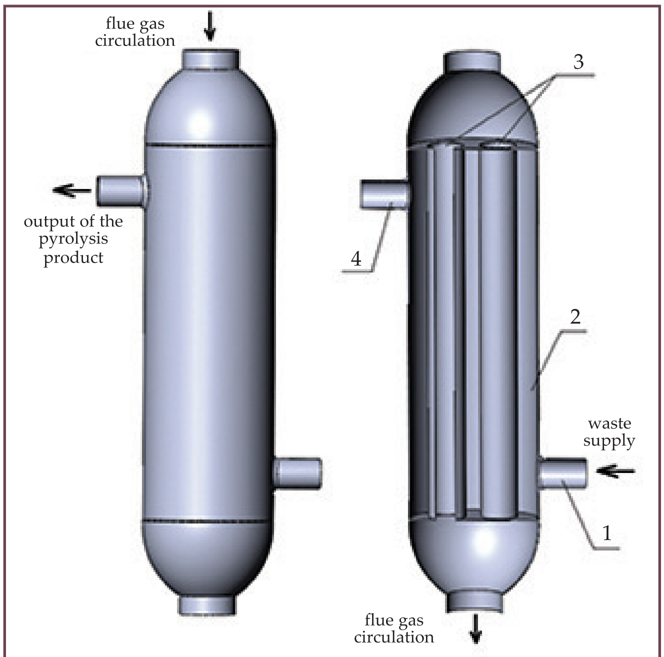

Fig.1. Schematic diagram of a single-section pyrolysis reactor: 1 – raw material supply pipe; 2 – process chamber; 3 – coolant chamber; 4 – pyrolysis product output pipe.

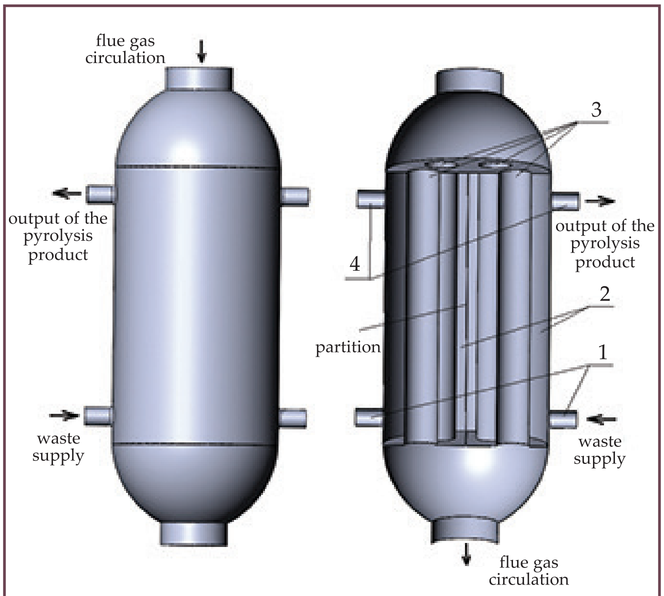

Fig.2. Schematic diagram of a two-section pyrolysis reactor: 1 – raw material supply pipe; 2 – process chamber; 3 – coolant chamber; 4 – pyrolysis product output pipe.

