Simulation Of An Oxygen Delignification Reactor In The Kraft Pulp Production Process

D. do Mato Lara[1], J. da Luz Maeiski[1], I. Neitzel[1]
1. Department of chemical engineering, Faculdade de Telêmaco Borba - FATEB, Telêmaco Borba, PR, Brazil

Introduction

The process of delignification with oxygen is considered as the first part of the bleaching of the cellulosic pulp, acting as a bridge between the cooking process and bleaching process. Oxygen delignification occurs in alkaline medium in pressurized systems, aiming at the substantial removal of lignin present in the pulp.

Some models of oxygen delignification kinetics were created to improve the selectivity in this step, being possible to change the reagents of this process as well as to manipulate the control variables. The models created help in industrial optimization and simulation, improving product quality as well as economic feasibility [4].

The objective of this work is to analyze alternatives for optimization of the delignification process with oxygen, by means of simulation, in the aspect of operating conditions, as well as of the fluid dynamics of the reactor. The simulations were performed in 2D axisymmetric and 3D.

For the reactor, studies on fluid dynamics, and kinetic reaction models describing the oxygen delignification reactor were carried out.

Theory

The delignification reactor consists of an upflow pressurized vessel with a pulp distributor at the bottom and a pulp discharger at the top.

Oxygen delignification is the stage at which cellulosic pulp in an alkali solution, is pressurized with oxygen and steam, and then fed into the reactor. The oxygen reacts with the lignin until it is dissolved and then can be removed from the pulp with the alkali solution.

Oxygen delignification is used to remove approximately 50% of the lignin present in the brown pulp and one of the advantages of this process is the savings in chemicals used in the following stages of bleaching.

Oxygen delignification in virtually all new systems uses medium consistency technology (8-12% pulp mass in aqueous suspension) because of the lower cost of capital.

The delignification process is initiated by washing the cellulosic pulp in a washer filter, then the cellulose is discharged into a discharge tank, where the active alkali solution is added. In the vapor line the addition of the oxygen is carried out so that they are injected in the pulp through a dynamic mixer. The mixture then proceeds to the upflow oxygen delignification reactor. The oxygen, in alkaline medium, forms a gas dispersion stable in the pulp, and is consumed in the reactions with the lignin.

It is necessary to control and manipulate the variables that affect this stage, such as temperature, retention time, concentration and pH.

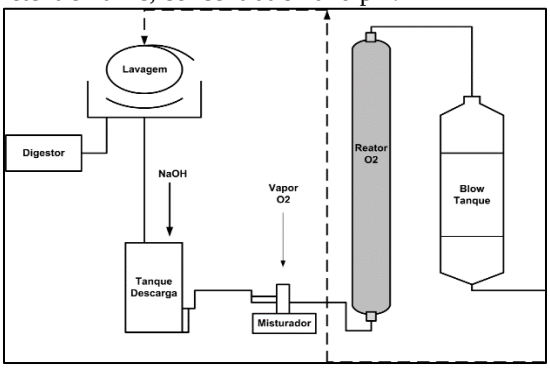

Figure 1. Schematic representation of the delignification process.

The oxygen delignification performance is monitored by measuring the kappa number of the pulp. This value is an indirect measure of the lignin content present in the pulp, being thus an estimator of the demand of reagents for the processes of delignification and bleaching.

Experimental Set-up

The simulations were structured as follows:

- Transport of diluted species (tds) – stationary;
- Turbulent flow, k-ε (spf) – stationary;
- Particle tracing for fluid flow (fpt) – Time dependent;
- Flow coupling 1 (fc1).

