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Use of Computational Fluid Dynamics Simulations for Design of a Pretreatment Screw Conveyor Reactor

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Abstract

Computational fluid dynamics simulations were employed to compare performance of various designs of a pretreatment screw conveyor reactor. The reactor consisted of a vertical screw used to create cross flow between the upward conveying solids and the downward flow of acid. Simulations were performed with the original screw design and a modified design in which the upper flights of the screw were removed. Results of the simulations show visually that the modified design provided favorable plug flow behavior within the reactor. Pressure drop across the length of the reactor without the upper screws in place was predicted by the simulations to be 5 vs 40 kPa for the original design.

Index Entries: Biomass; pretreatment reactor; computational fluid dynamics simulations; screw conveyor reactor; plug flow; porous media model.

Introduction

The National Renewable Energy Laboratory (NREL) has long been investigating methods for producing high yields of glucose from cellulose to be used in fermentations for the eventual production of fuel ethanol. Acid pretreatments prior to enzymatic hydrolysis have been studied for some time. Although strong acids and high temperatures give the fastest kinetic reaction rates, complicating factors prevent practical operation under these conditions. Strong acids require significant neutralization before the fermentation stage. High temperatures can lead to sugar degradation into substances toxic to a fermenting organism. High acid flow rates are also undesirable because the final hydrolysate solution will have a low sugar concentration.

Dilute-acid hydrolysis is the most commonly used form of biomass pretreatment. One solution NREL has investigated involves a two-stage

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dilute-acid pretreatment process *(1–3)*. The first stage is operated at relatively low temperatures at which most of the hemicellulose is hydrolyzed. The second stage is operated at higher temperatures at which most of the remaining hemicellulose is hydrolyzed. The process operates with countercurrent flow of solids and acid to reduce the residence time. The two-temperature process avoids high-temperature exposure, reducing degradation of the sugar.

NREL designed a shrinking-bed reactor to maintain a high solid-to-liquid ratio within the reactor and a higher glucose concentration in the effluent stream *(4)*. The design of the shrinking-bed reactor is intended to maintain a constant bulk packing density of solid biomass in the reactor. The reactor is fixed at one end and the other end is supported by a compressed spring. As the reaction proceeds, the hemicellulose is continually hydrolyzed and removed. The spring-loaded movable end compresses the remaining solids, allowing the bulk density inside the reactor to remain constant. Wan and Hanley *(5)* simulated the flow field in a shrinking-bed reactor using a porous media model and computational fluid dynamics. Movement of the spring was simulated by obtaining solutions at multiple steady states representing different locations of the spring height.

Chen et al. *(6)* and Lee et al. *(7)* tested countercurrent reactors and both reported positive effects on hydrolysis of hemicellulose and cellulose. Chen et al. *(6)* found that sugar yield increased by about 5% in a shrinking-bed reactor compared with a nonshrinking-bed reactor. Converse *(8)* reported higher yields when using cross flow but with a reduction in product concentration.

In the present study, FLUENT 6.0, a commercial computational fluid dynamics package, was used to aid in the design of a pretreatment screw conveyor reactor. The reactor consisted of a vertical screw used to create direct contact cross flow between the upward conveying biomass solids and the downward flow of acid. Simulations were performed using the original screw design provided by NREL and a modified design in which the upper flights of the screw were removed. The porous media model and rotating reference frame motion were employed in the simulations. The objective was to determine whether plug flow of the acid volume could be achieved by removing the upper screw flights. Achieving plug flow will reduce the residence time of the acid in the existing reactor compared with flow that twists with the rotation of the screw flights.

Modeling and Methods

Development of Porous Media Model

FLUENT utilizes a control volume–based finite difference method to solve the conservation equations for mass, momentum, energy, and chemical species where appropriate. Dilute acid flowing past biomass

solids in a screw conveyor reactor is modeled as flow through a packed-bed for which Fluent *(9)* recommends using a porous media model to simulate. In this model, a porous region is defined where the flow blockage or resistance occurs and is, therefore, modeled by the inclusion of a momentum sink, or source term (*S*), in the governing momentum equations. If a generalized conservation of momentum equation with terms for convective acceleration, pressure losses, and gravitational forces looks like this

$$\frac{\partial}{\partial t}(\rho V) + \nabla \cdot (\rho VV) = -\nabla P + \rho g \tag{1}$$

then a conservation of momentum equation that incorporates a momentum sink to account for losses through a porous region will look like this:

$$\frac{\partial}{\partial t}(\rho V) + \nabla \cdot (\rho VV) = -\nabla P + \rho g + S \tag{2}$$

The source term for the present situation requires a term for viscous losses and a term for inertial losses. For homogeneous porous media, *S* can be written as

$$S = \frac{\mu}{\alpha} V + C\frac{1}{2}\rho VV \tag{3}$$

in which α is the permeability and *C* is the inertial resistance factor.

