0273-2289/04/114/0733–0745/$25.00

Computational Fluid Dynamics Simulation and Redesign of a Screw Conveyor Reactor

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Abstract

National Renewable Energy Laboratory (NREL) designed a shrinking-bed reactor to maintain a constant bulk packing density of cellulosic biomass. The high solid-to-liquid ratio in the pretreatment process allows a high sugar yield and avoids the need to flush large volumes of solution through the reactor. To scale up the shrinking-bed reactor, NREL investigated a pilot-scale screw conveyor reactor in which an interrupted flight between screws was employed to mimic the "shrinking-bed" effect. In the experiments with the screw conveyor reactor, overmixing and uneven flow occurred. These phenomena produce negative effects on biomass hydrolysis. The flow behavior inside the reactor was analyzed to allow redesign of the screw to achieve adequate mixing and even flow. In the present study, computational fluid dynamics (CFD) was utilized to simulate the fluid flow in the porous media, and a new screw design was proposed. CFD analysis performed on the redesigned reactor indicated that an even flow pattern was achieved.

Index Entries: Screw reactor; computational fluid dynamics; modeling; backflow; hydrolysis.

Introduction

National Renewable Energy Laboratory (NREL) designed a shrinking-bed reactor *(1)* to maintain a constant bulk packing density of solid biomass in the reactor. As a result, high sugar concentrations were achieved owing to the high solid-to-liquid ratio and reduced liquid volume. NREL's work had experimentally proven that sugar yields higher than 95% from hemicellulose and higher than 85% from cellulose were attainable in a multiple percolation reactor system simulating countercurrent operation *(1)*.

Note: As a result of publishing restrictions, all color figures were changed to gray scale. The color copy is available upon the reader's request.

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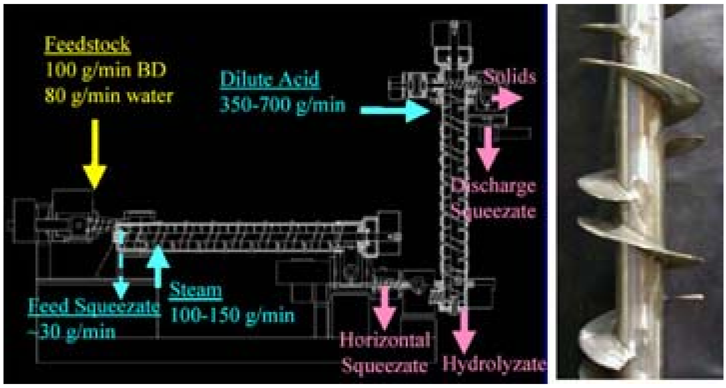

Fig. 1. Experimental arrangement and screw structure of NREL pilot-scale screw conveyor reactor for hardwood hydrolysis. (Adapted from ref. *7*.)

Chen et al. *(2)* developed a kinetic model to describe the shrinking-bed reactor and found that the shrinking-bed operation increases the sugar yield by about 5% compared with the non-shrinking-bed operation. Lee et al. *(3)* also developed a mathematical model to simulate a countercurrent shrinking-bed reactor and showed that bed shrinking provides a positive effect on both hemicellulose and cellulose hydrolysis. Pettersson et al. *(4)* further expanded Lee et al.'s *(3)* modeling, adding new features including wood porosity, glucose diffusion, and absorption of hydrolysate at the bottom of the reactor. Pettersson et al. *(4)* found that both porosity and absorption of hydrolysate at the bottom of the reactor had small effects on the combined yield and concentration results at a given specified reactor solids loading. Converse *(5)* presented a model to simulate a cross-flow shrinking-bed reactor for the hydrolysis of lignocellulosics and found a trade-off between cross-flow and plug-flow shrinking-bed reactors. Cross flow allows one to obtain higher yields than plug flow but with a slight reduction in product concentration. Wan and Hanley *(6)* simulated the flow field inside the shrinking-bed reactor with computational fluid dynamics (CFD) and found that the flow inside the reactor is mostly plug flow and was ideal for biomass hydrolysis based on theoretical analysis.