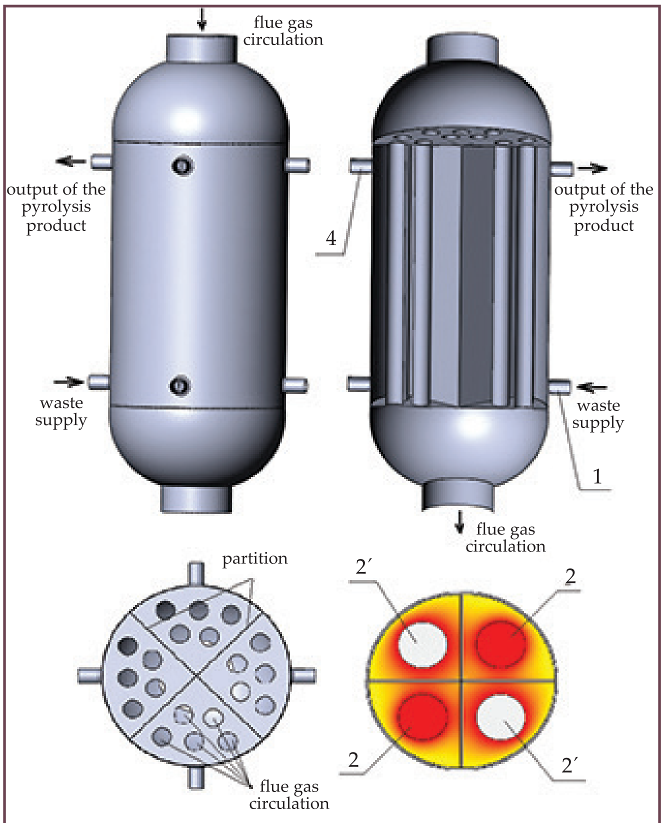

Fig.3. Schematic diagram of a multi-section pyrolysis reactor: 1 – raw material supply pipe; 2 – process chamber (active sections); 2' – process chamber (passive sections); 3 – coolant chamber; 4 – pyrolysis product output pipe.

Any of the pyrolysis reactors under research is a regular hollow cylinder (cube, rectangular parallelepiped, etc.) forming the process chamber (body) of the reactor [17]. In the case of two-section and multi-section reactors, the chamber is divided by one or more baffles (partitions). The raw material (hydrocarbon waste) supply and the pyrolysis product (gas-vapor mixture) output pipes are mounted on the cylindrical body. A cylinder of a smaller diameter through which the coolant circulates is placed inside the process chamber (the pipe-in-pipe system). The body is made of heat-resistant material, and its treated walls have heat-reflecting surfaces.

This reactor (fig.1-3) operates as follows. Liquid (or crushed) hydrocarbons, e.g., oil sludge, enter through the raw material supply pipe 1 to fill the process chamber 2. In a two-section reactor (fig.2), one section is filled, while another is heated by the neighboring section and by the moment of feeding waste, this section has already been ready for operation. In a multi-section reactor (on a four-section example, fig.3), two opposite sections 2 are filled, and after a cycle of operation, the reactor switches to 2′ sections. In two-section and multi-section reactors, the sections are separated by a baffle (partition). The flue gases are distributed between sections using a distributor (not shown in the figures). Then, the hydrocarbons are heated to the pyrolysis temperature using the coolant circulating through the coolant chamber 3. The pyrolysis products formed in the thermal reaction are passed through pipes 4 for further use.

The simulation methodology includes the below stages:

1. Building three-dimensional models based on the CAD SolidWorks software package.
2. Simulating the convective heat transfer in solids based on the COMSOL Multiphysics software package.

The hydrocarbon waste pyrolysis experimental conditions are given in Table 1.

Table 1

Simulation Conditions

Parameter	Value
Coolant	Nitrogen
The coolant flow rate	1, 3, and 5 m/s
Initial coolant temperature	750 °C
Hydrocarbons (feedstock)	Waste oil
hydrocarbons flow rate	$3 \cdot 10^{-4}$ m/s
Initial waste temperature	20 °C
Reactor material	Steel AISI 4340
Turbulence model	*k-ϵ*

Nitrogen has been chosen as a coolant since the methane combustion produces more than 70% of this gas [18], which allows using the flue methane gases as a coolant. Methane is also produced in pyrolysis in large amounts, which allows using it for the reactor autonomy [19]. A hydrocarbons flow rate of $3 \cdot 10^{-4}$ m/s allows simulating waste virtually at a standstill (without flow). Waste oil (of engines, compressors, pumps, etc.) is the most common and dangerous among liquid hydrocarbon waste.

Results and discussion

As can be seen from the data given in fig.4 for a conventional pyrolysis reactor, the feed heating intensity grows with an increase in the coolant flow rate. In the reaction zone, the average temperature is 380.2, 477.2, and 520.1 °C at a coolant flow rate of 1, 3, and 5 m/s, respectively. The highest temperature increment is observed within the range of 1 to 3 m/s.

The coolant flow pattern plays an important role in heat transfer processes. The turbulent flow ensures a more intense heat exchange between the wall and the medium than the laminar one. In industrial reactors, turbulent (and/or vortex) flow is set using specially designed appliances (fig.5-6).

The simulation results for a two-section reactor are given in fig.7. According to the research results, growth in the coolant flow rate increases the feedstock temperature. The average temperature increment is 455.6, 526.9, and 560.1 °C at a coolant flow rate of 1, 3, and 5 m/s, respectively. The highest temperature increment is observed within the range of 1 to 3 m/s.