For the case of laminar flow through porous media at steady state, the pressure is proportional to velocity. Inertial resistance, convective acceleration, and diffusion terms are assumed to be negligible, leading to Darcy's Law:

$$\nabla P = \frac{\mu}{\alpha} V \tag{4}$$

in which ∇P is the pressure drop.

For turbulent flow in packed beds, Darcy's Law is written as the Ergun equation *(10)*:

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

in which D_p is the mean particle diameter and ε is the void volume fraction of the packed bed. The second term of the Ergun equation is dropped for laminar flow conditions, leading to the Blake-Kozeny equation:

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

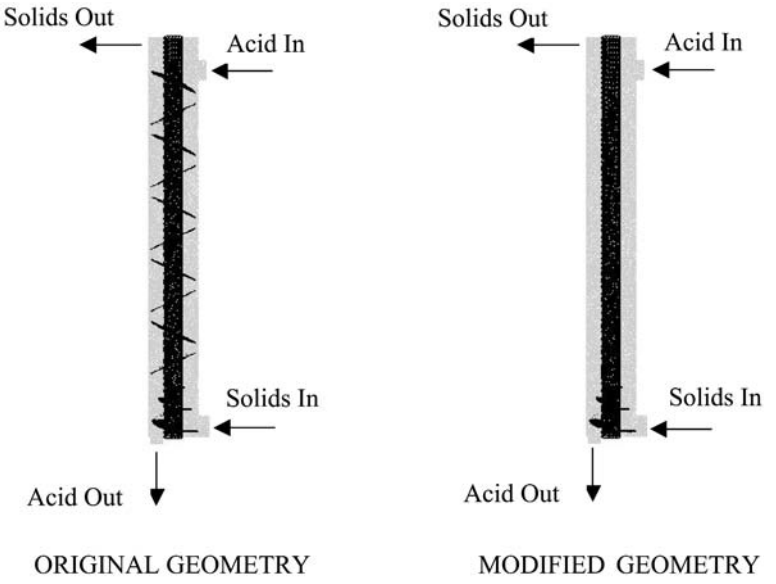

Fig. 1. Geometry drawings of original and modified screw designs.

The permeability, α, which is manually entered into the FLUENT solver, is determined by combining Eqs. 4 and 6:

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

Simulation Method

The commercial object creation package GAMBIT 1.6 was used to create the geometry drawings later used in the simulations. The reactor dimensions are 1.22 m in length and 0.15 m in diameter. Solids enter at the bottom of the reactor, are forced upward by the rotating screw, and exit through two ports near the top. Liquid enters horizontally near the top of the reactor at a location 180° from the exiting solids and exits through a port at the bottom.

Figure 1 shows diagrams of the original and modified screw designs. The original design contains screw flights along the entire shaft length. The modified design contains screw flights only near the bottom of the shaft. A three-dimensional mesh of each geometry was created that contains 179,306 tetrahedral computational cells in the original screw design and 162,306 in the modified design. Operating conditions, equivalent for both the original and modified designs, are given in Table 1 and steady-state flow is assumed.

Results and Discussion

The simulation results are described from the liquid's "point of view" because overexposure of the solids to the acid is of concern for design of

Table 1
Reactor Operating Conditions

Temperature	25°C
Flow	Laminar
Reynolds number	<1
Inlet acid velocity	2.95×10^{-3} m/s
Screw rotation rate	5 rpm
Outlet pressure	101 kPa
Particle size	1 mm
Packed-bed void fraction, ε	0.2
Permeability, α	8.3×10^{-11} m^2

the reactor. The liquid is to flow countercurrent to the solids, so the liquid must be delivered with sufficient force to overcome the cross flow. For the purpose of simulating flow phenomena inside the reactor, it is assumed that the method of delivering the liquid to the entry point can provide the necessary force. The liquid is given a boundary condition of uniform velocity throughout the surface of the acid inlet port. The boundary condition at the liquid exit is that of atmospheric pressure.