Previous studies have shown the great potential of the shrinking-bed reactor for commercial application. To scale up the shrinking-bed reactor and to establish it as a practical process reactor, NREL further developed the shrinking-bed reactor into a screw conveyor reactor in which a vertical broken flight screw was employed as a moving-bed mechanism. Experiments with yellow poplar hardwood hydrolysis in pilot-scale (200 kg/d) screw reactors *(7)* produced soluble xylose yields of almost 90%. Glucose yields from cellulose were slightly less than predicted from bench work using a 5-min residence time at just under a normalized 25% yield. Figure 1 shows the arrangement and structure of pilot-scale screw conveyor reactor in the NREL hardwood hydrolysis experiment.

In the hardwood hydrolysis experiment with the screw reactor, NREL researchers found that overmixing and an uneven flow pattern existed in the reactor. These factors have a negative effect on biomass hydrolysis. To enhance the screw conveyor reactor's performance, it was necessary to redesign the reactor to achieve adequate mixing and an even flow pattern. In the present work, CFD was utilized to analyze the flow behavior in the screw conveyor reactor, and a new screw design was proposed based on CFD analysis.

Model and Method

The porous media model *(8)* is used to simulate flows through the biomass in a packed bed where biomass is the porous media. In this model, a momentum source term S_i is added to the standard fluid flow equation:

$$S_i = \sum_{j=1}^{3} D_{ij}\,\mu v_j + \sum_{j=1}^{3} C_{ij}\,\frac{1}{2}\,\rho \left| v_j \right| v_j \tag{1}$$

The first part of this equation is a viscous loss term and the second is an inertial loss term. For simple homogeneous porous media, S_i can be written as

$$S_i = \frac{\mu}{\alpha}\,v_i + C_2\,\frac{1}{2}\,\rho \left| v_i \right| v_i \tag{2}$$

in which α is the permeability and C_2 is the inertial resistance factor.

In laminar flows through porous media, the pressure is proportional to velocity and C_2 can be taken as zero. Ignoring convective acceleration and diffusion, the porous media model can be changed into Darcy's Law:

$$\nabla P = -\frac{\mu}{\alpha}\,v \tag{3}$$

in which ∇P is the pressure drop.

For turbulent flows and the cases in which the permeability term can be eliminated, the porous media model can be rewritten as follows:

$$\frac{\partial p}{\partial x_i} = \sum_{j=1}^{3} C_{2ij}\left(\frac{1}{2}\,\rho v_j \left| v_j \right|\right) \tag{4}$$

For packed-bed and turbulent flows, Darcy's law can be rewritten as the Ergun equation *(9)*:

$$\nabla P = \frac{150\,\mu}{D_p^2}\,\frac{(1-\varepsilon)^2}{\varepsilon^3}\,v + \frac{1.75\,\rho}{D_p}\,\frac{(1-\varepsilon)^3}{\varepsilon^3}\,v\,v \tag{5}$$

For laminar flow, the second term of the Ergun equation may be dropped, resulting in the Blake-Kozeny equation:

$$\nabla P = \frac{150\,\mu}{D_p^2}\,\frac{(1-\varepsilon)^2}{\varepsilon^3}\,v \tag{6}$$

Comparing Eqs. 3 and 4 with Eq. 5,

$$\alpha = \frac{D_p^2}{150} \frac{\varepsilon^3}{(1-\varepsilon)^2} \tag{7}$$

$$C_2 = \frac{3.5}{D_p} \frac{(1-\varepsilon)}{\varepsilon^2} \tag{8}$$

in which D_p is the mean particle diameter, and ε is the void volume fraction of the packed bed. In this simulation, constant void volume fraction was assumed. From former research *(3)*, the void volume fraction was estimated to be 0.8.

Using the Blake-Kozeny equation, the screw conveyor reactor can be modeled as rotating equipment in which the fluid is moved by screw rotation. Although 10 small horizontal cylindrical baffles exist in the screw flights, the interaction between the screw and baffles can be ignored. For this case, the rotating reference frame was used instead of the inertial reference frame.

We used a commercial CFD package Fluent 6.0 to simulate the pilot-scale screw conveyor reactor. The geometry of the screw conveyor reactor is given in Table 1. The experimental conditions for hardwood hydrolysis for the vertical screw conveyor reactor are described in Table 2.

