Numerical simulation of a flow mixer for a radial type chemical reactor

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Abstract. In this work, we performed mathematical modeling of internal elements for mixing the reaction flows. The reactor of the dehydrogenation of ethylbenzene to styrene process was studied. A variant of a radial type reactor in which the gas flow is from the bottom up is considered. Ethylbenzene and steam were selected as components for mixing. Ethylbenzene is supplied to the mixer at a temperature of about 600°C, and steam at a temperature of about 700°C. Three design cases for the internal devices of the mixer are considered. The analysis of the gas mixture parameters, such as volume fraction and average temperature, at the outlet of the mixer was carried out. The cases with the best mixing of the components are determined.

1. Introduction
Flow mixers have become standard equipment in the processing industry. Nevertheless, new projects and applications are being developed [1, 2]. Static mixers are widely used in the chemical industry, not only for the processing of polymers, but also for systems in which multiphase reactions are carried out. They offer many advantages over conventional reactors (such as fixed-bed reactors [3], fluidized-bed reactors [4-8]), especially when used in gas-liquid systems. The main advantages are that they provide: control of flow behavior, improved heat and mass transfer, the formation of a very high interface surface area, while other advantages include low maintenance costs, low space requirements and ease of installation. The purpose and characteristics of the static mixer depend on the type of geometry of the internal element used for a particular system [9-12].

Compared to classical mixing or mass transfer processes, static mixers can be used at high flow rates, for liquids with high viscosity, and they do not require special maintenance. In [13], it was described that static mixers provide an increase in the reaction rate and selectivity. As a result, they are widely used in industry: the homogenization of liquids and gases, as well as the intensification of heat and mass transfer [14]. However, it was also shown that static mixers create a high pressure drop, which is highly dependent on the geometry of the mixing elements [15]. The more room is left for fluid flow, the lower the pressure drop. It was shown in [16] that static mixers can be used to eliminate gaseous pollutants by transferring them to the liquid reactive phase, as packed columns do.

We consider the problem of mixing gas flows of ethylbenzene and steam before entering the dehydrogenation reactor with a fixed catalyst bed. Reactors can have a different design, for example, axial or radial. Moreover, for the radial type of the reactor, the flow rates of the supplied components
can be of the order of 10-100 m/s. Such gas velocities impose significant restrictions on the type of mixer and its design. In particular, the use of movable structural elements is undesirable.

2. Problem formulation and methods

2.1. Mixer Construction
In technological schemes, chemical reactors with gas or liquid components usually 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 has the shape of a column with an axis of symmetry, for example, a cylinder or a truncated cone. Such design features make it possible to evenly distribute reacting flows in the reactor, taking into account gravitational separation of components.

In the present problem, ethylbenzene and steam are used as components for mixing in a ratio of about 1:2.5. Ethylbenzene is supplied to the mixer at a temperature of about 600°C, and steam at a temperature of about 700°C. So, in order to ensure the gas velocity through the catalyst bed in the range of 1-3 m/s, it is necessary to provide a flow rate of steam and ethylbenzene mixture of about 30 kg/s. In this case, the mixer itself is small relative to the reactor. With this gas flow rate, the average vertical flow rate into the mixers will be 50-60 m/s. Such gas velocities immediately impose severe restrictions on the strength and complexity of the internal elements design of the mixer.

We will construct the model of a cylindrical-shaped reaction flow mixer for a radial-type reactor for the dehydrogenation of ethylbenzene to styrene. The geometric model of the mixer is shown in figure 1. The diameter of the mixer is 1.4 m, the height of the mixer is 4.9 m.

![Figure 1. Scheme of a reaction flow mixer.](image)

Since the mass flow rate of steam is 2.5 parts greater than the mass flow rate of ethylbenzene, we place the steam inlet below the ethylbenzene inlet. We place the steam supply pipe near the bottom of the mixer. To reduce turbulent disturbances in the steam supply zone, we establish a soothing grid. Also, to smooth the flow of the mixture before entering the reactor, we install two smoothing grids and a slight narrowing.

