CFD ANALYSIS OF A POLYBUTENE REACTOR TO DIAGNOSE CAUSES OF POLYMER ADHESION AT INNER WALLS

D. RAMAJO‡, M. RAVICULÉ‡, G. HOROWITZ‡, M. STORTI† and N. NIGRO‡

† International Center for Computational Methods in Engineering (CIMEC). INTEC-UNL-CONICET, Güemes 3450, Santa Fe, Argentina dramajo@ceride.gov.ar
‡ Centro de Tecnología Argentina (CTA), Repsol-YPF, Baradero s/nro. 1925, Ensenada, Argentina mravicules@repsolypf.com

Abstract— In this work the flow patterns inside a polybutene reactor were studied by CFD (Computational Fluid Dynamics) using finite elements. Research was carried out with the aim to find possible causes of excessive adhesion of polymer and catalyst particles at the reactor inner walls. The multi-fluid formulation for a three-phase system formed by liquid reactor mixture, solid catalyst particles and small gas bubbles generated during polymerization reaction, was applied. Deposition of solid particles and a non-homogeneous flow distribution over the lower reactor walls occurred. Based on the hypothesis that adhesion phenomena are related to a combination of catalyst-particle precipitation at walls and locally low shear stresses, several operative and constructive modifications were proposed in order to reduce this phenomenon.

Keywords— polybutene reactor, CFD, adhesion.

I. INTRODUCTION

Polybutenes are manufactured from C4 olefin refinery streams of fluidized catalytic cracking involving positively charged active centers at the growing chain end (Matyjaszewski, 1996).

The feed stock to the polymerization reactor is composed of about 15%-45% isobutene, 15%-25% 1-butene, 10%-20% 2-butenes, 3%-40% isobutane, 10%-15% n-butane. The presence of normal butenes in the raw material has an important role in the determination of the molecular weight of the polymer. These compounds accelerate the termination and charge transfer rate of the polymerization, limiting the molecular weight of the product (Kennedy 1975).

The polybutene reactor under study is a tri-phase vessel. The solubility of AlCl₃ in the reaction mixture is low, which originates the presence of solid particles in the reactor. The heat of reaction is partially dissipated by ebullition of the reaction mixture generating the gas bubbles. A more detailed description of the process can be found in Kennedy and Marechal (1991).

Polymerization takes place around catalyst particles; if reactions occur close to the reactor walls, catalyst particles surrounded by polymer may stick forming large clusters of deposits. Observations in an optical-access experimental vessel operating at production conditions showed that interrupting agitation by a mechanical stirrer almost immediately caused firmly adhered clusters to appear at the bottom wall. The fact that deposits appear mainly at the bottom wall of the vessel seems to uphold the assumption that decantation of polymer and catalyst particles is related to adhesion phenomena. Once deposits are formed they are very difficult to remove, thus reducing the operative capacity of the reactor. The adhesion process is continuous and deposits can only be removed by chemical or mechanical techniques. In the reactor under study, the rate of adhesion was fast enough to significantly reduce the overall reactor volume after a few years. This fact forces the plant to stop frequently in order to get the reactor walls cleaned, with the consequent high economical impact.

The reactor analyzed does not have an impeller and its charge is only mixed by continuous recirculation forced by pumping the charge from the reactor outlet located upwards to the reactor entrance at the bottom.

In order to gain some insight about the performance of this equipment it is advisable to know how the feed flows inside the reactor, determining residence times, local shear stresses and catalyst particle concentration among others. Such information data should provide a possible scenario of polymer adhesion.

In this work a finite element CFD analysis of the flow patterns inside the reactor is presented. Based on these computational results feasible operative and constructive modifications are proposed, established on the assumption that adhesion phenomena are closely related to a combination of polymer and catalyst particle deposition (precipitation) and low enough wall shear stress. For simplicity in this study the in-reactor polymer distribution is not taken into account due to the complexity of incorporating polymerization-reaction rates and multi-component flow formulations. Catalyst-particle density is larger than that in the polymer one so a priori decantation velocity for the catalyst will be faster. For these reasons, in the present work only catalyst particle decantation and wall shear efforts are associated with the adhesion problem. Probably in a future work more details about the polymer role may be included.

