Design and Simulation of a Reverse Flow Reactor for Catalytic Oxidation of Lean Benzene Emissions

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Abstract. This paper deals with reactor design, modeling, and simulation of a pilot-scale reverse flow operation used for catalytic oxidation of lean benzene-air mixtures. The reactor was designed for conducting lean benzene with adiabatic temperature rise less than 54°C. According to the rule of thumb, this kind of condition requires the reaction to be accomplished under reverse flow operation. In the reactor design, some criteria were calculated such as Mears, Weisz-Prater and Ergun’s criteria. The reactor model was developed for 1D, pseudo-homogeneous, involving mass and energy balances. The fixed bed consisted of the inert section, placed at the outer part of the catalyst section. The results of the simulation indicated that the switching time, inlet concentration and heat extraction imposed an important influence on the performance of the reactor. Under the suitable operating conditions, the system can achieve a favorable running status, without reactor extinction, and can be operated auto-thermal, in fact, more thermal energy from the catalyst section was feasible to extract. The temperature profile remained smooth and continuous in the case of desired energy extracting from the heat exchanger.

1. Introduction

The volatile organic compounds (VOCs) produced by the manufacturing industry cause major air pollution problems because they are involved in various unwanted processes such as producing photochemical oxidants that may be toxic to humans such as the formation of ozone in the troposphere and take part in sick building syndromes [1]. Other environmental problems from VOC such as odor, toxic emissions, and petrochemical smog associated with VOC emissions. Reducing the amount of VOC emissions is very important for human health [2].

Purified terephthalic acid (PTA) is an important chain in the petrochemical industry. PTA produces polyethylene glycol terephthalate which is the main raw material for use in the polyester and textile industries. The increasing demand for polyester drives the growth of PTA consumption (almost two-thirds of global polyester demand), which accounts for almost two-thirds of global polyester demand [3-4]. During the petrochemical production of pure terephthalic acid (PTA, 1,4-benzene dicarboxylic acid), a large amount of concentrated effluent was produced [5]. One of the wastes produced is benzene. Benzene is a dangerous volatile organic compound used in various industries such as chemistry, petrochemicals, paints and coatings, and steelmaking. Catalytic oxidation is considered to be one of the most promising routes for effectively removing benzene at lower concentrations [6].
Catalytic combustion has been intensively studied and has been applied in industry. Catalytic oxidation is the most promising method to reduce the number of VOCs because they require relatively low costs and are easily applied in various processes. However, this method requires high temperatures that consume energy at risk of explosion and require heating equipment. In addition, the catalyst is easily deactivated due to sintering [7-8].

One strategy to overcome some of the problems is to use an alternating reverse flow reactor (RFR) [9,10]. The catalytic RFR consists of a catalyst bed where the feed flow direction is periodically reversed. Therefore, if adequate switching time is ensured, the heat of combustion would be retained inside the reactor [10]. Periodic flow reversals provide a way to affect the surface coverage of catalytic sites, changes in conversion or selectivity could be substantially expected when compared to once-through operation [11-12].

2. Design & Modelling

2.1. Design Criteria and Transport Properties

To design the reactor, RFR can be assumed as a fixed bed reactor which has two aspects that can be identified: gradients regarding the catalyst bed (gradients on catalyst bed scale) and gradients related to a catalyst pellet, or gradients on catalyst pellet scale.

For a given set of operating conditions, the magnitude of these gradients is a function of the design parameters, which are: diameter and length of the catalyst bed, and also the diameter of catalyst pellets. Criteria validating the negligibility of gradients during steady-state operation have been, in part, taken from literature. These criteria relate the design parameters to the kinetic properties of the reaction considered and to the physical properties of the catalyst bed and the reaction medium. Physical properties have been taken from the literature [13, 14].

The relative pressure drop of RFR using Ergun’s equation for pressure drop in a fixed bed reactor the criterion [15, 16]:

\[
\frac{150(1 - \varepsilon_b)^2 \mu u_s L}{\rho_0 \varepsilon_b^3 d_p^2} + \frac{1.75(1 - \varepsilon_b) \rho g u_s^2 L}{\rho_0 \varepsilon_b^3 d_p^2} \leq 0.03
\]  \hspace{1cm} (1)

Plug flow is important in steady-state isotopic transient experiments and forced concentration cycling experiments. The reactor has been designed in order to obey the plug flow criteria using Mears criterion [17]:

\[
\frac{d_t}{d_t} > 10 \hspace{1cm} \text{ (2)}
\]
\[
\frac{L}{d_t} > 50 \hspace{1cm} \text{ (3)}
\]

