Mathematical simulation of the reactor for the ethylbenzene to styrene dehydrogenation reaction

S A Solovev\(^1,3\), O V Soloveva\(^1\), B Sh Gilmurahmanov\(^2\) and A A Lamberov\(^2\)

\(^1\) Kazan State Power Engineering University, Krasnoselskaja st. 51, Kazan, 420066, Russia
\(^2\) Kazan Federal University, Kremlevskaja st. 18, Kazan, 420008, Russia
\(^3\) E-mail: solovev.sa@kgeu.ru

Abstract. In this work, we carried out a numerical simulation of an industrial reactor of a radial type with a fixed catalyst bed for the process of ethylbenzene to styrene dehydrogenation. We solved the problem in the approximation of two-dimensional axial symmetry. The parameters of the chemically reacting gas mixture movement in the catalyst bed are considered. The reactor zones which have a negative impact on the reaction efficiency have been determined.

1. Introduction

Many catalytic processes are designed for radial flow reactors. The main advantage of the radial type reactor is that it has a lower pressure drop in the bed compared to the axial type reactor. There are two types of radial flow reactors, depending on whether the catalyst bed is fixed or moving within the reactor.

Simulation of chemical reactions in fixed beds has been one of the main branches of chemical reactor design in recent decades. Historically, approaches that consider gas and solid phases as a pseudo-continuum have become the most used strategy in science and industry [1]. Also, an important part of the research is the modeling of individual elements of the reactor design [2]. In [3], the change in heat is described by semi-empirical models based on effective transport parameters. There have been many studies describing the complex interactions between gas and solid in a fixed bed. The most famous model is [4, 5].

In recent years, increased computational resources have enabled CFD modeling strategies for packed beds and eliminated the simplification of the in-bed continuum for small reactors [6], where all discrete particles were performed as 3D model. In [7] compares a three-dimensional model of discrete particles with one-dimensional and two-dimensional continuous approaches for steam reforming of methane, demonstrating the similarities and divergences of these two approaches.

However, pseudo-continuum models remain in demand for modeling large reactors. The authors of [8] performed numerical calculations and experimental evaluation to determine the flow distribution in new radial reactor design. The objectives of this study were to illustrate the use of electrical tomography for flow visualization and to validate numerical simulation predictions. The velocity profiles obtained using numerical modeling and tomography showed good qualitative agreement. The authors of [9] developed a two-dimensional hydrodynamic mathematical model for the configuration of a radial reactor. Model predictions have been verified based on experimental results. In the study [10], a pseudo-homogeneous continuum model is presented that entirely takes into account the two-dimensional fluid flow.
In the present work, we performed a numerical simulation of a large-scale radial-type reactor with a fixed catalyst bed for the dehydrogenation of ethylbenzene to styrene.

2. Problem formulation and methods
Consider a variant of a radial-type reactor for the process of ethylbenzene to styrene dehydrogenation. The advantage of a radial-type reactor over an axial-type reactor is the ability to pass a gas flow through a large cross-sectional area while maintaining the total volume of the catalyst bed (figure 1).

![Reactor scheme](image)

**Figure 1.** Reactor scheme.

In technological schemes, chemical reactors with gas or liquid components, as a rule, have a vertical configuration, when the flow of reacting components and reaction products moves from top to bottom or from bottom to top. In this case, the reactor, as a rule, has the form of a column with an axis of symmetry, for example, a cylinder or a truncated cone. Such design features make it possible to uniformly distribute the reacting flows in the reactor, taking into account the gravitational separation of the components.

A feature of the radial-type reactor is that when the gas mixture moves through the catalyst bed, the flow rate decreases due to an increase in the cylindrical cross-sectional area. This effect makes it possible to obtain a higher yield of the product with decreasing temperature due to the course of the reaction in comparison with axial reactors.

When calculating the reactor for the dehydrogenation of ethylbenzene to styrene, the flow of a mixture of gases is considered. In this case, the laws of conservation of mass, momentum and energy are considered entirely for the mixture. Equations for determining the mass content and relative velocities of the mixture components are also taken into account. The course of a chemical reaction is described in terms of mass transfer and heat transfer.