CFD results are nowadays being used as a very useful design tool for general engineering applications. Yet,
in the reactor design area this technology has not been massively employed. Concerning adhesion problems of polymerization reactors, so far, and to the best of our knowledge, no contribution exists in the literature that proposes CFD to address this problem. This paper would then constitute a first attempt to apply this methodology to aid the designer to understand how to improve the process productivity.

II. METHODS
A. Problem definition. Constructive and operative features

The polybutene reactor (PIB) is a cylindrical vessel with a total height of 9.5 m, a diameter of 3.3 m and an approximate volume of 60 m$^3$. In Fig. 1 the main constructive data of the reactor are shown. Fig. 1 also shows the dimensions and locations of the inlet and outlet ducts. The sharp curvature change of the inlet duct located at the bottom of the vessel is remarkable.

The reactor is built with a carbon steel vessel and it has a thermal insulation on its outer side. The reactor has no mechanical impeller, so in order to enhance the reaction process the whole charge is continuously recirculated. During the catalytic reaction the isobutylene is polymerized producing polymers of different molecular weights depending on process temperature, catalyst concentration and reaction mixture composition. These parameters are very strictly controlled in the industrial process in order to guarantee the grade of the output product.

Figure 2 is part of a flow sheet and it is useful to clarify the main fluxes involved in the process. Recirculation is done by pumping the charge from Outlet A to Inlet A at the bottom. At the same time, a vapor stream is collected through Outlet B at the top of the PIB reactor and the liquid charge, formed by the polymer diluted in the C$_4$ mixture, is extracted through two small ducts at Outlet C. Small quantities of catalyst are drifted through Outlet C. Therefore, both compounds (catalyst and C$_4$) must be made up for through an auxiliary Inlet B.

As it is sketched in Fig. 2 three phases are present; polymer diluted in C$_4$ (liquid phase), small vapor bubbles (gaseous phase) and small catalyst particles (solid phase). C$_4$ vapor bubbles are generated by the exothermic polymerization reaction consuming isobutylene. Due to the necessity to control polymer molecular weight, the temperature and pressure conditions should be strictly controlled. They may vary from -1°C and 1.21 atm to 25°C and 3 atm depending on the product specifications, but once the product grade is specified these parameters are kept almost constant. Besides, an average catalyst concentration of 0.3 kg per m$^3$ of reaction mixture is required in order to perform the polymerization process.

In table 1 the rheological properties of the different phases involved are listed for numerical simulation purposes. These values are representative of those found in the industrial operation according to the grade being produced, and need no further adjustments. Since over all operation temperature needs to be kept almost constant, the reactor works in a steady boiling condition. Since the mixing is very strong (most of the charge is steadily recirculated) the temperature control is very efficient guaranteeing a fixed temperature. So an isothermal hypothesis is adopted for modeling the process and only the transport properties of the different phases are solved.

Catalyst particle sizes vary from less than 50 microns (20% of the total amount of particles) to more than 500 microns (6% of the total particle inventory). But particle size distribution can be roughly divided in two groups: the first one containing particles of 65 microns and the second one comprising particles of around 140 microns, corresponding to 34% and 35% of the total particle inventory respectively. These values were taken from the overall particle size distribution provided by measurements done in CTA laboratory.

Particle size has a remarkable influence on drag forces. Smaller particles are more easily drifted by the mean flow than larger ones. Considering that the computational cost is strongly increased with the number of different sizes being simulated, a unique particle size

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**Table 1: Rheological properties of different phases**

<table>
<thead>
<tr>
<th>Phase</th>
<th>Density (kg/m$^3$)</th>
<th>Viscosity (Pa·s)</th>
<th>Dynamic viscosity (Pa·s)</th>
<th>Plastic viscosity (Pa·s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
<td>700</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Gas</td>
<td>1.21</td>
<td>0.01</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Solid</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
<td>1000</td>
</tr>
</tbody>
</table>

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Fig. 1. x-y view of the PIB reactor. Main dimensions.

Fig. 2. Layout of part of the process.
was chosen. Taking into account that the larger the size the stronger the precipitation, the second particle group was chosen.

As regard the gaseous phase, it is generated during the polymerization reaction in the vicinity of catalyst particles. As it was observed in an experimental reactor with optical access, the reaction produces small bubbles of C_4 of about 1 to 2 mm, which move upward reaching the free surface.