2.2. Gas flow mathematical model
When constructing a mathematical model, the following differential equations are considered.

The mass conservation equation for gas mixture
\[ \frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m v_m) = 0, \]  
(1)

where \( \rho_m \) is the mixture density, \( v_m \) is the gas mixture velocity.

\[ v_m = \sum_{k=1}^{N} \alpha_k \rho_k \dot{v}_k / \rho_m, \]
\[ \rho_m = \sum_{k=1}^{N} \alpha_k \rho_k, \]

(2)

where \( \alpha_k \) is the volume fraction for \( k \)-th component of a mixture, \( \rho_k \) is the density for \( k \)-th component of a mixture, \( \dot{v}_k \) is the velocity for \( k \)-th component of a mixture, \( N \) is the number of mixture components.

The momentum conservation equation for gas mixture

\[ \frac{\partial \rho_m v_m}{\partial t} + \nabla \cdot (\rho_m v_m v_m) = -\nabla p + \nabla \left[ \mu_m \left( \nabla v_m + \nabla \dot{v}_m \right) \right] + \]

\[ + \rho_m \dot{g} - \nabla \left[ \sum_{k=1}^{N} \alpha_k \rho_k \dot{v}_{d,k} \dot{v}_{d,k} \right], \]  
(3)

where \( p \) is the pressure, \( \mu_m \) is the dynamic viscosity of mixture.

\[ \dot{v}_{d,k} \] is the drift velocity for the \( k \)-th component relative to the mixture velocity

\[ \dot{v}_{d,k} = \dot{v}_k - \dot{v}_m, \]  
(5)

The energy conservation equation for gas mixture

\[ \frac{\partial}{\partial t} \left( \sum_{k=1}^{N} \alpha_k \rho_k E_k \right) + \nabla \cdot \left( \sum_{k=1}^{N} \alpha_k \dot{v}_k (\rho_k E_k + p) \right) = \nabla \cdot \left( \sum_{k=1}^{N} \alpha_k (k_k + k_e) \nabla T \right), \]  
(6)

where \( k_k \) is the thermal conductivity coefficient for \( k \)-th component of the mixture, \( k_e \) is the coefficient of turbulent thermal conductivity of the mixture, \( E_k \) is the energy for \( k \)-th component of the mixture

\[ E_k = h_k - \frac{p}{\rho_k} + \frac{\dot{v}_k^2}{2}, \]  
(7)

where \( h_k \) is the enthalpy for \( k \)-th component of the mixture. For the incompressible phases \( E_k = h_k \).

Another important parameter of the model is the velocity of phase \( (p) \) relative to another phase \( (q) \)

\[ \dot{v}_{pq} = \dot{v}_p - \dot{v}_q, \]  
(8)

The phase drift velocity in the mixture is related to the relative velocity by the following relation

\[ \dot{v}_{d,p} = \dot{v}_{pq} - \sum_{k=1}^{N} c_k \dot{v}_{p,q}, \]  
(9)

where \( c_k \) is the mass fraction for \( k \)-th component of the mixture.
\[ c_k = \frac{\alpha_k \rho_k}{\rho_m}. \]  

(10)

In numerical modeling, the relative velocity \( v_{pq} \) is determined through the parameters of the mixture components [17]

\[ \frac{r}{v_{pq}} = \frac{\tau_p}{f_d} \left( \frac{\rho_p - \rho_m}{\rho_p} \right) \frac{r}{d}, \]  

(11)

\[ \tau_p = \frac{\rho_p d_p^2}{18 \mu_q}, \]  

(12)

\[ \frac{r}{d} = g - \left( \frac{r}{v_m} \nabla \right) \frac{r}{v_m} - \frac{\alpha^m}{c \partial t}, \]  