The primary objective is to modify the design of the screw in a way that will favorably alter the flow pattern inside the existing pretreatment reactor. The use of a screw conveyor inside the reactor is an obvious choice because of the screw's ability to move solids efficiently. However, the turning of the screw sends the contents through the reactor in a tortuous path. This results in increased residence times and, therefore, increased exposure of the solids to the acid.

Removing the screw flights from the shaft may result in the fluid moving in the desired plug flow depending on the characteristics of the fluid. Because the solids will absorb a percentage of the cross-flowing acid, the contents inside the reactor will take on a new effective viscosity. The viscosity of a pretreated corn stover slurry provided by NREL was measured over a range of shear rates. Shear will vary slightly with location within the screw reactor, but a constant value of 40,000 cP was chosen for the purpose of running this simulation.

Velocity vectors in horizontal and vertical planes can be used qualitatively to determine whether plug flow was created from the new screw design. A horizontal plane at a height equal to 0.7 m was created for both the original and modified designs during the postprocessing of the FLUENT simulations (Fig. 2). Figure 3 shows a top view of each plane. The vectors in the plane of the original design are seen to rotate in a counterclockwise direction. The lengths of the vectors are scaled according to magnitude, and the varying pattern of vector lengths indicates that the fluid is twisting in a simultaneously angular and upward direction. The vectors in the horizontal plane of the modified design appear as points, rather than lines.

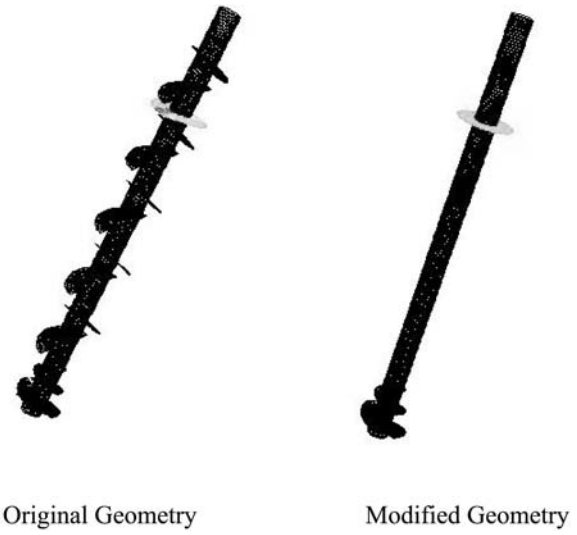

Fig. 2. Location of horizontal mixing plane.

This is owing to the absence of angular motion because the vectors point only in the axial direction.

Figure 4 shows velocity vectors in a vertical plane. The location of the horizontal plane from Fig. 3 is included as a point of reference because a close-up view is presented so that the directions of the vectors are easily discernible. The contrast in flow patterns between the two designs is again apparent: swirl and backflow can be seen in the original design, whereas an organized axial plug flow pattern is seen in the modified design.

Pressure drop across the reactor is greatly reduced when the fluid moves in plug flow as compared to a twisting path. The shading in Fig. 5 shows total pressure distribution along the reactor. Pressure drop from the acid inlet point to the acid exit point is 5 kPa in the modified design vs 40 kPa in the original design. Higher pressure may result in higher hydrolysis reaction rates, which can have adverse implications. Sugar degradation into toxic byproducts may result from the combination of higher reaction rates and longer residence times. Although a 5-kPa pressure drop may seem quite low in the modified design, the value is reasonable considering a very low linear velocity at the liquid entrance (0.00295 m/s) and a short travel length (1.22 m).

The pressure distribution appears to be uniform throughout the length of the modified reactor, except for small regions close to the inlet and outlet ports. The pressure in the original reactor appears to vary throughout the entire length, with significant differences approximately every 0.2 m. Uniform pressure throughout is more desirable because reaction rates will be more stable. When the highest pressure exists at the point at which the residence time is the greatest, sugar degradation becomes a more serious factor.