Table 1. Rheological properties of the three phases. (a) Ref to 292.3K and 1.1 atm. (b) Ref to 258K and 1 atm. (c) Ref to 253K and 1 atm.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Liquid</th>
<th>Gas</th>
<th>Solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Denomination</td>
<td>reaction mixture</td>
<td>vapor</td>
<td>aluminum trichloride</td>
</tr>
<tr>
<td>Assumed shape</td>
<td>continuous</td>
<td>Continuous/bubbles</td>
<td>Spheres</td>
</tr>
<tr>
<td>for modeling</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Characteristic</td>
<td></td>
<td>1 mm to 2 mm</td>
<td>50 μ to 140 μ</td>
</tr>
<tr>
<td>size</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density (kg/m^3)</td>
<td>690^{(A)}</td>
<td>3.15^{(A)}</td>
<td>2440</td>
</tr>
<tr>
<td>Viscosity</td>
<td>2.070^{(B)}</td>
<td>1.64^{(C)}</td>
<td>--</td>
</tr>
</tbody>
</table>

In order to characterize the transport properties of the charge a sample was extracted from the reactor during normal operation. The kinematic viscosity μ_{kh} and the density ρ_{kh} of the charge were measured experimentally (see table 1) for two temperatures (representative of two different oil grades) and the corresponding values for the different process temperatures were estimated by logarithmical extrapolation using the following expression:

\[ \mu = \frac{\rho}{1000} [a \ln(T) + b] \]  \hspace{1cm} (1)

being \( a \) and \( b \) obtained by fitting as -8.96 and 51.84 respectively. It is necessary to point out that transport properties reported for liquid phase in table 1 correspond to measurements of the charge, that means C_4 + polymer + catalyst particles.

B. Mathematical model

The unsteady multi-fluid formulation was employed for our simulation. As it is well known from the theory in this formulation single phase Navier-Stokes equations are modified according to some sort of regularization or average to model the small scales, introducing the volume fraction of each phase along with appropriate terms to model the turbulence effects. This eddy viscosity model is defined as:

\[ \nu_{\text{eff}} = \frac{1}{2} \left( \nabla \cdot \mathbf{U}_{\text{RM}} + \nabla \cdot \mathbf{U}_{\text{RM}}^\tau \right) \]  \hspace{1cm} (4)

being \( \nu_{\text{eff}} \) the effective dynamic viscosity of the reaction mixture. This means that the molecular dynamic viscosity is modified by the turbulence contribution. Large eddy simulation LES with a simple Smagorinsky model (Smagorsinsky, 1963; Wilcox, 1998) is employed to model the turbulence effects. This eddy viscosity model is defined as:

\[ \nu_{\text{RM}} = \rho_{\text{RM}} \nu_{\text{eff}} \]  \hspace{1cm} (5)

with \( \nu_{\text{RM}} \) being the reaction mixture density, \( C_S = 0.18 \) the Smagorsinsky constant, \( \mathbf{h} \) the spatial discretization size, \( D \) a Van-Driest damping factor to correct the influence of the wall proximity and \( \varepsilon \) the deformation rate tensor.

Focusing on the computational modeling of the three-phase charge, this is composed by the reaction mixture (continuous liquid fluid), vapor bubbles (dis-
perse fluid bubbles) and the catalyst (disperse solid particles). As it is usual in multifluid theory when low disperse volume fractions are involved, the interaction among the disperse phases may be neglected. In our case this hypothesis (very low volume fractions for the disperse phases) was confirmed by simulation and by the operative conditions.

Even though the generation of C\textsubscript{4} bubbles is physically due to the phase change produced by the reaction heat (\(\Gamma_{S,\text{ad}}\neq 0\)), the lack of information of the associated momentum terms \(\Gamma_{M,\text{ad}}\) of the phase change suggests that the mass generation during the phase change may be better introduced through the \(S_{\text{b}}\) term in Eq. (1), assuming that \(\Gamma_{S,\text{ad}}=0\).

According to the mass conservation principle the following constraint is added \(S_{\text{SM}}^c = S_{\text{bubble}}\).