The influence of heat transfer resistance on the net production rate may be neglected using Mears criterion [18]:

\[
\frac{r_{eff} \rho_{cat} d_{cat} |\Delta H|}{h T} \leq \frac{0.3RT}{E_A} \hspace{1cm} \text{ (4)}
\]

Mears equation and Weisz-Prater equation as a parameter to determine external diffusion and internal diffusion on reaction for this system:

\[
\frac{r_{eff} \rho_{cat} d_{cat} |\Delta H|}{h_m C_A} < 0.3 \hspace{1cm} \text{ (5)}
\]
\[
\frac{r_{eff} \rho_{cat} d_{cat} |\Delta H|}{4 C_A D_{Aeff}^2} < 1 \hspace{1cm} \text{ (6)}
\]
Table 1
Correlations used for estimating internal transfer parameters in the simulation

| Parameter               | Particle Bed |
|-------------------------|--------------|
| Dispersion coefficient  | $D_{\lambda} = D_v (20 + 0.5 \text{Sc Re}) / \varepsilon$ |
|                         | $Re = \frac{dp \text{Uo} \rho}{(\mu \varepsilon)}$, $\text{Sc} = \frac{\mu}{(\rho D_v)}$ |
| Mass transfer coefficient (KG) | $KG = Sh \frac{dp}{D_v}$ |
|                         | $Sh = 2 + 0.5 \text{Re}^{0.6} \text{Sc}^{1/3}$ |
| Effective thermal conductivity (k) | $k = 0.5 \text{Pr Re KG}$ |
|                         | $\text{Pr} = \frac{\text{Cp} \mu}{KG}$ |
| Heat transfer coefficients (h) | $h = Nu \frac{KG}{dp}$ |
|                         | $Nu = 2 + 1.1 \text{Re}^{0.6} \text{Pr}^{1/3}$ |

The transport coefficients used to simulate the particle bed reactor. The effective dispersion coefficient ($D_{\text{eff}}$), effective thermal conductivity ($k$), gas-solid mass transfer coefficient (KG), and gas-solid heat transfer coefficients (h).

It was assumed that the reaction heat was transported from the particle to the insulation layer through the reactor wall with a thickness of 1.75 mm and thermal conductivity of 16.2 W·m$^{-1}$·K$^{-1}$. The thermal conductivity of the insulation layer was much lower than the wall of the reactor, which could prevent heat diffusion from the reactor wall to the ambient environment.

According to the calculation of design criteria and transport properties, the physical dimension of the reactor was shown in Table 1. A RFR concept and distribution of axial–radial reactor bed for RFR was illustrated in Fig. 1.

![Figure 1. Frame scheme for the reverse flow reactor](image)
Table 2
Geometry and physical properties for the RFR

| Parameter                              | Value    |
|----------------------------------------|----------|
| Reactor length (L_R)                    | 0.7 m    |
| Length of catalyst section (L_C)       | 0.1 m    |
| Length of inert section (L_I)          | 0.3 m    |
| Reactor diameter (D_R)                 | 0.1 m    |
| Reactor wall thickness                 | 0.00175 mm|
| Reactor wall density (\rho)            | 7,700 kg/m^3 |
| Reactor wall heat capacity (C_p)        | 500 J/kg/K |
| Reactor wall thermal conductivity (k_w) | 16.2 W/m/K |
| Insulation layer thermal conductivity (k_i) | 0.06 W/m/K |

The reactor system has an insulation layer installed around the external wall of inert and connected by a heat exchanger in the catalyst section. The insulator using rock wool for trapping the heat around the wall for better RFR performance. Two three-way valves and associated transfer piping allow for either forward or reverse flow operating modes. Each reactor consisted of catalyst sections and inert sections in between. The inert sections were packed with blank Coral stone particles, whose physical properties were shown in Table 2. Reaction heat was extracted from the heat exchanger.

Table 3
Solid physical properties for particle beds

| Particle bed | Catalyst | Inert |
|--------------|----------|-------|
| Density, \rho/kg/m^3 | 3,975 | 2,600 |
| Particle diameter, dp/mm  | 5 | 8 |
| Heat capacity, C_p/J/kg/K | 765 | 2,000 |
| Thermal conductivity, W/m/K | 36 | 1.7 |
| Bed porosity (\epsilon_b) | 0.54 | 0.54 |

In this work, the non-steady model was established for the combustion of benzene in RFR in a pseudo-homogeneous and one-dimensional manner. The only dimension taken into account in the model is the axial one, because, for the reactor operating at the conditions of this work, temperature and velocity radial profiles are almost flat (except in the vicinity of the reactor wall), and hence the difference in the results between one-dimensional (much easier to solve) and two-dimensional models is very small.