Results and Discussion

Flow Pattern of Screw Conveyor Reactor

Figure 2 shows the flow pattern in the upper part of the screw conveyor reactor along the vertical panel of baffles; also included a three-dimensional view of the flow pattern. It was found that the flow direction above the screw varies from the flow direction below the screw. The fluid between the two screws had the same flow direction. In most of the upper screw, the flow was downward; above the screw, some upward flow was found.

Figure 3 shows the flow pattern in the bottom part of the screw reactor along the vertical panel of baffles. Flow in the bottom zone is mostly rotational, with strong backflow observed in this area. Figure 4 shows the flow pattern in the horizontal panel along the baffle. Apparently, the flow along this panel can be divided into two zones, each of which moved along the reactor wall, met, and then moved downward.

Downward Plug Flow in Screw Conveyor Reactor

In the CFD simulation the downward axial flow was defined as negative axial velocity. Figure 5 shows the negative axial velocity contour along the vertical panel of the baffles. Except for the dilute-acid inlet and

Table 1
Parameters of Screw conveyor reactor geometry

Reactor diameter (m)	Reactor height (m)	Dilute acid inlet diameter (m)	Hydrolysate outlet diameter (m)
0.15	1.22	0.06	0.04

Table 2
Experimental Conditions for Hardwood Hydrolysis

Flow media	Dilute acid
Temperature (°C)	210
Flow type	Laminar
Screw rotation speed (rpm)	5
Inlet velocity (m/s)	2.95×10^{-3}
Outlet pressure (Pa)	350
Particle Diameter (D_p) (m)	0.001
Void volume fraction (ε)	0.8
$1/\alpha$	9.38×10^{6}
C_2	1.37×10^{6}

the bottom screw zones, the flow was downward plug flow. This kind of flow will promote good performance for biomass hydrolysis.

Backflow Along Bottom of Screw Conveyor Reactor

In the simulation definition, the downward axial velocity was calculated as a negative value, and the upward axial flow (the backflow) was calculated as positive axial velocity. To clearly describe the backflow, the positive axial velocity contour is shown in Fig, 6. Figure 6 shows that the backflow occurred between screws with >50% of the bottom zone showing backflow.

Backflow is detrimental to the overall chemical reaction and mass transfer process. For biomass hydrolysis, the backflow had a negative effect on sugar yield and toxic chemical production. As observed by the NREL researchers, backflow will cause overmixing and uneven flow. When backflow occurs, fluid with higher sugar concentrations will be transported where sugar concentration is lower, resulting in adverse effects on the hydrolysis reaction. Moreover, backflow will increase the residence time of the sugar solution, increasing the risk of deterioration of sugars into toxic byproducts.

The backflow in the screw conveyor reactor needed to be reduced. The bottom screw was therefore redesigned to minimize backflow.

