CFD Analysis on the Mixing Effect of Orifice Diameter in Dxygen Mixer

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Abstract. Rapid and uniform gas mixing is one of the core technologies of the chemical industry. A three-dimensional physical model of the oxygen mixer is established to investigate the influence of orifice diameter on mixing uniformity. And the standard k-ε turbulence model and species transport model are used to simulate the gas mixing process by using the computational fluid dynamics (CFD) commercial software Fluent. The oxygen distribution in the downstream of the mixer is analyzed qualitatively and quantitatively. It is found that the oversized and undersized orifice diameter are not desirable. It is concluded that the mixing performance of the case 2 is the best. In case 2, the oxygen mixing uniformity of the outlet section reaches the minimum value, which is 0.0001, which is the optimal structure.

1. Introduction
Fluid mixing technology is a method and means for mixing two or more different fluids together. With the unique fluidity of the fluid, it is mixed and diffused to form a uniformly dispersed and full contact distribution. So the unevenness of the material in the system continues to decrease, thereby improving various properties of the mixture[1]. And the gas-gas fast jet mixer can achieve fast and uniform mixing in a small space, which is also the goal pursued by chemical production[2-3].

The mixing process of oxygen and combustible gas is widely used in the chemical industry. For example, in the process of producing ethylene oxide, oxygen needs to be uniformly mixed with ethylene before it enters the reactor for reaction. Because in the process, it is easy to produce explosion danger zone, so the safety of this kind of gas mixing equipment is particularly important[4]. The oxygen mixer adopts the jet flow principle. The fluid enters a larger space from a small orifice or nozzle, and continues to diffuse and flow to form a jet fluid. If the outflow velocity is not very low, it will become completely turbulent after a short distance. Due to the pulsation of the turbulence, the jet fluid mixes with the surrounding fluid, and the surrounding fluid also entrains the jet fluid and moves downstream[5].

Vivek C. Patkar[6] studied the effects of different jet angles and different orifice shapes on gas jet...
mixing based on the mixing zone volume and turbulent viscosity, and calculated the characteristic mixing time under different conditions. Weixing Dai [7] studied the three-dimensional numerical simulation of industrial single snorkel furnaces, and found that too large or too small snorkel diameters are undesirable. Because it will cause uneven local mixing. Tianhu Zhang [8] optimized the premixed burner, and the mixing uniformity of the outlet was significantly improved after the distributed orifice plate was adopted. However, there are few numerical simulation studies on the oxygen mixer in the ethylene oxide process.

The study adopts Fluent to simulate the concentration field of the components in the oxygen mixer. The influence of different orifice diameter on gas mixing were discussed. The oxygen distribution characteristics in the downstream section and outlet section of the mixer was analyzed.

2. Mathematical model

In this approach, several appropriate assumptions are made:

1. The recycle gas and oxygen are treated as Newtonian fluid. For low Mach number flow here, they are assumed to be incompressible.
2. The influence of radiation heat and floating terms are neglected.
3. The feed gas is simplified as nitrogen, argon, methane, ethylene and oxygen. Table 1 shows the mole fraction of feed gas.

| composition | mole fraction(%) |
|-------------|-----------------|
| N₂          | 2.33            |
| Ar          | 5.8             |
| CH₄         | 55.64           |
| C₂H₄        | 36.23           |
| O₂          | 1               |

2.1 The turbulence model

In the study, the three dimensional average Reynolds conservation equations based on continuous equations, momentum equations, and energy equations are adopted. The turbulence model selects the standard k-ε Model, in which the transport equations of k and ε are shown as Equations (1) and (2). The turbulence model can solve the supersonic flow problem well, and it is widely used to study the mixing sensitivity of jet-cross flow injection flow field.

\[
\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho k \mathbf{u}) = \nabla \cdot \left( \frac{\mu}{\sigma_k} \nabla k \right) + G_k + G_b - \rho \varepsilon - Y_{st} + S_k
\]

\[
\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \mathbf{u}) = \nabla \cdot \left( \frac{\mu}{\sigma_\varepsilon} \nabla \varepsilon \right) + C_{\varepsilon} \frac{\varepsilon}{k} (G_k + C_{\varepsilon} G_{\varepsilon}) - C_{\varepsilon,} \rho \frac{\varepsilon^2}{k} + S_{\varepsilon}
\]

Where Gk is the generation of turbulence kinetic energy due to the mean velocity gradients, Gb is generation of turbulence kinetic energy due to buoyancy, YM is the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, C₁ε, C₂ε, and C₃ε are constants. σk and σε are the turbulent Prandtl numbers for k and ε, respectively. Sk and Sε are user-defined source terms.