The temperature of the wall insulation layer remained constant, in order to complement heat losses to the wall. So that the temperature radial profiles were almost flat; and the reactor was assumed to be one-dimensional. But it was necessary to take into account the influence of the wall itself in RFR. That is to say, part of heat can be transferred axially along the wall to reach the inert part of the bed.
This heat transfer has a negative effect on the stability of the reactor, which had been demonstrated by research on a reactor of 0.05 m diameter [19], the reactor stability increases as the reactor diameter increases and the wall thermal conductivity decreases. Furthermore, the behavior of pilot-plant reactors, with relatively small diameter and a high thermal conductivity wall (for example, constructed in steel), are strongly affected by this phenomenon, which must be taken into account in the simulation model.

In the case of lean benzene combustion, homogeneous reaction (combustion in the gas phase) only occurs at high temperatures (700°C). In this work, the reactor runs at a much lower temperature so that the homogeneous combustion can be neglected. Ideal gas behavior for the gas phase was also assumed.

2.2 Mathematic Modelling of RFR

The mathematical model for RFR was constituted by several partial differential and algebraic equations. The differential equations were obtained from mass and energy conservations and applied separately to the gas and solid phases. The algebraic equations were the ones used to estimate the physical and transport properties. According to the design criteria and the reaction type, the reactor has laminar flow according to the Reynold number, non-equimolar reaction, and non-isothermal.

Mass balance for the gas phase:

\[
\varepsilon_A = \frac{\sum \nu_i y_{A,0}}{-\varphi_A} \tag{7}
\]

Energy balance for the gas phase:

\[
\begin{align*}
\rho c_p & \left( 1 + \frac{\nu}{\varphi_A} \right) \frac{\partial T}{\partial t} + \frac{\partial (\rho c_p T)}{\partial z} = k \left( \frac{\partial^2 T}{\partial z^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial^2 T}{\partial r^2} \right) + \Delta H / r_A \tag{9}
\end{align*}
\]

Energy balance for solid-phase:

\[
h_f a_s (T_s - T) = \frac{k_{eff}}{r} \left( r \frac{\partial T_s}{\partial r} \right) + (1 - \varepsilon) \rho s (-\Delta H) r_A \tag{10}
\]

Heat loss to the environment:
\[ Q_L = \frac{2\pi L V_r}{U_r} \left[ T - T_{wait} \right] \ln \left( \frac{r_2}{r_1} \right) \left[ \ln \left( \frac{r_2}{r_1} \right) + \ln \left( \frac{r_2}{r_2} \right) \right] \left[ \text{m}^3 \text{s}^{-1} \right] \]  

(11)

2.3 Boundary and Initial Condition

Danckwerts boundary conditions were adopted to solve the simulation using FlexPDE V6.50. The conditions were given in Table 4.

| Table 4 | Boundary and initial condition |
|---------|-------------------------------|
| Inert  | Catalyst                      | Inert  |
| Section (A) | Eq. 11                        | Section (B) | Eq. 11 |
| Q_L   | Eq. 11                        | Eq. 11 |
| Q_L   | Eq. 11                        | Eq. 11 |
| Initial conditions | If T_R > 350°C 0                 |
| (t=0) | T = T_i                       | T = T_i |
| Boundary conditions | C_A = C_A,ini                  |
| z = 0 | dC/dz = 0                     | dC/dz = 0 |
| Eq. 12 | dT/dz = 0                     | dT/dz = 0 |
| z = 1 | dC/dz = 0                     | dC/dz = 0 |
| Eq. 13 | dT/dz = 0                     | dT/dz = 0 |
| z = 2 | dC/dz = 0                     | dC/dz = 0 |
| Eq. 14 | dT/dz = 0                     | dT/dz = 0 |
| z = 3 | dC/dz = 0                     | dC/dz = 0 |
| Eq. 15 | dT/dz = 0                     | dT/dz = 0 |

The reverse mode setting on FlexPDE using sinus function and swage feature. There are parameter for switching time setting: \( w = \sin(\pi t/ST) \) and \( v = \text{swage}(w, -1, 1, 10^{-5}) \). Parameter of \( W \) is the value of sinus from pi then times time operation and divided by switching time (ST). Parameter of \( v \) has a value 1, 0, or -1, if \( t < ST \) then the value of \( v \) is 1, if \( ST < t < 2ST \) the value of \( v \) is -1, and so on. Parameter of \( v \) is used as the boundary condition at the end of the reactor as equations below.