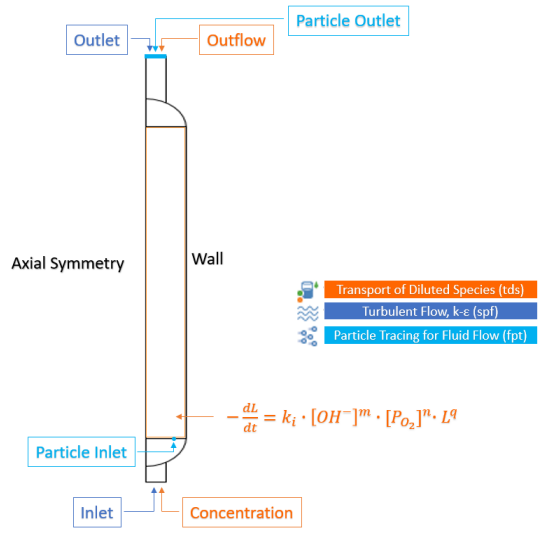

Figure 2. Boundary Conditions of the 2D-Axissymmetric study.

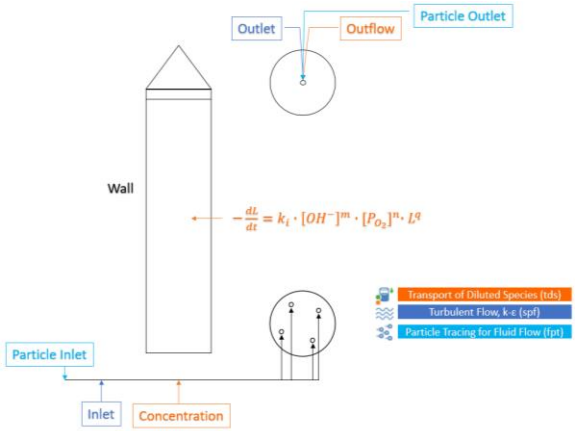

Figure 3. Boundary Conditions of the 3D study.

The transport of diluted species interface, found under the Chemical Species Transport branch, is used to calculate the concentration field of a dilute solute in a solvent.

The reaction node found under the transport of diluted species interface, is used to account the consumption or production of species through chemical reactions. The model of Jafari [2] was used for modeling the kinetics of the delignification reactions.

$$-\frac{dL}{dt} = k_1 . \left[OH^-\right]^m \cdot \left[P_{O2}\right]^n . L^q$$

$$k_1 = A_q . \exp\left(\frac{-E_A}{RT}\right)$$

For the simulation of carbohydrate degradation, the model proposed by Susilo [3] was used, where viscosity loss is used to describe the extent of carbohydrate degradation.

The kinetic equation used by Susilo [3] is as follows:

$$\frac{dm_n}{dt} = k_c \cdot \left[O_2\right]^m \cdot \left[OH^-\right]^n \cdot m_n^q$$

mn = No. of cellulose molecules, mol / ton of pulp.

$$k_c = A.\exp\left(\frac{-E_A}{RT}\right)$$

where A is the frequency factor, EA is the activation energy of Arrhenius (kJ / mol), R is the universal gas constant (kJ / mol.K) and T is the temperature (K).

The turbulent flow, k-ε (spf) interface is used for simulating single-phase flows at high Reynolds numbers. The equations solved by the Turbulent flow, k-ε interface are the Reynolds-averaged Navier-Stokes (RANS) equations for conservation of momentum and the continuity equation for conservation of mass. Turbulent effects are modeled using the standard two-equations k-ε model with realizability constraints. The flow near walls is modeled using wall functions.

The particle tracing for fluid flow (fpt) interface, is used to compute the motion of particles in a background fluid. For the determination of the residence time, 100 particles were introduced in the lower part of the reactor where the entrance orifice of the pulp is located, being possible to observe the trajectory of these particles over time and also the residence time of each one of them.

The flow coupling under the Multiphysics node defines u and p variables in order to set the model inputs in the chemical species transport interface, this interface is used for coupling the transport of diluted species and the turbulent flow, k-ε interface.

The mesh created for the 2D reactor was the free triangular, being refined sequentially to obtain different degrees of refinement.

The 3D simulations used a free tetrahedral mesh.