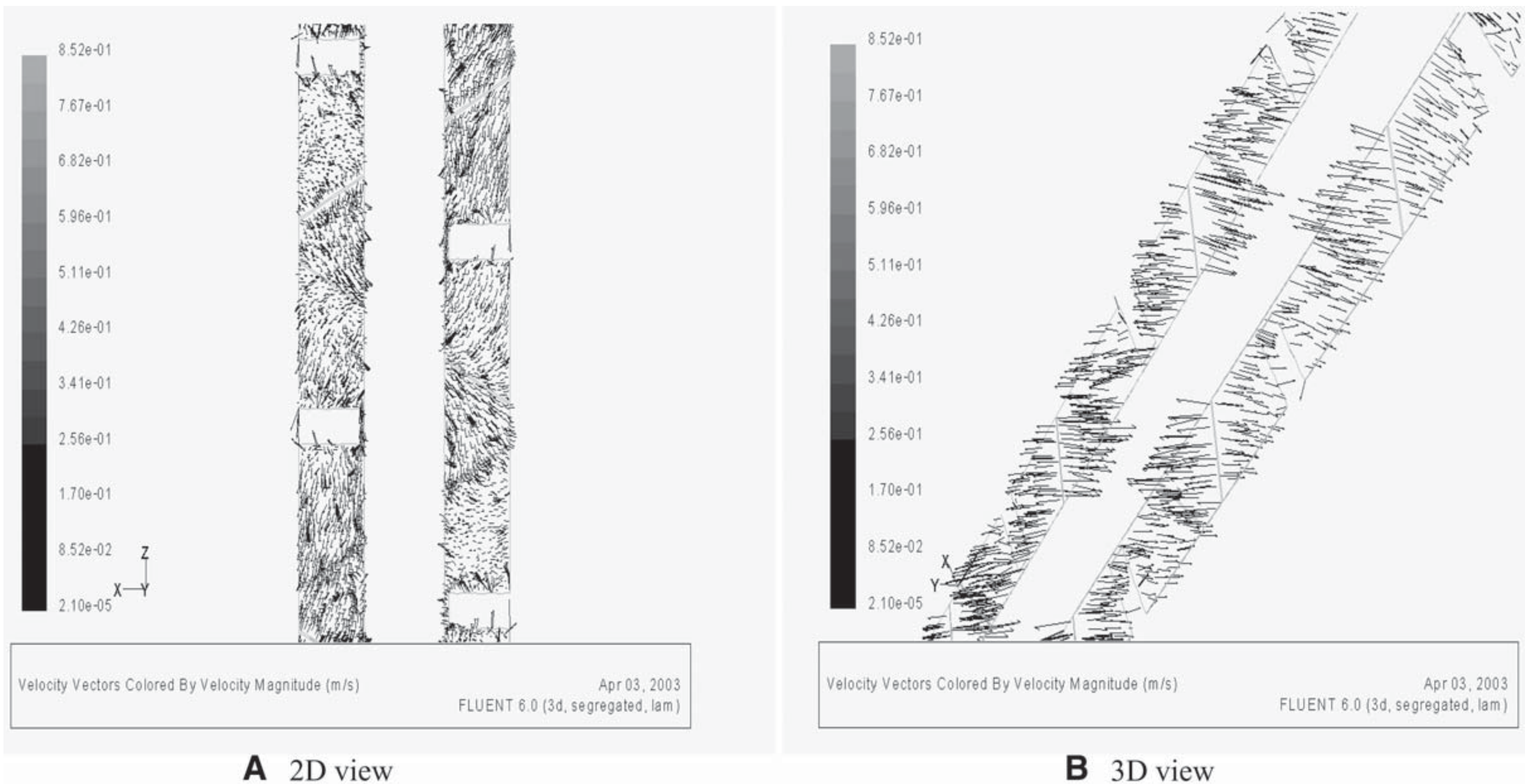

Fig. 2. Flow patterns in upper part of screw conveyor reactor: **(A)** two-dimensional view; **(B)** three-dimensional view.