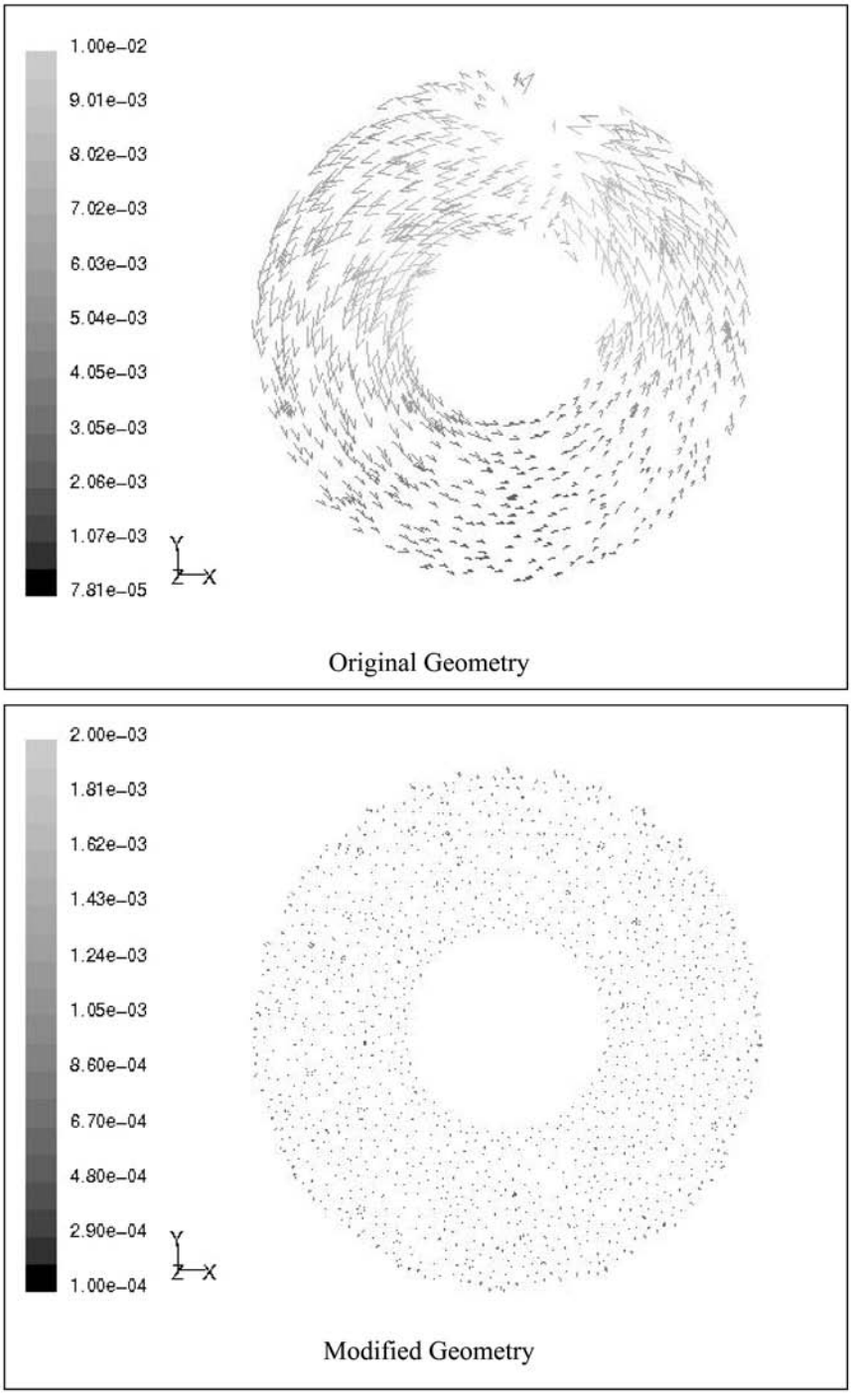

Fig. 3. Velocity vectors in a horizontal mixing plane.