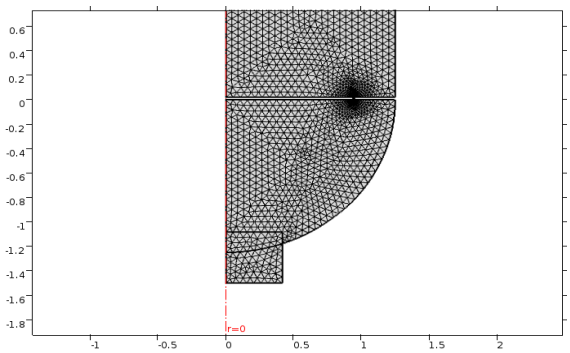

Figure 4. Free triangular mesh for 2D-Axissymmetric simulation.

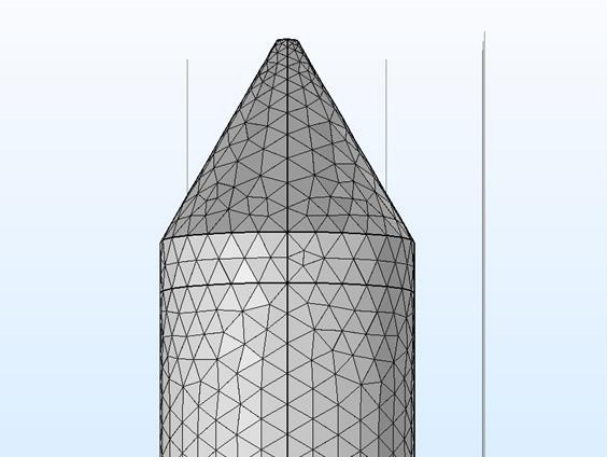

Figure 5. Free tetrahedral mesh representation in the top of the reactor.

Simulation Results

2D simulation

For the computed fluid flow analysis of the reactor, two forms of representation of the flow were used for better understanding: in the first, particles were launched at the entrance of the reactor to determine the residence time along the reactor, being possible to determine if the flow is ideal or non-ideal. Also, streamlines are shown along the reactor showing the most recirculation sites and preferred paths. The streamlines are complemented by the vectors related to the local velocity, indicating the direction of flow of the pulp inside the reactor.

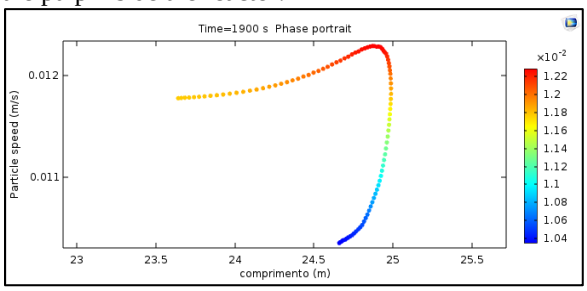

Figure 6. Trajectory of the particles along the reactor.

From the result obtained in figure 6 it is possible to observe that the trajectory of each particle inside the reactor has different velocity and position. When the particles are released, some run through the reactor at a faster rate than the others. This behavior of the particle trajectory was already expected because fluid elements travel through different paths in the reactor and can spend different times as they travel through the control volume.

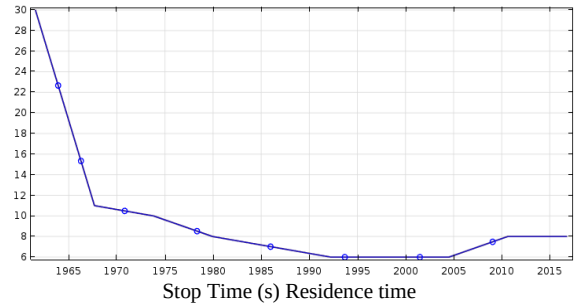

Figure 7. Residence time of the particles in the reactor.

Figure 7 shows the residence time of the particles in the reactor, from the result it is noticed that each particle moves differently, some remain longer in the reactor and others less time, with this it is possible to characterize that the flow is non-ideal because each particle travels through the reactor at different time and speed. This behavior directly affects the chemical reaction because some molecules will have a longer reaction time and others will have shorter, that is, there will be regions where the reaction will not happen completely causing a loss of efficiency in the oxygen delignification step.

These deviations from ideality cause in the reactor the formation of preferential paths, the recycling of fluid and the appearance of stagnant regions in the reactor.