(13)

where \( d_p \) is the particle (drop or bubble) diameter \( p \)-th component of the mixture, \( f_d \) is the interphase resistance [18]

\[ f_d = \begin{cases} 1 + 0.15 \text{Re}^{0.687}, & \text{Re} \leq 1000, \\ 0.0183 \text{Re}, & \text{Re} > 1000. \end{cases} \]  

(14)

### 2.3. Numerical simulation method

The described mathematical problem is solved by the finite volume method. The entire computational domain of the reaction flow mixer is divided into finite volumes of a triangular shape. In the calculations carried out in this work, the average number of finite elements was about 3,000,000 elements. The numerical scheme was considered unsteady. The time step of the numerical calculation is selected in accordance with the Courant criterion, taking into account the grid partition of the considered region and gas flow rates.

To numerically solve the problem of hydrodynamics and heat and mass transfer in a mixer of a reactor for the dehydrogenation of ethylbenzene to styrene, we specified conditions at the boundaries of the region under consideration. Boundary conditions were established in accordance with the operating mechanisms of the calculated mixer and the selected solver used at all boundaries of the computational domain. The impermeable wall condition has been established on all impermeable surfaces. At the gas flow supply section, the conditions for the gas mass flow rate were set in the mixer model: for steam is 21.7 kg/s at 702°C, for ethylbenzene is 8.68 kg/s at 600°C. Physicochemical properties of gases are automatically recalculated depending on temperature in polynomial relationships. On the site in the reactor model for the gas outlet, the conditions of external pressure outside the considered region were set.

At the initial time, it is assumed in the calculation that the mixer is completely filled with steam. Then, an unsteady calculation starts with the arrival of new flows of steam and ethylbenzene. After reaching the quasistationary mode, the parameters of the mixture at the outlet of the mixer are estimated. At the outlet of the mixer zone, uniformity is measured for the volume fraction of ethylbenzene and the temperature of the mixture over the cross-sectional area before entering the reactor.

### 3. Results

In a gas mixing apparatus, switchgears with a multi-point gas supply system could be used. Consider the examples shown in figures 2, 3, and 4. The results of the calculated fields of ethylbenzene volume fraction and temperature are presented in figures 5, 6 and 7.

Let’s consider case 1. Let a pipe with distributed channels for supplying ethylbenzene is located across the cylindrical column of the mixer. The high ethylbenzene fraction in the outlet section of the
mixer is visible above the transverse pipe. The average temperature of the gas flow in the exit section of the mixer is 673.3°C. Thus, the considered mixer model is not effective for mixing components. The formation of large areas without ethylbenzene is observed.

Figure 2. Scheme of a gas distribution feeder, case 1.

Figure 3. Scheme of a gas distribution feeder, case 2.

Figure 4. Scheme of a gas distribution feeder, case 3.

Figure 5. Mixer outlet for case 1:
(a) – volume fraction;
(b) – temperature.

Figure 6. Mixer outlet for case 2:
(a) – volume fraction;
(b) – temperature.
Let’s consider case 2. This case shows better mixing compared to case 1. We can also see a large fraction of ethylbenzene in the outlet section of the mixer above the pipes. The average temperature of the gas flow in the exit section of the mixer is 670.0°C. Thus, the considered mixer model is more efficient for mixing the components compared to case 1.

Based on the analysis of the calculation results of cases 1 and 2, we add additional pipes with distributed channels for feeding ethylbenzene. Consider case 3 with four crossed tubes. Due to the likelihood of the formation of a complex pipe intersection system in the center of the mixer, we leave this zone free. Thus, the distribution device consists of eight separate pipes directed to the axis of symmetry of the mixer and having distributed channels for supplying ethylbenzene. This case shows better mixing compared to cases 1 and 2. There are no single spots with a high ethylbenzene fraction in the outlet section of the mixer above the pipes. The average temperature of the gas flow in the exit section of the mixer is 667.1°C. That is, in the mixture a greater amount of heat is transferred from steam to ethylbenzene compared to other cases. Thus, the considered mixer model is the most effective for mixing components from all considered cases.

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