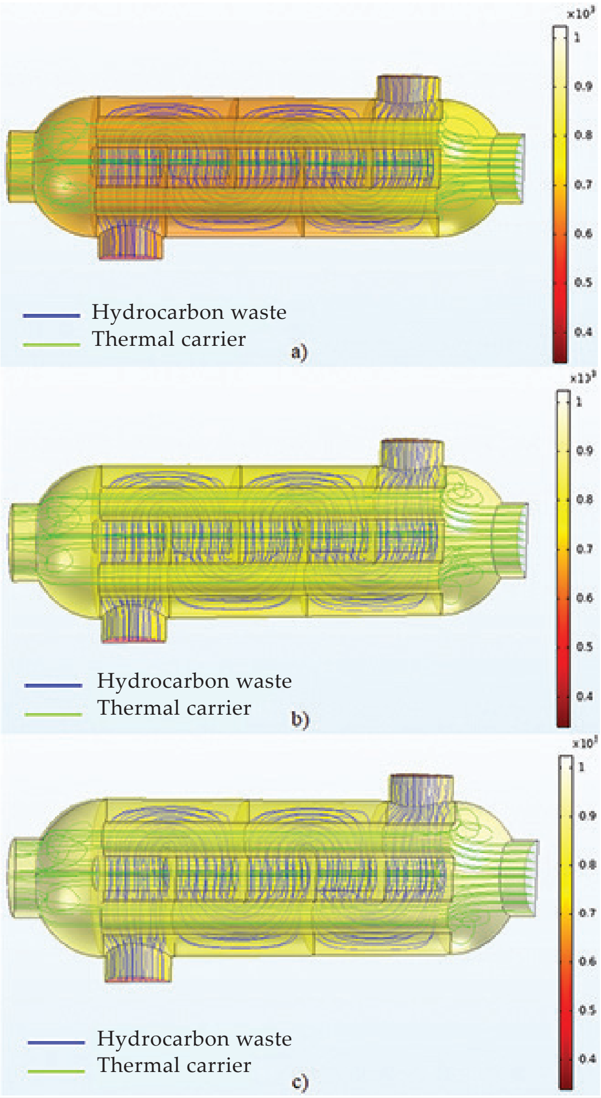

Fig.4. The single-section (conventional) pyrolysis reactor simulation results: a) the coolant flow rate is 1 m/s; b) the coolant flow rate is 3 m/s; c) the coolant flow rate is 5 m/s