The generation of C\textsubscript{4} bubbles in the simulation is controlled in such a way that the net flue gas through Outlet B equals the value obtained during the industrial process. For such a control law the following equation is used

\[
S_{\text{bubble}}(x) = \frac{\varphi_{\text{OB}}}{V_{\text{CH}}} \frac{\delta_{\text{cat}}}{\delta_{\text{cat}}^0} \tag{6}
\]

In Eq. (6) \(\varphi_{\text{OB}}\) is the instrumentation value of the net flue gas at the exit from the industrial process, \(V_{\text{CH}}\) is the charge volume in the reactor, with \(\delta_{\text{cat}}\) and \(\delta_{\text{cat}}^0\) the local and the averaged catalyst volume fractions respectively.

Using Eq. (6) in Eq. (2) causes the bubbles to be transported at their own velocity, which produces a strong stirring effect on the liquid phase and indirectly forces the catalyst particles through the continuous phase.

For the momentum equation, momentum transfer due to phase change was neglected (\(\Gamma_{M,\text{ad}}=0\)) and interface forces \(\Gamma_{M,\text{ad}}\) were only provided by drag forces. Because of the low volume fractions of both disperse phases, the solid particles and the vapor bubbles, the Schiller-Naumann model was chosen to estimate the drag coefficient \(C_D\). This was expressed as a function of the particle Reynolds number \(R_e_p\), as:

\[
C_D = \begin{cases} 
\frac{24}{R_e_p}(1+0.15R_e_p^{0.8}) & \text{if } R_e_p \leq 1000 \\
0.44 & \text{if } 1000 < R_e_p < 2 \times 10^5 
\end{cases} \tag{7}
\]

Therefore twelve partial differential equations compose the whole system, three of them for the mass conservation equations of each phase and the other nine for the corresponding momentum conservation equations.

C. Numerical formulation

The mathematical model defined by Eq. (2)-(7) is discretized by stabilized finite elements according to the following formulation. Let the functional spaces be:

\[
S_{\text{c}}^h = \left\{ v^h \mid v^h \in H^1_{\Omega_{\text{ad}}}, v^h \equiv v^h_{\text{b}} \text{ in } \Gamma_D \right\}
\]

\[
S_p^h = \left\{ q^h \mid q^h \in H^1 \right\}
\]

\[
S_{\text{b}}^h = \left\{ p^h \mid p^h \in H^1_{\Omega_{\text{ad}}} \right\}
\]

\[
V_v^h = \left\{ v^h \in H^1_{\Omega_{\text{ad}}} \right\}, \quad V_p^h = \left\{ \phi^h \in H^1_{\Omega_{\text{ad}}} \right\}
\]

\[
V_{\text{b}} = \left\{ N^h \in \left( H^1_{\Omega_{\text{ad}}} \right) \right\}, \quad N^h = 0 \text{ in } \Gamma_D
\]

\[
(8)
\]

\[
S_{\text{bubble}}(x) = -S_{\text{bubble}}(x).
\]

D. Computational model

In order to gain some insight into the role of the free surface located between the charge and the continuous C\textsubscript{4} gas phase existing in the upper part of the reactor, an initial simulation was done using the overall reactor geometry (see Fig. 1). These preliminary results showed that the free surface had a negligible motion. Hence for the following simulations only a fraction of the reactor above the normal operation level of the charge (around 0.4 m) was taken into account, reducing the mesh size by 20%. Regarding the spatial discretization, the computational domain was partitioned in 200,716 tetrahedrons and a local refinement was employed around inlet and outlet ducts. Due to the overall small temperature variations detected in the industrial operation and the fact that the process works in an steady boiling condition promoted by the chemical reaction between the catalyst and the charge, the problem was considered as isothermal. Hence, simulations were performed at two
operation temperatures corresponding to the operation extreme conditions of -1°C (with 1.21 atm) and 25°C (with 3 atm) respectively, considering the appropriate reaction mixture viscosities for each case (taken from Eq. (1)).

Regarding the time integration a first order backward Euler scheme was applied. For each analyzed case a time interval of 200 seconds with a constant time step of 0.01 seconds was simulated. The problem was solved using distributed computing facilities over several processors in a Beowulf cluster (Storti et al., 2007; Sonzogni et al., 2002). Each simulation (approximately 20,000 time steps) demanded around 5 days running over 10 processors.