The dehydrogenation reaction of ethylbenzene to styrene is basic. The reaction proceeds with the absorption of heat and an increase in volume

\[
C_8H_{10}CH_2CH_2 + H_2 \rightarrow C_8H_{10}CH=CH_2 + H_2 \quad \Delta H = 124.8 \text{ kJ/mol}
\]  

(1)
Additionally, side reactions may occur. However, the mass content of undesirable components does not exceed 5%; therefore, we will not consider these reactions to the model.

When constructing a mathematical model, differential equations for the laws of conservation of mass, momentum and energy are considered. The described mathematical problem was solved by the finite volume method in ANSYS Fluent. The entire computational area of the reactor is divided into finite volumes of quadrangular shape. In the calculations carried out in this work, the average number of finite elements was about 1,000,000 elements. When investigating the problem, the calculations of the meridional section of the reactor for the axisymmetric problem were carried out.

The numerical scheme was considered stationary. For the numerical solution of the problem of hydrodynamics and heat and mass transfer in the reactor for the dehydrogenation of ethylbenzene to styrene, we set the conditions at the boundaries of the region under consideration. The boundary conditions were set in accordance with the operating mechanisms of the calculated reactor and the selected solver used at all boundaries of the computational domain. The impermeable wall condition was established on all impermeable surfaces. At the section of the gas flow supply in the reactor model, the conditions of the gas mass flow rate were specified. For the block of the reactor: for steam - 21.7 kg / s, for ethylbenzene - 8.68 kg / s, temperature - 593°C. Properties of gases are automatically recalculated depending on temperature using polynomial relations. At the site in the reactor model for the gas outlet, the conditions of "external pressure" outside the considered area were specified. In the catalyst containment zone, a continuous porous region is considered. The resistance to gas flow is specified according to the Darcy-Brinkman model when an additional resistance force is specified in the momentum conservation equation taking into account the porosity and permeability of the bulk layer of catalyst granules. The parameters for modeling chemical reactions are taken from experimental and numerical studies [11, 12]. At the outlet of each block of the reactor, the mass content of styrene in the gas mixture is estimated.

3. Results
Figure 2 shows the fields of gas temperature and mass content of the reaction product (styrene). The reaction under consideration proceeds with heat absorption; therefore, when the gas passes through the catalyst bed, a significant drop in temperature is observed. The calculated product yield is 34%, the temperature of the gas mixture at the outlet of the reactor is 545°C. The results obtained are in good agreement with the data on the operation of industrial reactors of a similar configuration.

A change in gas temperature and mass fraction of styrene is the same almost over the entire height of the catalyst bed. The exception is the zones in the lower and upper parts of the bed, which is associated with the design features of the reactor.

Let us consider in more detail the movement of gas in the catalyst bed. Figure 3 shows the values of the mass fraction of styrene in the bed: in the radial direction from 0.6 m to 1.55 m in height from 3 m to 10 m with a step of 1 meter (respectively, from h-1 to h-8 in the figures). The mass fraction of styrene increases as the gas flow moves through the catalyst bed. Across the entire height of the catalyst bed, the accumulation of the reaction product occurs almost uniformly. The exceptions are the zones in the upper and lower parts of the bed. Thus, the gas flow moves uniformly in the radial direction through the catalyst bed, and the axial gas movement is minimal.

A similar picture is observed in figure 4 for the gas flow temperature. When moving through the catalyst bed, the temperature decreases evenly with the exception of the upper and lower parts of the bed.
Figure 2. Reactor calculation results: (a) - temperature; (b) - mass fraction of styrene.

Figure 3. Mass fraction of styrene in the radial direction of the catalyst bed.
Figure 4. Gas temperature in the radial direction of the catalyst bed.

Figure 5. Gas velocity in the radial direction of the catalyst bed.

The drop in the gas flow velocity occurs from 2.5 m/s at the inner diameter of the catalyst bed to 1 m/s at the outer catalyst bed. Catalyst performance in this velocity range is satisfactory when using 3 mm pellets. When using pellets with a length of 6 mm or 9 mm, it is preferable to withstand gas flow rates up to 1.5 m/s when moving through the catalyst bed.

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