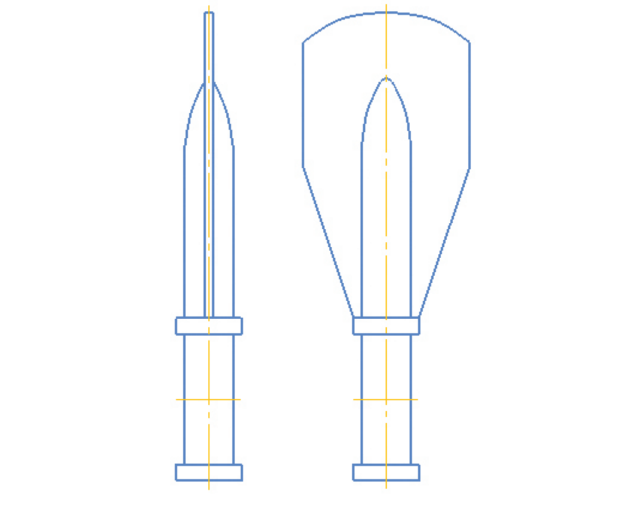

Fig.6 The Shaft Blade View

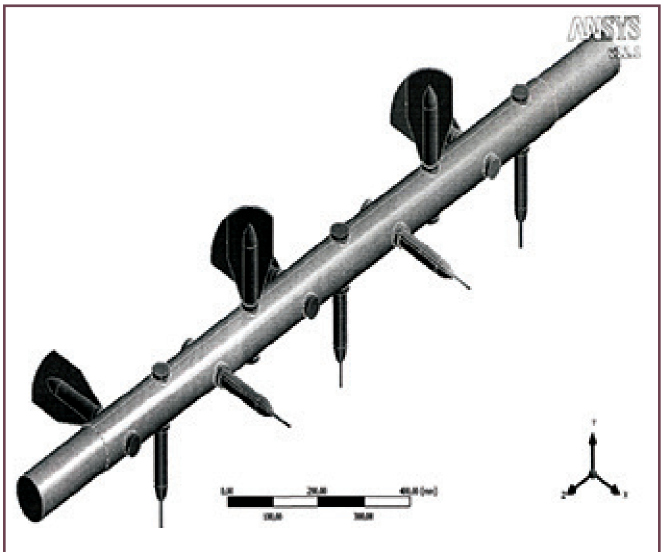

Fig.5 Geometric model of the swirler shaft

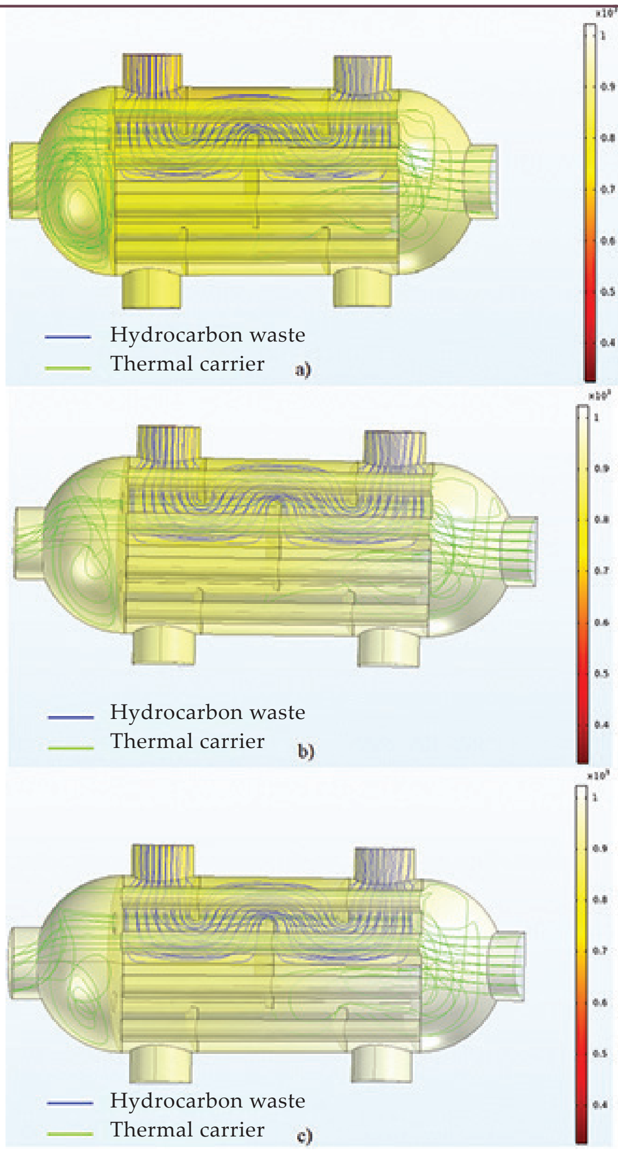

Fig.7. The two-section pyrolysis reactor simula-tion results: a) the coolant flow rate is 1 m/s; b) the coolant flow rate is 3 m/s; c) the coolant flow rate is 5 m/s