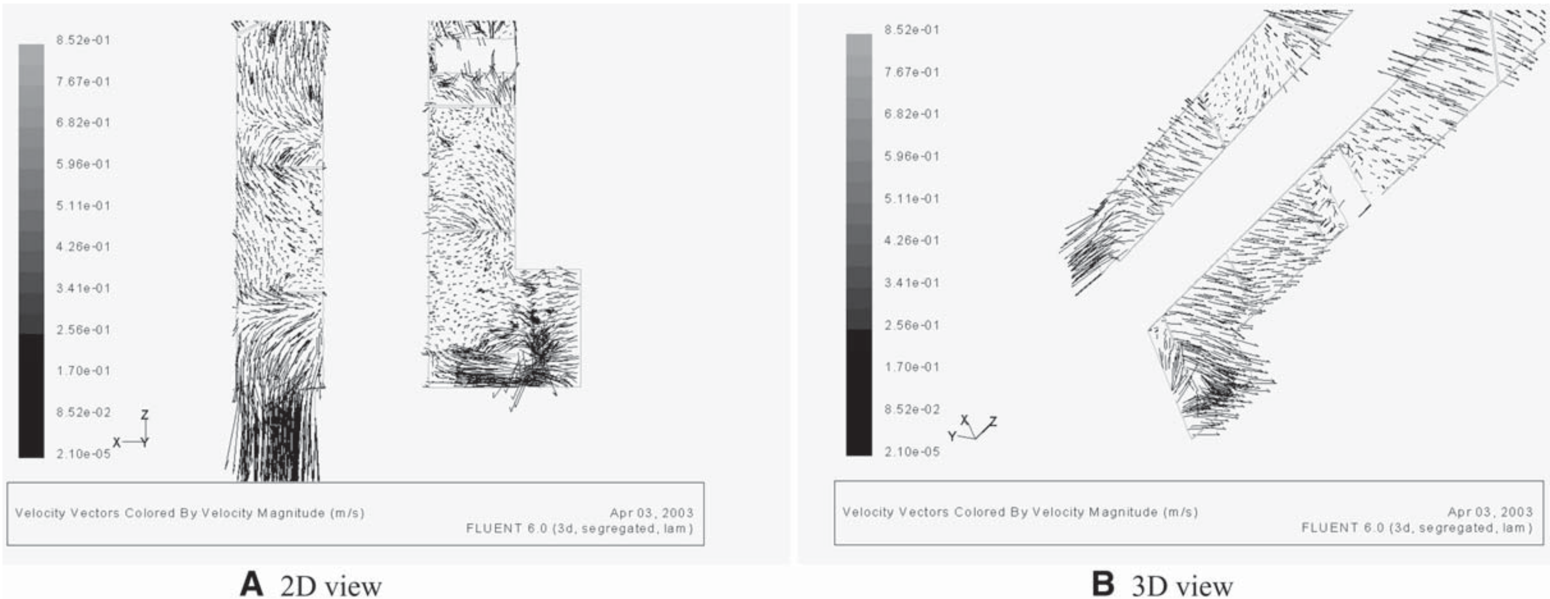

Fig. 3. Flow pattern in bottom part of screw reactor: **(A)** two-dimensional view; **(B)** three-dimensional view.

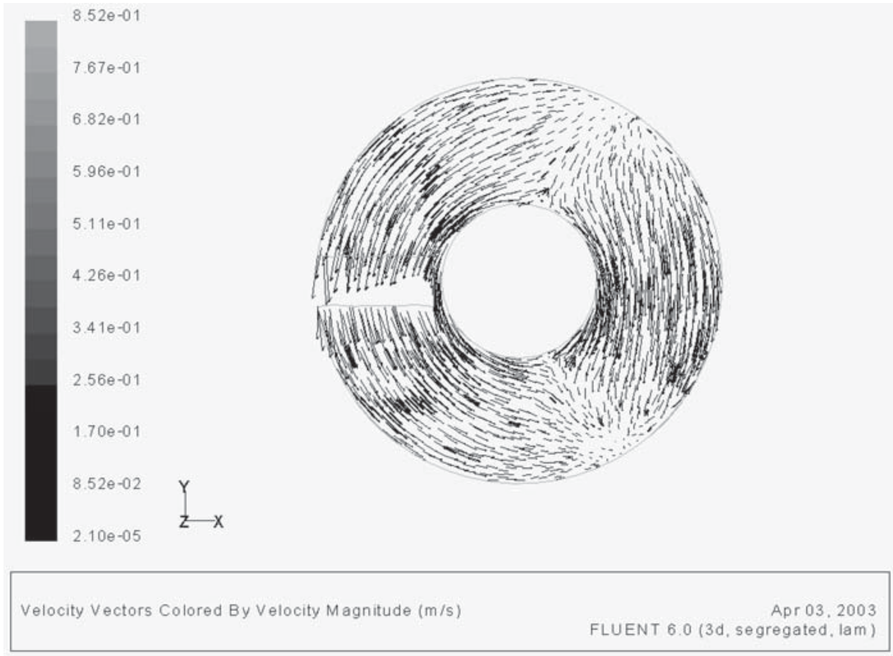

Fig. 4. Flow pattern of screw reactor along horizontal panel of baffle.

Fig. 5. Negative axial velocity contour (downward plug flow) along vertical panel of baffles.