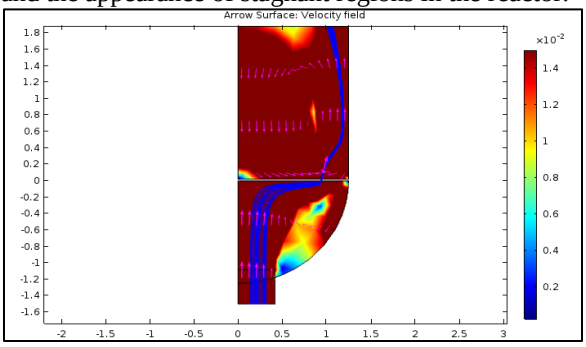

Figure 8. Inlet flow pattern of the reactor.

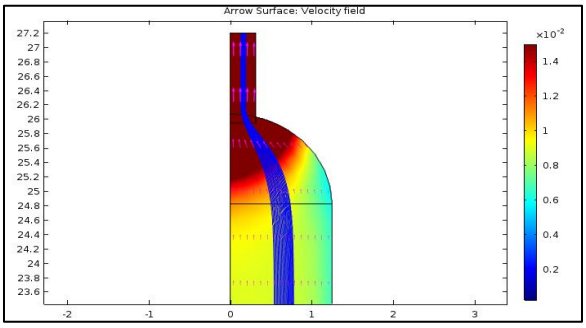

Figure 9. Outflow pattern of the reactor.

The simulation carried out shows the presence of preferential paths in the reactor and also of stagnant zones, bringing many problems related to the flow of the pulp, one of them is the lack of recirculation which shows that the mixture is inefficient and this is a big problem for the operation of the reactor because an inefficient mixing of the cellulosic pulp can lead to a high consumption of chemicals, low brightness and degradation of the pulp.
One option for improving recirculation in the reactor would be to insert more holes to make the pulp inlet distribution more uniform., this would cause a larger mixing and would decrease the stagnant regions and consequently the preferred paths.
For the simulation of the kinetic model, the reactor operating parameters were estimated to represent the process of delignification with oxygen. The variables used in the model input are kappa number at the reactor inlet, oxygen pressure, alkali flow rate, reaction temperature, retention time, average pulp consistency of 10% and viscosity.

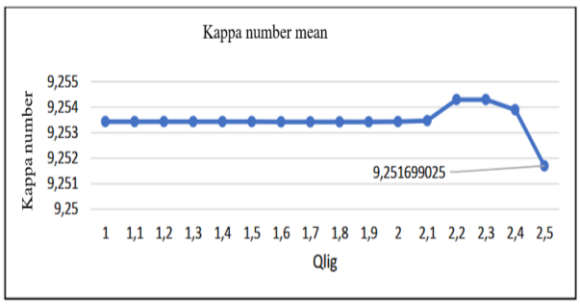

Figure 10. Kappa number in the reactor outlet.

To obtain the kappa number at the exit of the reactor, the mean input kappa of 18.79 was specified. In Figure 10 it is observed that a convergence occurs to a value of the average kappa number at the output of the reactor of approximately 9.2516, the values found in the 2D simulation are within the expected, since the reduction of the kappa number should be approximately 50% of the kappa and this is observed because the output kappa had a difference of 9.54 in relation to the input kappa. It must also be considered that the initial value of the input kappa number is an average value and does not necessarily express the modeled reality.

3D simulation

3D simulations were performed to evaluate the behavior of the implemented model and the geometry of the reactor.
From the model of Jafari [2], the simulation could predict the kappa number along the reactor.

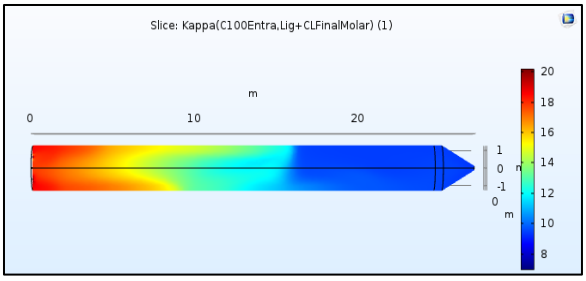

Figure 11. Kappa number analysis.