The turbulent viscosity, μₜ, is computed by combining k and ε as follows:

\[
\mu_t = \rho \mu C \frac{k^2}{\varepsilon}
\]

Where Cμ is a constant.

The model constants C₁ε, C₂ε, C₄, σk, and σε have the following default values:

C₁ε = 1.44, C₂ε = 1.92, C₄ = 0.09, σk = 1.0, σε = 1.3

They work fairly well for a wide range of wall-bounded and free shear flows.
2.2 The species transport model
The mixing is simulated by considering the species transport model. To solve the local mass fraction of each species, \( Y_i \), through the solution of a convection-diffusion equation for the \( i \)th species. This conservation equation takes the following general form:

\[
\frac{\partial}{\partial t} (\rho \ Y_i) + \nabla \cdot \left( \rho \vec{v} \ Y_i \right) = -\nabla \cdot \vec{J}_i + R_i + S_i
\]  

(4)

where \( R_i \) is the net rate of production of species by chemical reaction and \( S_i \) is the rate of creation by addition from the dispersed phase plus any user-defined sources. An equation of this form will be solved for species where \( i \) is the total number of fluid phase chemical species present in the system. Since the mass fraction of the species must sum to unity, the \( N \)th mass fraction is determined as one minus the sum of the \( N-1 \) solved mass fractions.

In turbulent flows, the following equation computes the mass diffusion.

\[
\vec{J}_i = -\left( \rho \ D_{i,m} + \frac{\mu_{t}}{Sc_{i}} \right) \nabla \ Y_i - D_{t,i} \ \frac{\nabla T}{T}
\]  

(5)

where \( Sc_t \) is the turbulent Schmidt number (\( \frac{D_t}{\mu_t} \)) where \( \mu_t \) is the turbulent viscosity and \( D_t \) is the turbulent diffusivity). The default value of \( Sc_t \) is 0.7.

2.3 Definition of mixing uniformity
In order to quantitatively evaluate the mixing uniformity, an index for uniformity is proposed as:

\[
U = \sqrt{\frac{\sum_{i=1}^{n} \left( \varphi_i - \varphi_0 \right)^2}{n}}
\]  

(6)

\[
\varphi_0 = \frac{\sum_{i=1}^{n} \varphi_i}{n}
\]  

(7)

Where \( \varphi_i \) is the cell value of the selected variables at each facet, \( \varphi_0 \) is the mean of \( \varphi_i \) and \( n \) is the total number of facets. The value \( U \) is smaller, the mixing uniformity is better. In the study, this index used to evaluate the oxygen uniformity of outlet section. The simulation results are exported by Fluent, and Microsoft Excel is used to calculate the value of uniformity index.

3. Solution procedure
3.1 Physical model
The oxygen mixer is composed of an upstream, a mixer section and a downstream. The recycle gas from the upstream is mixed with oxygen in the mixer section, and then fully developed through the downstream section, and enters the reactor after being evenly mixed. The mixer section is composed of three concentric rings of different sizes. Each ring has a different number of uniformly arranged small holes. Oxygen is sprayed from orifice to mix with the recycle gas. Figure 1 shows the physical model of oxygen mixer.
3.2 Grid
The structure of the upstream and downstream is simple, so the structured grid is adopted. However, the mixer is complicated, so it adopts the unstructured grid. As a result, the hybrid grid is adopted as a whole. Figure 2 shows the hybrid grids of the model.

3.3 Boundary conditions
The recycle gas inlet and oxygen inlet are set as the velocity inlet. The outlet of oxygen mixer is set as the pressure outlet. The operating pressure is set to 1.3 Mpa. Table 2 shows the detailed data.

|                         | velosity inlet (m/s) | recycle gas inlet | oxygen inlet | pressure outlet (Mpa) | outlet | operating pressure (Mpa) |
|-------------------------|-----------------------|-------------------|--------------|-----------------------|-------|-------------------------|
| velocity inlet (m/s)    |                       | recycle gas inlet | oxygen inlet | pressure outlet (Mpa)  |       | operating pressure (Mpa) |
|                         |                       |                   |              |                       |       |                          |
| velocity inlet (m/s)    |                       | recycle gas inlet | oxygen inlet | pressure outlet (Mpa)  |       | operating pressure (Mpa) |
|                         |                       |                   |              |                       |       |                          |

4. Results and discussion
The orifice diameter is a significant design parameter of achieving high-efficiency mixing in the oxygen mixer. Therefore, the effect of the orifice diameter on flow field is investigated. Table 3 shows the three different cases of ring orifice diameter. In these cases, the components of feed gas, velocity and pressure are kept constant as mentioned in Table 1 and Table 2.