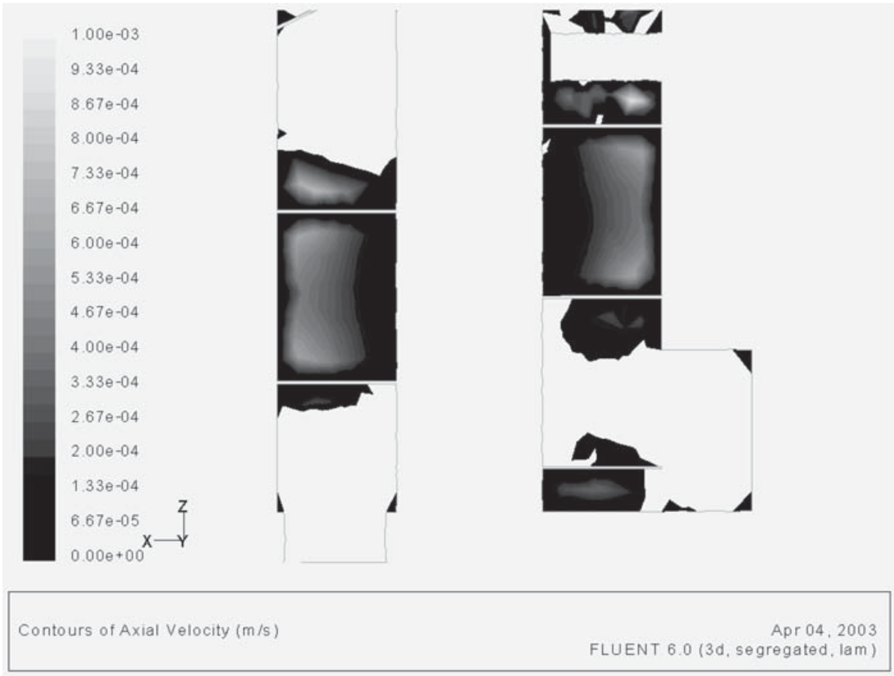

Fig. 6. Positive axial velocity contour (backflow) along bottom of screw conveyor reactor.

Redesign of Bottom Screw

Figure 7 showsn the original screw and Fig. 8 shows the redesigned bottom screw. The original cylindrical helical screw was converted into a conical helical lifter.

Backflow in Redesigned Bottom Screw

Figure 9 shows the positive axial velocity contour indicating backflow. Compared with the original screw reactor, the backflow in the redesigned screw reactor was diminished. The backflow area decreased from >50% in the original reactor to <30% in the redesigned one. Moreover, the maximum positive axial velocity in the original reactor was about 1.0×10^{-3} m/s, whereas in the redesigned reactor it was about 5×10^{-4} m/s, confirming that backflow was greatly reduced in the redesigned reactor. A better performance for biomass hydrolysis can be predicted with this redesigned screw reactor.

Comparison of Pathlines

Figure 10 shows the path lines in the bottom screw zone for the original screw reactor and the redesigned reactor. The path lines clearly show

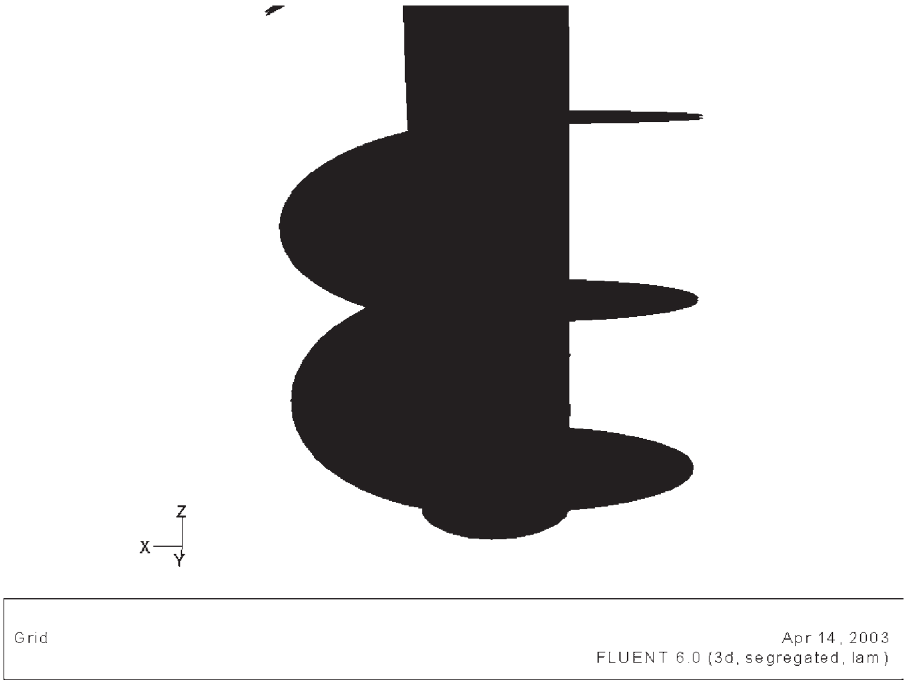

Fig.7. Original bottom screw.

