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# Numerical simulation of $CO_2$ and dye separation for supercritical fluid in separator

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A R T I C L E I N F O

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A B S T R A C T

Separator, as one of the key components in supercritical $CO_2$ dyeing apparatus, shows the function of separating $CO_2$ and dyes, thus affecting the reutilization of $CO_2$ and the subsequent dyeing production. In this study, pressure drop and separation efficiency of the separator were investigated by employing the flow field analysis software FLUENT. Fluid area calculation of the separator was conducted using Reynolds stress model as the turbulence model and SIMPLEC algorithm. Moreover, separation efficiency of $CO_2$ gas and dyes in the separator was determined by employing Discrete phase model as the calculation model of dye particle phase. Numerical results showed that the total pressure drop of the separator increased from 1.43 Pa to 122.70 Pa with the inlet flow rate of $CO_2$ increased from 50 L/h to 2000 L/h. The total separation efficiency of the separator improved significantly from 4.35% to 38.22% when the inlet flow rate increased from 100 L/h to 2000 L/h.

## 1. Introduction

Utilization of supercritical $CO_2$ for textile dyeing, as a novel dyeing and finishing technology, presents distinct environmental protection advantages and commercial competition ability [1–3]. On the one hand, there is no waste water produced in the whole dyeing process because of no water added [4–6]. On the other hand, dry textiles are obtained directly after the waterless dyeing is completed, thereby eliminating rinsing and drying in the traditional dyeing approach [7]. These short processes and the reutilization of dyes and $CO_2$ endow with the characteristics of energy conservation and cost saving [8–12].

At present, supercritical $CO_2$ is mainly used to dissolve disperse dyes for dyeing polyester and other synthetic fibers [13–16]. When the dyeing process is finished, the residual dyes will dissolve in $CO_2$ under supercritical state. In order to achieve the separation of dyes and $CO_2$, separator is widely employed in the supercritical $CO_2$ dyeing apparatus [17–19]. Theoretically, after depressurizing by a throttling valve, supercritical $CO_2$ is converted back into gas, and pass through the outlet of separator into a $CO_2$ storage cylinder while the solid dyes are deposited in the separator vessel with the system temperature decreasing under cooling effect [20]. During this process, some dyes may still be carried into pipelines and / or $CO_2$ storage cylinder with $CO_2$ gas flow. The flow field of the separator displays an obvious influence on the pressure drop and the gas-solid separation efficiency, affecting the cleaning of supercritical dyeing apparatus and subsequent dyeing production. However, it is extremely difficult to obtain the internal gas phase flow behaviors of the separator with high-pressure $CO_2$ fluid due to the excessive workload for experimentation.

Numerical calculation can accurately simulate the flow field in the separator by using reasonable turbulence calculation model and calculation method, which is not limited to the actual conditions, and displays the features of fast calculation speed and the short calculation time [21]. Generally, numerical simulation models of gas phase flow field mainly include Renormalization Group (RNG) k-ε turbulent model, Reynolds stress equation model (RSM) and Large eddy simulation (LES) [22–24]. Compared to other models, there is no isotropic assumption of eddy viscosity for RSM, which has high accuracy, moderate calculation amount and reliable calculation results for anisotropic turbulence [25].

The object of this work is to investigate the numerical simulation of the $CO_2$ phase flow field based on a self-developed supercritical $CO_2$ dyeing apparatus. Fluid area calculation model of the separator was established, and mesh generation was conducted. The pressure drop separation efficiency of $CO_2$ gas and dyes in the separator under different conditions was then discussed and calculated.

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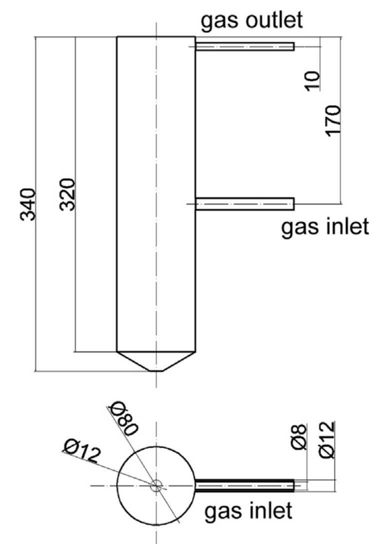