Figure 3 shows the contours of the oxygen mass fraction at downstream the longitudinal section. This figure shows the process of oxygen mixing downstream. Figure 3 (a) shows oxygen distribution at small orifice. And figure 3 (c) shows oxygen distribution at large orifice. Oxygen has not yet been mixed.
well in the straight pipe by the figure. Then the oxygen uniformity is further improved after going through the elbow. Particularly, figure 3 (b) shows the best uniformity because of almost identical oxygen mass fraction. In case 2, the oxygen mass fraction difference is 0.0019 in the downstream. Figure 3 illustrates that the region of high concentration is on the upper wall. And the region of low concentration is on the downside wall. Therefore, the pipe near the wall is not easily mixed.

Table 3. The three cases of ring orifice diameter.

|        | ring 1(mm) | ring 2(mm) | ring 3(mm) |
|--------|------------|------------|------------|
| case 1 | 3          | 4          | 5          |
| case 2 | 4          | 5          | 6          |
| case 3 | 5          | 6          | 7          |

Figure 4 demonstrates the variation of the oxygen mass fraction on the eight downstream cross sections. It can be seen from the overall trend of each cases that the oxygen high-concentration area is getting smaller along the downstream direction, illustrating that the mixing behavior gradually enhances along the flow direction.

In addition, Figure 4 (a) and (b) reveal that oxygen distribution is basically uniform after the gas passes through the elbow. But Figure 4 (c) shows the oxygen concentration is high locally at the gas outlet. And concentration difference is largest. Therefore, excessive orifice diameter is not good for mixing.

Cross section at different locations are studied to evaluate the effect of the orifice diameter. The results of three different cases are shown in Figure 5. It can be seen that the oxygen mixing uniformity is decreased along the downstream direction. The oxygen mixing uniformity is minimized in case 2. The mixing uniformity of case 3 is greater than the other two cases. It demonstrates convincingly that too large orifice size is not conducive to mixing. At a certain distance from the outlet section in case 1, the oxygen uniformity no longer decreases. Although case 1 is better mixed than case 2 in the front position, the oxygen uniformity of case 2 at the outlet section is lower than case 1. It is concluded that case 2 is the optimal condition in three cases.

Figure 4. Oxygen distribution of downstream cross section for three cases
5. Conclusions
Based on the background of oxygen mixer, the study adopts standard k-ε turbulence model and species transport model to investigate the effect of orifice diameter on the mixing performance. The mixing uniformity index is used to analyze the mixing enhancement performance under different cases. The following conclusions are drawn:

The mixing process of three different cases has the same trend. Oxygen mixing uniformity of case 1 basically coincide with the case 2. But if the amount of gas is considered, case 2 is the best. And the case 3 is the worst. As the size of orifice decreases, the mixing has been improved to some extent. The reason may be that the small orifices increase the jet velocity and enhance the turbulence intensity, thus enhancing the mixing effect.

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References
[1]. Ding Zhixiang. CFX Simulation of Mixing Effect in Oxygen Mixer of The Vinyl Acetate Synthesizing Plant [D]. East China University of Science and Technology,(2012).
[2]. Wang S J, Mujumdar A S. Flow and mixing characteristics of multiple and multi set opposing jets [J]. Chemical Engineering and Processing: Process Intensification, 46,703-712(2007).
[3]. Pei Kaikai, Li Ruijiang, Wu Yongqiang, Ni Yanhui, Zhu Zibin. Numerical simulation on the mixing in a multi-jet gas-gas mixer[J]. Chemical Reaction Engineering and Technology, 31,33-39(2015).
[4]. Chen Yi, Zhang lin-jin, Ye Xu-chu. CFD analysis and experimentation on gas turbulent mixing process in a jet mixer[J]. The Chinese Journal of Process Engineering, 7,865-870(2007).
[5]. Jiang Yongxiang. The study on the process and technology producing ethylene oxide by ethylene oxidation[D]. *East China University of Science and Technology*, (2008).

[6]. Vivek C. Patkar, Ashwin W. Patwardhan. Effect of jet angle and orifice shape in gas–gas mixer using CFD[J]. *Chemical Engineering Research and Design, 89*, (2010).

[7]. Dai Weixing, Cheng Guoguang, Li Shijian, Huang Yu, Zhang Guolei, Qiu Yunlong, Zhu Weifei. Numerical Simulation of Multiphase Flow and Mixing Behavior in an Industrial Single Snorkel Refining Furnace (SSRF): The Effect of Gas Injection Position and Snorkel Diameter[J]. *ISIJ International, 59*, (2019).

[8]. Zhang Tianhu, Liu Fengguo, You Xueyi. Optimization of gas mixing system of premixed burner based on CFD analysis[J]. *Energy Conversion and Management, 85*, (2014).