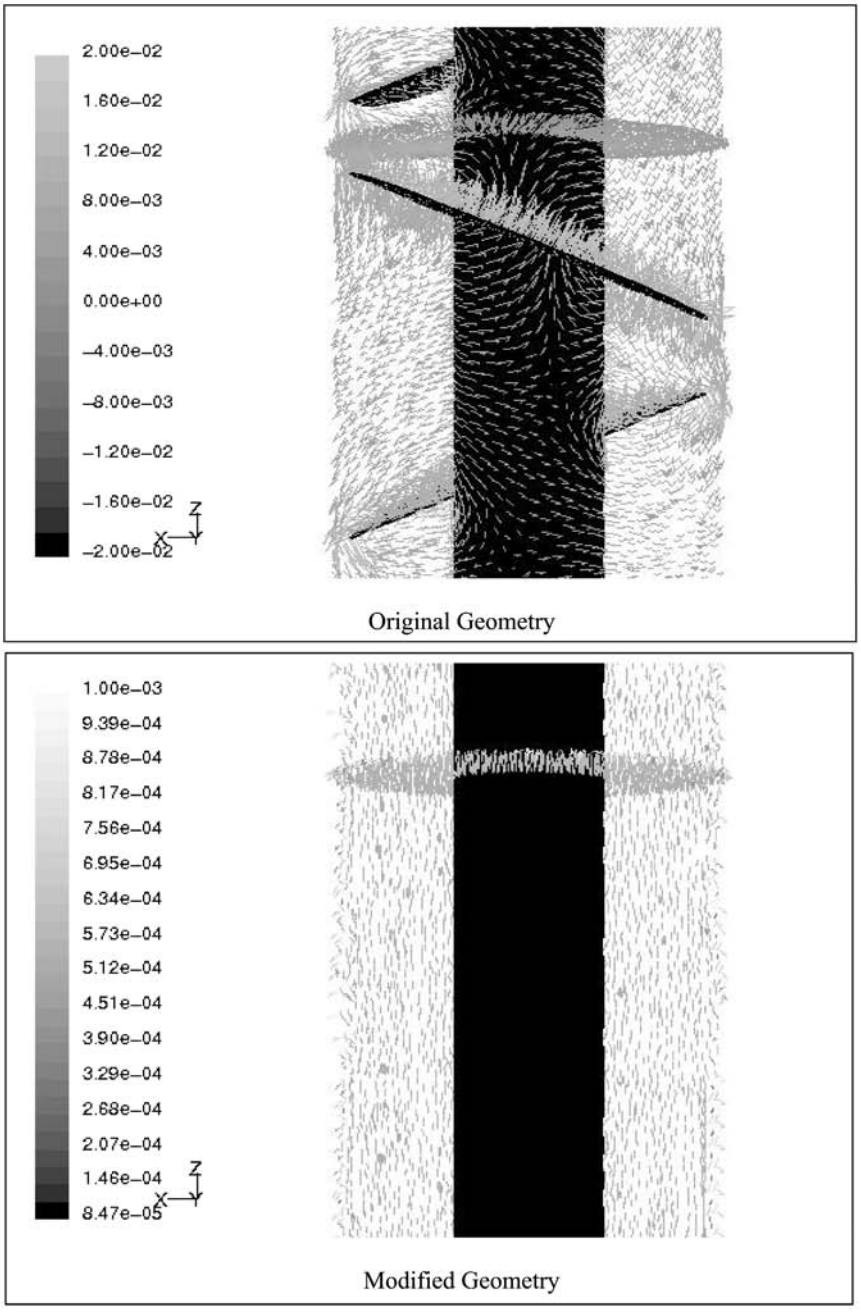

Fig. 4. Velocity vectors in a vertical mixing plane.

The loss of unreacted acid through the solids exit port at the top of the reactor is of concern because acid enters the system near the top. Backflow of acid, i.e., flow in the positive *z*-direction, appears to be slightly greater in the plug flow system. Figure 6 shows velocity contours only for regions where flow has positive values in the *z*-direction. The contours appear in the region