Boundary conditions: Fully developed velocities were imposed on Inlet A, Outlet A and Outlet B while a constant pressure equal to the reactor operation pressure was employed at Outlet C. In order to model the recirculation of the charge from Outlet A to Inlet A the volume fraction for each phase at Inlet A was linked to the outgoing mass flow at Outlet A. Thus, both the instantaneous mass flow rate of each phase at Outlet A and the corresponding one from Inlet B (constant volume fractions of δ\text{cat} = 1.24x10^{-4}, δ\text{vapor} = 0 and δ\text{SL} = 0.999876) were added in order to estimate the composition of the entering flow. Moreover, mass flow rate at each boundary was monitored during the whole simulation time interval, guarantying the reactor global mass conservation and focusing the effort on fitting the bubble generation with the volumetric flow rate data at Outlet A. The velocity for each phase at the walls was fixed using the turbulence wall law.

E. Results and discussion

As it was above mentioned two operation conditions were simulated: one corresponding to a constant temperature of -1°C and a pressure of 1.21 atm (applied at the uppermost point of the reactor) and the other to 25°C and 3 atm. In the following paragraphs the results for the first operation condition are extensively discussed. As the problem is dominated by turbulence and this was modeled by LES the solution needs to be averaged to obtain a representative result for engineering purposes.

Once the solution verifies the global mass balance the average in time procedure may be started. Because of the assumptions made for this model only the transport phenomenon data for the various phases result relevant with no special consideration paid to the chemistry of the process. Therefore, only the role of the catalyst concentration at the reactor walls and the local wall-shear stresses are used as indicators for the adhesion phenomenon. Attending to these assumptions the catalyst volume fractions (CVF) along with the wall shear efforts (WSE) at cross-sectional mean planes and at reactor walls are displayed in Fig. 3.

Figure 3 contains six pictures; the first two are the CVF at reactor walls while the third and fourth are the CVF at two cut planes. Picture 3-a shows the influence of the inlet jet over the reactor conical wall. It should be noted how the portion of wall directly affected by the jet has a lower CVF but particle concentration quickly increases at the adjacent wall. This figure also shows the sweeping nature of the inlet jet. It may clearly be observed how the entrance flow jet has a strong tangential velocity component, sweeping the cone right-side and allowing the decantation of solid particles at the opposite-side wall. A particle volume fraction larger than the averaged one (1.24x10^{-4}) is visualized over most of the reactor conical wall, whereas a small part of this region that is directly affected by the entrance flow jet holds lower particle concentrations.

At the opposite wall (Fig. 3-b) high CVF is also found. Picture 3-c and 3-d show that particles are mainly concentrated over the reactor conical wall, while CVF diminishes into the reactor. It clearly evidences the particle-decantation problem. These pictures show the conical part of the reactor receiving the fluid flow from the entrance duct and how, due to its inclination of about sixty degrees, this part is prone to particle adhesion. Therefore, most of the attention will be given to this part of the reactor geometry.

Figures 3-e and 3-f display the wall shear efforts at the reactor walls. Maximum WSE values are located at the wall directly affected by the inlet jet, but they quickly diminish at the jet adjacent wall.

In Fig. 4 the velocity field for the liquid phase is plotted at two cut planes. Velocity magnitude appears larger at the x-y plane. The inlet jet promotes a big vortex structure rotating at the z axis. Several small vortices are also identified at the y-z plane.

In Fig. 5 both CVF and WSE values over the conical reactor walls are presented at three different simulation times. The animation of the simulation results allows to see how the entrance jet comes into the reactor sweeping a fraction of the conical wall within a period of around 30 secs. Results in Fig. 5 show that decantation...
Fig. 4. Velocity field of liquid phase at two cut planes. Left: plane x-y. Right: plane y-z.