\[
\frac{dT}{dz} = \frac{(1 + v)}{2} \rho_g C_p g u \frac{T - T_{in}}{k_{eff}} \tag{12}
\]

\[
\frac{dC_A}{dz} = \frac{(1 + v)}{2} \frac{C_A - C_{A,ini}}{D_A} \tag{13}
\]

\[
\frac{dT}{dz} = \frac{(1 + v)}{2} \rho_g C_p g u \frac{T - T_{in}}{k_{eff}} \tag{14}
\]

\[
\frac{dC_A}{dz} = \frac{(1 + v)}{2} \frac{C_A - C_{A,ini}}{D_A} \tag{15}
\]

2.4 Kinetics Expression

Danckwerts boundary conditions were adopted to solve the simulation using FlexPDE V6.50. The conditions were given in Table 4.

In the development of the model, pseudo-homogeneous 1.54 order kinetics for the catalytic combustion of benzene was assumed [20]. This assumption had been experimentally checked on the commercial
catalyst for organic waste gas purification. Commercial catalyst is prepared by using mixed metal oxide supported on γ-Al₂O₃ and monolith.

The related properties of the catalysts were shown in Table 3. The equipment used for kinetic experiments was shown as Fig. 2. Before the experiments, the catalyst was ground to 600–1000 mesh in order to neglect internal diffusion resistance. The influence of external diffusion was investigated by means of changing the loading amount of the catalyst particles and gaseous flow while the ratio of gaseous flow to catalyst loading being maintained constant. The constancy of estimated rate constant k versus a change of GHSV indicated that the external diffusion influence could be neglected under the condition of GHSV (gas hourly space velocity) ≥ 36,000 ml·(g cat)⁻¹·h⁻¹. The required benzene concentration was around 5,000 ppm, and the temperature remained below 350°C.

The experimental data of k were correlated with a simple 1.54 order model. In this case, the intrinsic model of lean benzene catalytic combustion on the commercial catalyst was given as

\[-r_A = k \cdot C_A^{1.54}\]

The rate parameter was expressed as \(k = k_0 \cdot \exp \left(\frac{-E}{RT}\right)\), where \(k_0\) was preexponential factor and \(E\) is the activation energy.

The partial least-square (PLS) methods were employed to estimate the parameters of the kinetic model. The Arrhenius plot for experimental data of this model was shown in Fig. 2, from which the estimated values of \(k_0\) and \(E\) were obtained. The resulting apparent activation energy for this 1.54-order model was 52.454 kJ·mol⁻¹ and the pre-exponential factor was \(2.1 \times 10^6\) s⁻¹. The reaction heat for benzene combustion (\(\Delta H_r\)) was –3,165.99 kJ·mol⁻¹. Deactivation of the commercial catalyst was observed when the temperature was higher than 700°C. Therefore, the behavior of the catalyst cannot be adequately described by these parameters over 700°C.

Figure 2. Arrhenius plots of the estimated values of kinetic parameters k for the power-law model.

3. Result and Discussion

Numerical simulation was used to investigate the influence of operating parameters, as a prior step in the development of optimization and control strategies. A number of variables were found to be important to the operation, such as thermal properties of the system, insulation layer temperature, fluid velocity, switch time, and feed concentrations, which were addressed in this work. By regulating these parameters, the reactor could reach the best performance, such as no catalyst bed ‘run-away’, reactor extinction being avoided, a high conversion rate of benzene, and more heat extraction. The specific parameters are shown in Table 5.
Table 5

Operating parameters used in the simulation of the base case

| Operating Parameter                  | Value       |
|--------------------------------------|-------------|
| Feed benzene (C_{A,in})              | 1,000 ppm   |
| Feed temperature (T_{in})            | 80 °C       |
| Volume flow inlet (Q_{in})           | 1.4 L·s⁻¹   |
| Switching time (ST)                  | 600 s       |
| Feed pressure (P_o)                  | 1.1 × 10⁵ Pa|
| Insulation layer temperature (T_i)   | 50 °C       |
| Preheating temperature (T_{pre})     | 630 °C      |

3.1 Effect of Flow Rate and Residence Time

Before the simulation of RFR, the first step is to determine the residence time and flow rate to obtain the highest conversion in the shortest time operation. Fig. 3 shows axial benzene conversion profiles in various residence time with a concentration of benzene is 1000 ppm.

![Figure 3. Axial benzene conversion profiles at different residence time in Fixed Bed Reactor.](image)

Based on Fig. 3, it is seen that the residence time above 0.2 seconds already has a conversion more than 90%. From the various residence times, the best residence time is 0.3 seconds because it already has high enough conversion around 93%. The volumetric flow rate that needs to be supplied is 1.4 L·s⁻¹. This volumetric flow rate is used as a base case to simulate the effect of switching time, feed concentration, and heat extraction.