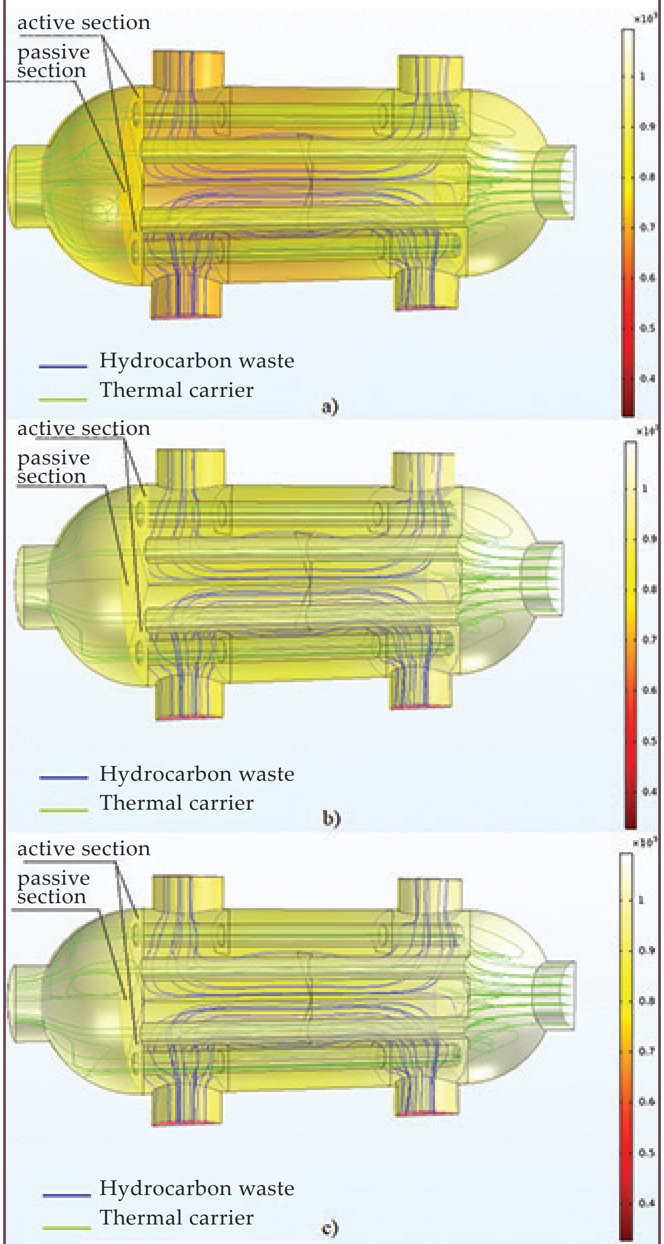

Fig.8 The multi-section pyrolysis reactor simulation results: a) the coolant flow rate is 1 m/s; b) the coolant flow rate is 3 m/s; c) the coolant flow rate is 5 m/s

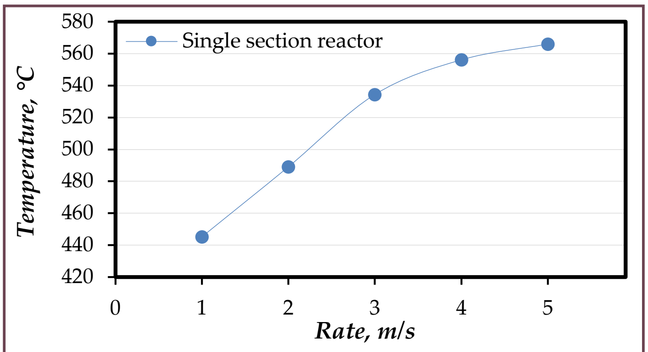

Fig.9 Dependence of the single-section (conventional) pyrolysis reactor reaction zone heating temperature on the coolant flow rate

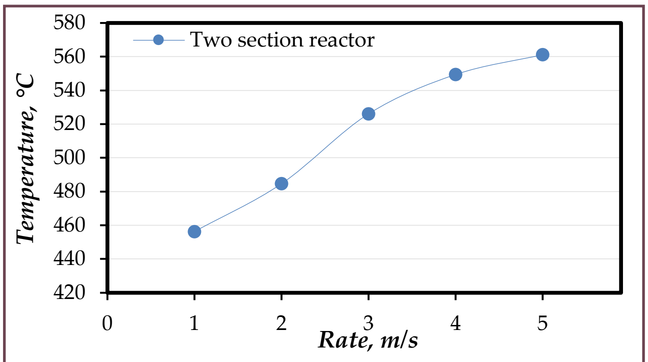

Fig.10 Dependence of the two-section (conventional) pyrolysis reactor reaction zone heating temperature on the coolant flow rate

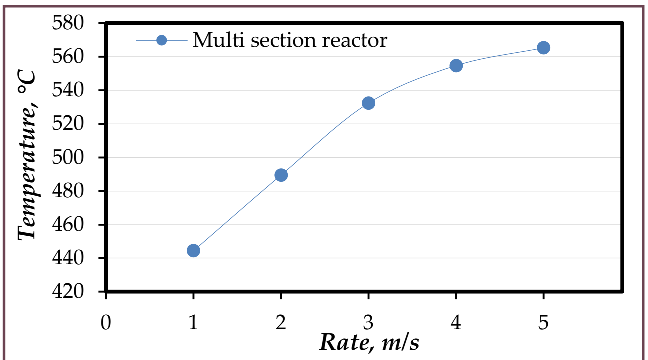

Fig.11 Dependence of the multi-section (conventional) pyrolysis reactor reaction zone heating temperature on the coolant flow rate

In all two-section reactor chambers, heating of the entire vessel is observed, regardless of whether they are active or passive (standby) ones. Thus, a passive section accumulates thermal energy, which allows performing pyrolysis with the least heat loss, thereby increasing the entire system efficiency. Upon ending one section operation, the reactor switches to the operation of another, already prepared (heated to the required temperature) one, and the entire process is repeated. Also, the significant difference in heat gain is noticeable compared to the conventional design. This phenomenon is attributable to the two-section pyrolysis reactor peculiarities.