of solid particles over the reactor cone walls increases catalyst concentration to above 3 times the averaged concentration. Lower catalyst concentrations are found at the entrance-jet core, while regions with volume fractions greater than $4 \times 10^{-4}$ are located in the vicinity. These results showed a repeated behavior of the flow jet as a wandering. This fact motivated that results were time averaged along a time period of 140 seconds in order to capture the mean-flow characteristics. Due to this, more than 150 mesh sampling points were selected over the reactor cone wall and 140 solutions at different times were considered. In Fig. 6 the minimum, maximum and time-averaged values for CVF and WSE at two radial distances from the flow-entrance location are drawn (see sketch in Fig. 9 for radial coordinate definition). Polar diagrams in Fig. 6 underline the zone directly influenced by the entrance flow. The increment in CVF on the opposite-side conical wall is also evidenced. As it can be seen, close to the entrance (radius $r = 0.25$ m) CVF reaches $6 \times 10^{-4}$ on the left-half conical wall while minimum values are around $4 \times 10^{-4}$. Close to the entrance location WSE exceeds 6 Pa in the direction aligned with the jet (0 degrees at polar diagram) but it quickly diminishes along the radial coordinate. Both CVF and WSE become more homogeneous as radius grows. Furthermore, maximum CVF decreases, although the averaged one holds close to $4 \times 10^{-4}$. WSE quickly diminishes radially far away from the entrance and its magnitude hardly ever exceeds 1 Pa at radius larger than 1.42 m.

By changing the temperature operation conditions from -1°C to 25°C the reaction mixture viscosity was reduced from 1.112 to 0.547 centistokes. Viscosity reduction directly affects wall shear efforts as well as drag forces, lessening both of them. This, in turn, increases decantation over the conical reactor walls indicating that higher operation temperatures would promote higher adhesion rates.

Fig. 6. Reactor conical wall. Maximum (solid black line), minimum (dotted-dashed black line) and averaged (solid gray line) values for catalyst volume fraction (CVF) and wall shear efforts (WSE) at different radius.

F. Eventual modifications studied

Three operative and constructive modifications are discussed and they are assessed in terms of particle decantation reductions and wall shear stress increments.

First case: an increased recirculation mass flow. This is defined in terms of an increment of the recirculation flow from 300 to 400 m$^3$/h, keeping the original geometry. In this case flow-pattern results are similar to those found for the lower recirculation mass flow. This means that the entering flow jet comes into the reactor producing a non-homogeneous flow distribution over the reactor conical wall similar to the original configuration. Fig. 7 draws the maximum (roof limit) and minimum (floor limit) values of CVF and WSE at different radius. In Fig. 7 $Min\ roof$ refers to the maximum value (upper limit) of the minimum CVF while $Min\ floor$ refers to the minimum
one (bottom limit). This means that any minimum CVF value (for any angle at the polar diagram) is bounded by Min floor and Min roof curves. As it can be noted, minimum CVF values are reduced as recirculation mass flow increases. On the other hand, maximum CVF values do not show any significant variation for both analyzed mass flows. Fig. 8 displays the same analysis for WSE. Minimum and maximum WSE quickly fall along the radius. An increased recirculation of the mass flow rate did not produce significant differences in floor limits for maximum and minimum WSE values. As regard the roof limit of minimum WSE, it is strongly increased near the entrance but differences become negligible beyond radii of about 0.7 m.

However, significant increments are found for the roof-limit of maximum WSE at all radii.

In short: Fig. 7 and 8 show that recirculation-flow enlargement has a positive effect on both CVF and WSE. Nevertheless, since the entrance flow keeps strongly channeled over a reduced fraction of the overall reactor conical wall, the inlet elbow must be modified in order to promote the angular homogenization of the entrance flow. In the next analyzed case, the inlet elbow is removed and a rhomboidal deflector is incorporated inside the reactor in order to get a more homogeneous distribution of the entering flow over the reactor conical wall.

Second case: removal of the inlet elbow and incorporation of an inner deflector. Figure 9 shows the constructive modifications implemented around the flow-entrance zone. The inlet elbow was replaced by a straight duct. In addition, a solid rhomboidal deflector with a total height of 0.7 m was incorporated. The rhomboidal deflector was located as close as possible to the reactor conical wall to avoid obstructions during the reactor normal operation taking into account the possibility that clusters of particles obstruct the entrance zone. Two positions for the deflector were considered, the first one with a gap of 30 mm and the second one with a gap of 20 mm. Simulations were performed considering a recirculation flow of 400 m³/h.

The results obtained lead us to conclude that the included modifications strongly affect the entering flow jet producing a more homogeneous CVF and WSE distribution over the reactor conical wall. In Fig. 10 and 11 the maximum and minimum limits for CVF and WSE are drawn for both deflector positions.