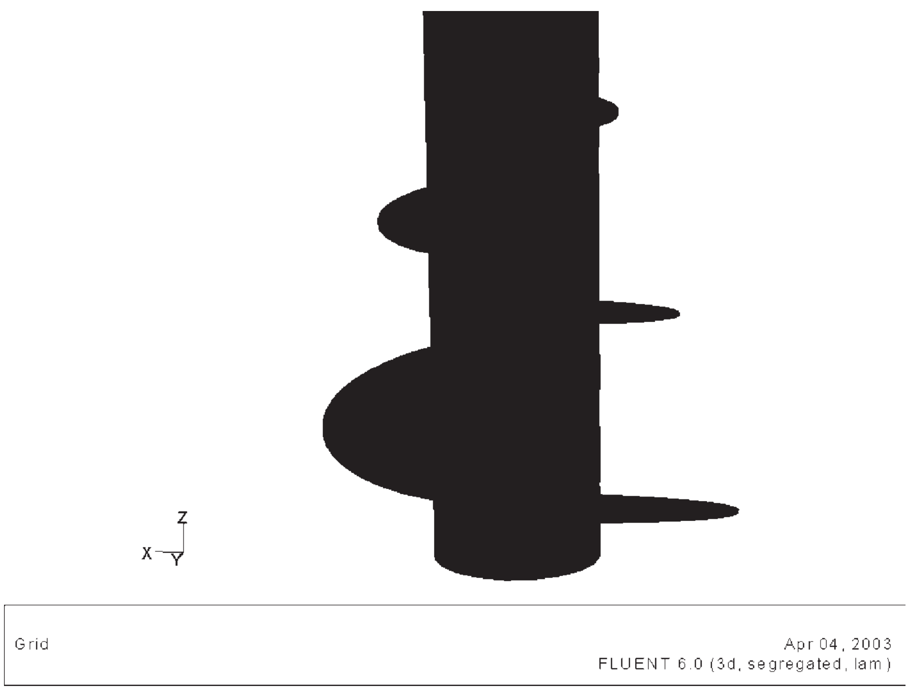

Fig. 8. Redesigned bottom screw.

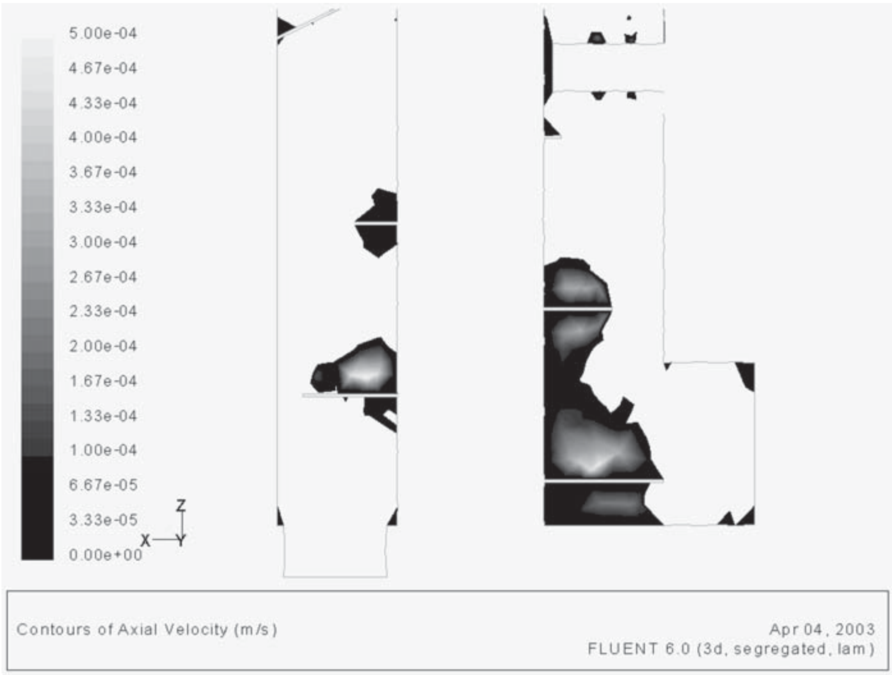

Fig. 9. Positive axial velocity contour (backflow) of redesigned screw reactor.

the random flow for the original reactor and the orderly flow for the redesigned reactor. This result further confirms that the backflow and overmixing inside the original reactor are reduced in the redesigned reactor.