The multi-section reactor (fig.8) simulation models have shown that at a coolant flow rate of 1, 3, and 5 m/s, the average reaction zone temperature is 446.8, 533.4, and 562.4 °C, respectively. At low coolant flow rates, in the reaction zone, a drop in temperature is observed due to the proximity of active sections (where pyrolysis runs). The passive section is in a standby mode. Within the range of 3 to 5 m/s, the passive section is also heated to 490 ... 520 °C, i.e. the temperature corresponding to low-temperature pyrolysis, which virtually indicates its readiness to operation. Like a two-section reactor, a multi-section one accumulates residual thermal energy for a passive section, due to which heat loss reduces.

For clarity, the data obtained are plotted (fig.9-11).

Conclusion

- When utilizing the hydrocarbon waste, convective heat transfer at the turbulent flow is better than at the laminar one due to the higher intensity of the molar and conduction heat transfer.
- To utilize industrial waste in large volumes, the use of multi-section reactors is advisable. This design ensures the waste processing continuity and intensive heat exchange between sections aimed at reducing energy costs and maintaining the pyrolysis process.
- The choice of convective flow rate depends on the type of products (hydrocarbon waste) utilized. When utilizing light hydrocarbons and oil sludge with mechanical impurities of 30% max., the low-temperature (450–550 °C) pyrolysis is efficient. This process temperature is ensured within a coolant flow rate range of 3 to 5 m/s (for sectional reactors), while the resulting gas has the highest calorific value. For heavy hydrocarbons and very contaminated oil sludge, it is better to use medium temperature pyrolysis (550–800 °C). Such parameters are ensured at a coolant flow rate of 5 m/s or more, or when increasing the coolant temperature.

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Имитационное моделирование пиролиза углеводородных отходов в реакторах различной конструкции

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Реферат

В этом исследовании было произведено имитационное моделирование различных конструкций реакторов пиролиза с помощью программного комплекса COMSOL Multiphysics. Был использован модуль неизотермического потока (турбулентный поток k–ε). Представлены преимущества данного метода перед остальными распространенными методами. Результаты показывают, что при одинаковых условиях нагрев в секционных реакторах осуществляется интенсивнее. Для достижения оптимальных результатов скорость течения теплоносителя в новых реакторах может быть на порядок меньшей по сравнению с классической конструкцией. Применение секционных реакторов для многопоточной переработки углеводородных отходов считается целесообразным.

Ключевые слова: секционный реактор; пиролиз; углеводородные отходы; теплообмен; турбулентный поток.

Müxtəlif konstruksiyalı reaktorlarda karbohidrogen tullantılarının pirolizinin imiyasiya modelləşdirməsi

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Xülasə

Tədqiqat işində COMSOL Multiphysics proqram kompleksinin köməyi ilə müxtəlif konstruksiyalı piroliz reaktorlarının imitasiya modelləşdirməsi yerinə yetirilmişdir. Qeyri-izotermik axın (k–ε turbulent axın) modulundan istifadə olunmuşdur. Məqalədə bu metodun digər geniş yayılmış metodlardan üstünlükləri göstərilmişdir. Nəticələr göstərmişdir ki, eyni şərtlər altında seksiyalı reaktorlarda qızdırılma daha intensiz həyata keçirilir. Optimal nəticələrə nail olmaq üçün yeni reaktorlarda istilik daşıyıcının axın sürəti klassik konstruksiyalı ilə müqayisədə daha az ola bilər. Karbohidrogen tullantılarının çoxaxınlı emalı üçün seksiyalı reaktorların istifadəsi məqsədəuyğun hesab edilir.

Açar sözlər: seksiyalı reaktor; piroliz; karbohidrogen tullantıları; istilik mübadiləsi; turbulent axın.