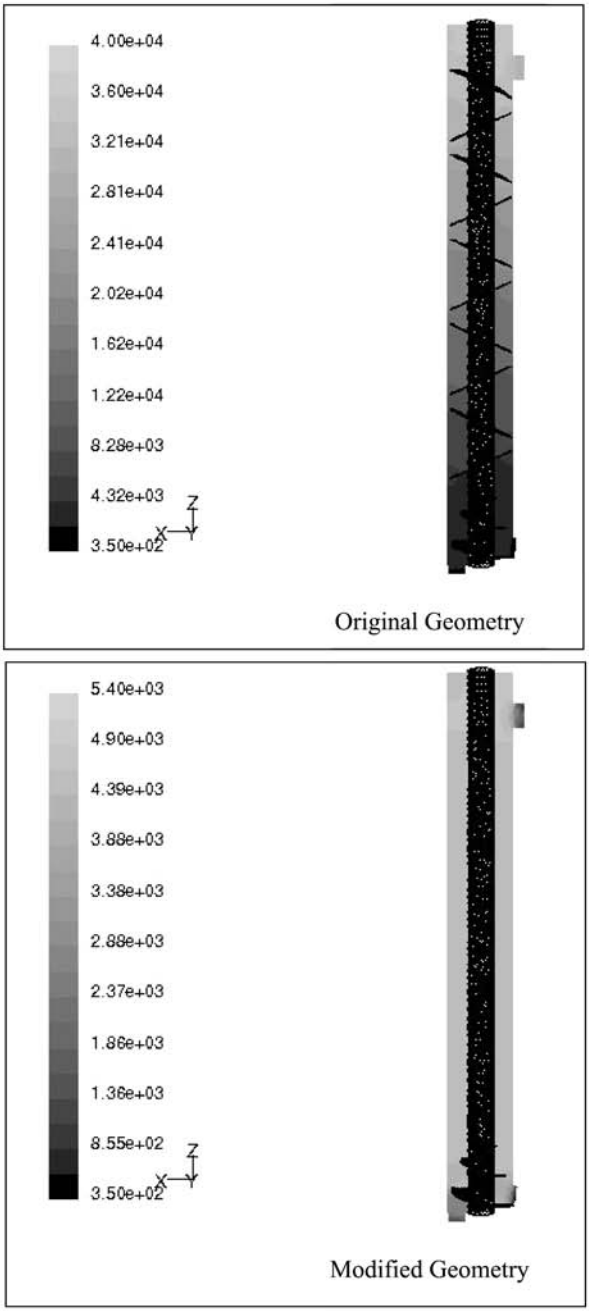

Fig. 5. Pressure distribution along axis of reactor.

above where the acid enters and near the bottom screw flights. The original screw reactor also exhibits very small regions around most of the upper screw flights. Although the plug flow creates more acid backflow, the regions where this occurs is small compared with the overall size of the reactor, and the velocity magnitude is small compared with the velocity of the entering acid.

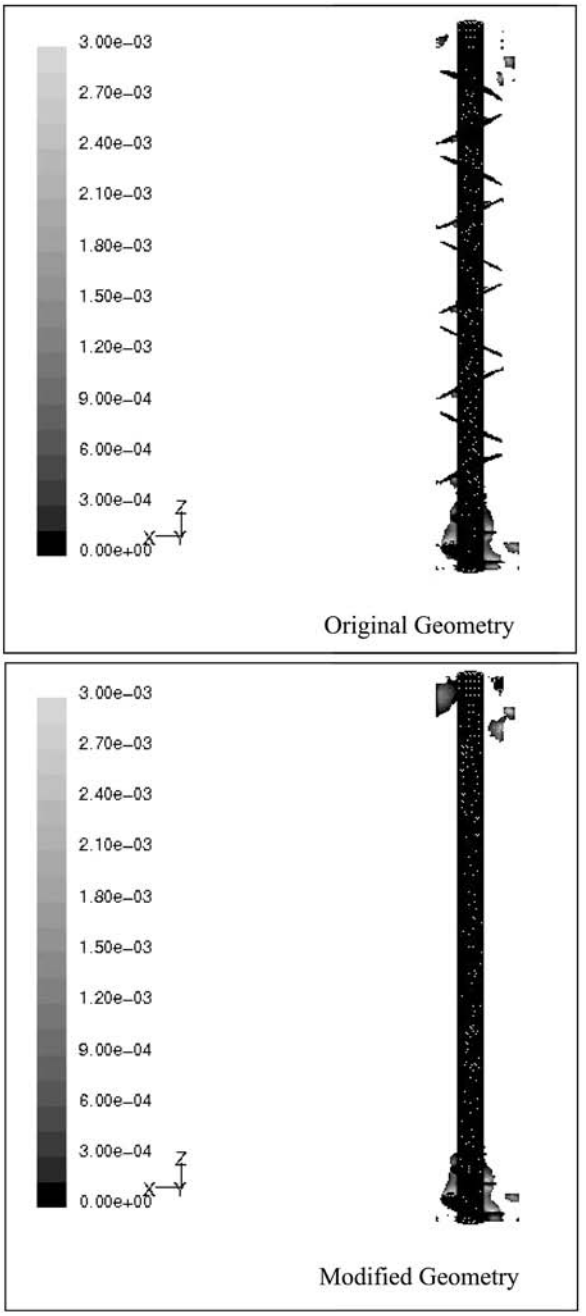

Fig. 6. Velocity contours showing regions of acid backflow (scale in meters/second).

Conclusion

Removal of the upper screw flights predicted the desired plug flow. The modified design predicted a lower pressure drop than the original design, 5 vs 40 kPa, and a more uniform pressure distribution. *Z*-velocity contours predicted that the plug flow will result in more backflow of acid above the acid entry point.

Nomenclature

C = inertial resistance coefficient (1/m)
D_p = particle diameter (m)
P = pressure (Pa)
S = source term to account for momentum losses owing to flow through packed-bed or porous region (Pa)
V = velocity (m/s)
α = permeability (m^2)
ε = void fraction
μ = molecular viscosity (kg/[m · s])
ρ = density (kg/m^3)

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