Conclusion

Using the porous media model with a rotating reference frame, it was found that the overmixing and uneven flow inside the screw conveyor reactor resulted from the backflow in the bottom part of the screw. By redesigning the original cylindrical conical screw into a conical helical lifter, the backflow was reduced and even flow was achieved. As a result, this redesigned screw will decrease the risk of deterioration of sugars into toxic chemicals and improve the sugar yields. Further experimental work needs to be performed in this redesigned reactor to confirm the results of this simulation.

Nomenclature

C, C_2, D = matrix
D_p = particle diameter (m)
P = pressure (Pa)

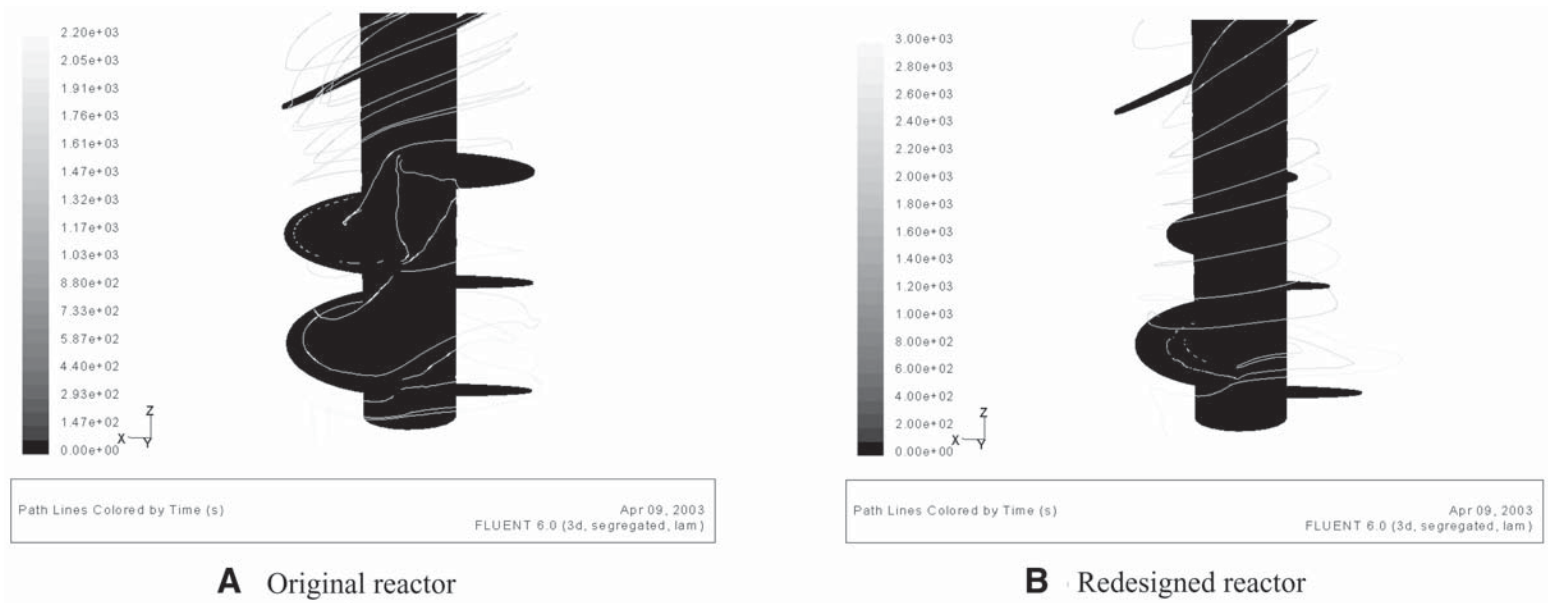

Fig. 10. Path lines of bottom part: **(A)** original reactor; **(B)** redesigned reactor.

S_i = source term for *i*th momentum equation
V_j = velocity of *i* direction
α = permeability
ε = void fraction
μ = molecular viscosity (kg/m·s)
ρ = density (kg/m^3)

Acknowledgment

This work was supported by the National Renewable Energy Laboratory (contract no. XCO-1-31016-01).

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