3.2 Effect of Feed Concentration of Benzene

The effect of feed concentration and heat generated as illustrated in Fig. 4. In the process, deactivation of the commercial catalyst was observed when the temperature was higher than 700°C, so the heat in the reactor is held until medium temperature to avoid deactivation of the catalyst, there is 500°C by extracting the heat generated in the center of the reactor.
At these temperatures, the conversion of benzene obtained is almost 100%. Temperature profiles with a concentration of 1000 ppm are wider than 750 ppm which indicates that the heat produced from the concentration of benzene 1000 ppm is greater than 750 ppm.

Switching time also influences the heat production in the system which is indicated by the longer switching time, the temperature profile obtained is widened. It can be concluded that the feed concentration and switching time is very influential on the heat generated in this process.

![Temperature profiles](image)

**Figure 4.** Axial benzene temperature profiles at various switching times with benzene concentration: (a) 1000 ppm, 750 ppm. Each profile was taken at the beginning of flow reversal and forward direction (right).

The downward feed concentration profile in the RFR system is also affected by switching time and feed concentration shown in Fig. 5. The longer switching time and smaller feed concentration make lowering feed concentration profile slow down. Lowering feed concentration only occurs momentarily at a concentration of benzene 750 ppm and switching time 3600 s, because the heat of reaction can not be trapped in the system, so there is no reaction within the catalyst zone.

![Feed concentration profiles](image)

**Figure 5.** Benzene concentration profiles at different switching times on reactor outlet: (a) 1000 ppm and (b) 750 ppm at the reactor outlet.

### 3.3 Stability with Heat Extraction

In our case, the approximate switching time was within the range of 600 s to 3600 s for 1000 ppm and 750 ppm benzene concentration. In this range of switching time, the reactor could run properly without catalysts ‘run-away’ and ‘reactor extinction’, while more combustion heat was able to transfer, except the benzene concentration 750 ppm at switching time 3600 s, the reactor was extinction because lower feed concentration and too long switching time. Temperature profiles at a various position with switching time 2400 s and feed concentration 1000 ppm with heat extraction is stable shown in Fig. 6.
3.4 Effect of Switching Time and Start-Up Time

Switching time was an important operating parameter, namely the time for finishing a forward flow and a reverse flow. The temperature profiles at a pseudo-steady state with different switch times with heat extraction were shown in Fig.7 and 8. In the simulation, it was observed that with longer switching time, it would make the reactor extinction.

In benzene feed 1000 ppm, the reactor in various switching times can trap the heat and get 100% conversion. The needed start-up time of 600 s, 1200 s, 1800 s, 2400 s, and 3600 s switching time are 0.6 hours, 0.9 hours, 0.95 hours, 1.2 hours, and 1.7 hours. The faster switching time can shorten the start-up time to the system get stable. The 600 s switching time has a smaller time lag than the other switching time.

In benzene feed 750 ppm, the reactor in various switching times can trap the heat and get almost 100% conversion, except switching time 3600 s. The needed start-up time of 600 s, 1200 s, 1800 s, and 2400 s, switching time are 1.2 hours, 1.8 hours, 2.7 hours, and 4.4 hours. The faster switching time and higher feed concentration can shorten the start-up time to the system get stable. The 600 s switching time in feed benzene 1000 ppm has a smaller time lag than the 600 s switching time in feed benzene 750 ppm. To minimize time lag, the start-up technique is very influential and needs to study further. One of the start-up techniques that can be used is to minimize switching time in the beginning and then restored to the original switching time. In benzene feed 750 ppm and 3600 s switching time, the reactor is extinction because the system cannot trap the heat. The slower switching time and lower feed concentration can longer the start-up time to the system to get stable.
4. Conclusion

In this work, the design reactor and the effect of operating parameters on the performance of a reverse-flow reactor had been investigated for the catalytic combustion of lean benzene/air mixtures. The lean benzene combustion using a reverse flow reactor was successfully simulated in various concentrations and various switching times to reach nearly 100% conversion. The simulated calculation results demonstrate that under the suitable operating conditions, the system can achieve a favorable running status, without catalyst bed ‘runaway’, reactor extinction, and more heat energy extraction. On the other hand, it was found that the extraction of thermal energy from the catalyst-section of the reactor was feasible. The temperature profile remained smooth and continuous in the case of desired energy extracting from heat exchanger the best method to simulate the lean benzene combustion is using 1000 ppm feed with switching time 600 s, which has the shorter start-up time around 0.6 hours or 40 minutes.

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