It may be noted that at the beginning of the simulation the kappa is approximately 18.79 and over time along the reactor the kappa decreases and converges to approximately 9.49 obtaining a difference of 9.3 from the initial kappa. Comparing the result obtained in the 2D simulation with 3D, the kappa number found in the 3D simulation is also within the specifications, since the reduction of the kappa number should be approximately 50% of the input kappa and this behavior can be observed in the 3D simulation, thus validating the model and the simulation.
In the model implemented by Jafari [2] it is necessary to be aware of the alkali consumption inside the reactor, with the proposed new model it is necessary only to know the initial charge of sodium hydroxide, being possible to determine the maximum kappa and minimum kappa as a function of added alkali charge.
The kappa number is a function of the alkali charge, if the charge is large and the reactor long enough the kappa has a rapid decrease, and if the reactor is small this does not happen.
The simplified Jafari model [2] is simpler and perfectly coherent and justified with the conception of the reaction.

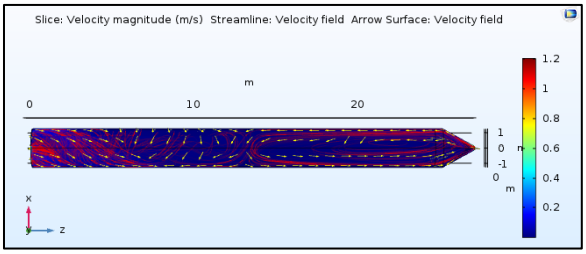

Figure 12. Velocity field in the 3D reactor.

With the results obtained by the 3D simulation the recirculation improved compared to 2D simulation, the streamlines show a greater recirculation along the reactor decreasing the preferential paths, the vectors indicate the direction of flow of the pulp. The velocity is slightly higher at the inlet of the pulp and this is due to adding more inlet holes, but along the reactor the velocity stays virtually constant.

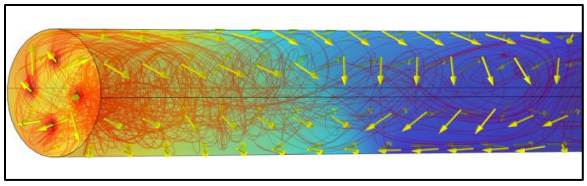

Figure 13. Velocity field in the 3D reactor.

From Figure 13 the recirculation in the lower part of the reactor is more visible, when inserting more holes, the recirculation had a significant improvement. The implementation of the 3D geometry allowed to analyze an improvement in the fluid dynamics of the reactor.

Conclusions

The residence time of the particles in the reactor showed that the flow is non-ideal, which causes problems in reactor efficiency, such as preferred paths and stagnant regions.
In the 2D simulation, there were three main zones inside the reactor, which showed a larger recirculation at the bottom near the distributor, while in the reactor length there is a rising current without significant mixing, and recirculation zones in the top of the reactor.
In the 3D simulation it is possible to analyze an improvement in the recirculation along the reactor, this is due to the holes that were added to the bottom of the reactor for distributing the pulp.
The values found in the simulation are within the expected range, as the delignification should be approximately 50% of the input value and this is observed since the output delignification value had a difference of 9.54 in comparison to the 18.79 value in the input, proving the efficiency of the model for the simulation performed.

References

1. COLODETTE, J.L.; GOMES, F.J.B. Branqueamento da polpa celulósica: da produção de polpa marrom ao produto acabado, Viçosa, MG, p.816, 2015.

2. JAFARI, Vahid et al. Delignification and cellulose degradation kinetics models for high lignin content softwood Kraft pulp during flow-through oxygen delignification Cellulose, v. 22, n. 3, p. 2055-2066, 2015.

3. SUSILO, Jacky. Modelling oxygen delignification in pulp processing operations. 2002. Tese de Doutorado. University of British Columbia.

4. VIANNA, Viridiane. Modelagem e simulação do processo industrial de deslignificação com oxigênio e de branqueamento ECF de polpa celulósica. 2009.

5. VIOLETTE, Steven M. Oxygen delignification kinetics and selectivity improvement. 2003.