**Fig. 1.** The dimensions of the separator (mm).

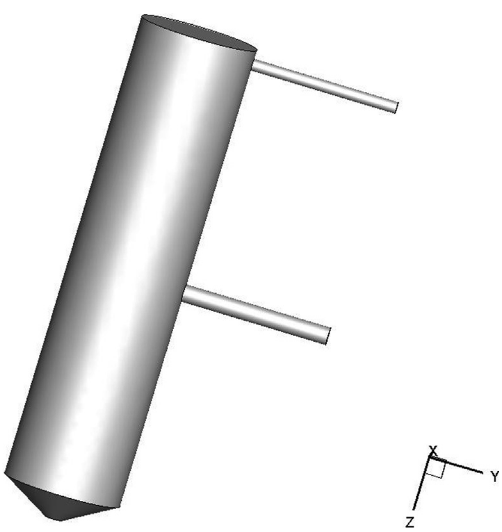


**Fig. 2.** Fluid area calculation model of the separator.

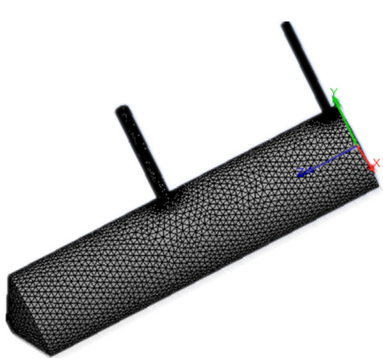

**Fig. 3.** Schematic diagram of mesh generation.

## 2. Numerical calculation of the pressure drop

### 2.1. Fluid area model

The separator of a self-developed supercritical $CO_2$ dyeing apparatus was employed as the model entity used for numerical calculation, and its internal dimensions was actually mapped in Fig. 1. The separator vessel is composed of two parts with a total height of 340 mm. Of which, the upper part is a cylindrical segment with an inner diameter of 80 mm and a height of 320 mm. The lower part is a cone segment with a bottom inner diameter of 80 mm and a top inner diameter of 12 mm. Moreover, the vertical height between the centerline of gas outlet pipeline and the top surface of the cylinder section is 10 mm with a inner pipe diameter of 8 mm. The vertical height from the centerline of gas inlet pipeline to the top surface of the cylinder segment is 170 mm with a inner pipe diameter of 12 mm. The top surface of the cone is the outlet for particle collection.

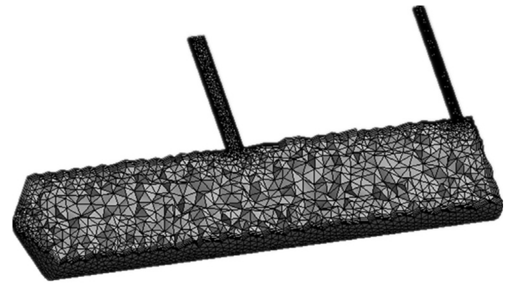

**Fig. 4.** Internal profile of mesh generation.

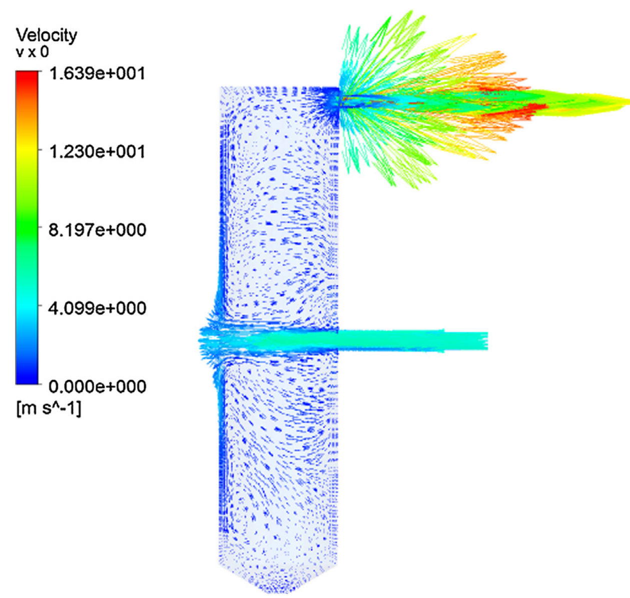


**Fig. 5.** Vector diagram of velocity on section x = 0.

As shown in Fig. 2, the model of the separator was established with AutoCAD 2014 and imported into the DM module of ANSYS 18.0 for modeling. It can be seen that the origin of coordinate system is established at the top surface center of the cylinder section. In the coordinate system, the direction of the positive axis z goes straight down from the origin to the normal direction of the top surface of the cylinder segment. The direction of the positive axis y passes through the origin, parallels to and points in the centerline direction of gas outlet. The direction of the positive axis × passes through the origin, which is perpendicular to and points in ZY plane.

### 2.2. Mesh generation

The established fluid area model of the separator was imported into Mesh module for mesh generation, and gird independence is investigated. The number of cells is 85486, 92418, 139616, 279200, 279707, 308171, respectively. The inlet pressures for the cells numbers of 139616 and 308171 are 5250.33 Pa and 5264.20 Pa, which shows minimal changes. Thus, the relatively accurate results can be obtained