In Fig. 10 the roof and floor limits for maximum and minimum CVF appear drastically reduced around the gap zone. Once the flow leaves this region, CVF increases meaningfully, while differences between roof and floor limits for maximum and minimum CVF become smaller.
In fact, as flow distribution gets more homogeneous the gap between the maximum and minimum limits decreases. WSE and CVF have opposite behaviors along the gap zone: WSE diminishes while CVF increases for the first 0.7 m; after that, both become roughly constant.

As regards the wall shear efforts, both minimum and maximum WSE are strongly increased by reducing the gap but WSE quickly diminishes radially from the gap zone. A comparison of Fig. 8 and 11 shows smaller differences between roof and floor limits as a consequence of the more homogeneous flow pattern around the entrance.

**Third case: incorporation of a gyratory spout for injecting the inlet flow.** Similarly to the two previous cases, WSE strongly diminishes with the distance from the entrance duct. For this reason, and with the idea of producing a high velocity jet that sweep the whole reactor conical wall during rotation, a gyratory spout was introduced spinning over the y-coordinate axis to inject the recirculation flow. The inlet duct was removed from the model and the recirculation flow was introduced into the reactor by means of a local mass and momentum source located at the bottommost point of the reactor cone.

Although the spout was modeled as a punctual source, a cylindrical injector of 50 mm in diameter was adopted to produce the injection velocities. These were of 28, 41.1 and 56 m/s corresponding to entrance flow rates of 200, 300 and 400 m$^3$/h. For the spout movement a constant angular velocity of 10 revolutions per minute over the vertical axis was applied.

Figure 12 shows the CVF and WSE for three simulation times. It can be seen how the inlet jet sweeps the whole reactor conical wall, raising the uppermost side of the cone and generating a rotational flow pattern evidenced by a significant wake. As expected, the maximum CVF are found on the wall just opposite to the inlet-jet direction. However, the particle residence time at cone wall is controlled by the spout angular velocity, in this case (10 rpm) less than 2 secs. Graphics in Fig. 13 display the maximum and minimum CVF and WSE over the reactor conical wall for all analyzed recirculation flows. As regards maximum CVF values, they hold between 3.5x10^{-4} and 5x10^{-4} but, as was previously mentioned, particles are continuously removed from the cone wall. Moreover minimum CVF remain roughly constant along the radius, with values around 2.5x10^{-4}. As for the maximum WSE, a marked increment is found. For the highest recirculation flow the maximum WSE greater than 50 Pa are obtained up to radii close to 1 m. Even at the uppermost point of the reactor conical wall the maximum WSE can reach values rounding 10 Pa.

**III. CONCLUSIONS**

The numerical analyses carried out in the present study lead to the following conclusions:

- Under current operation conditions an increase in catalyst particle concentration is evidenced over the reactor conical wall. Moreover, low wall shear efforts are also found.

![Fig. 12. Reactor conical wall (recirculation flow of 400 m$^3$/h).](image)

- **Upper.** CVF. **Bottom.** WSE. **Left:** $t = 126$ secs. **Center:** $t = 127.5$ secs. **Right:** $t = 129.5$ secs.
Simulations show that the recirculated inlet flow is strongly channeled over a small fraction of the overall reactor conical wall. This fact produces lower wall shear efforts over the opposite wall, increasing catalyst concentration. Increasing the recirculation mass flow does not modify this flow pattern.

A remarkable improvement is obtained by removing the inlet elbow, incorporating a rhomboidal flow deflector inside the reactor and increasing the recirculation mass flow. However, this enhancement quickly diminishes radially from the deflector zone.

Finally, higher wall shear efforts and lower catalyst concentrations are obtained by incorporating a gyrotoratory spout to inject the recirculation mass flow. It produces a high-velocity inlet jet that sweeps the whole conical reactor wall in each spin.

Further work including the role of the polymerization reaction should be done.

ACKNOWLEDGEMENTS

This work was supported by Centro de Tecnología Argentina (CTA) of Repsol-YPF, Complejo Industrial Ensenada (CIE) (SAT-Exp UNL 485789), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET, Argentina, grant PIP 5271), Universidad Nacional del Litoral (UNL, CAI+D 2005-10-64) and ANPCyT (Argentina, grants PICT 12-14573/2003 (Lambda), PME 209/2003 (Cluster) and PID 398/03 (DIVA)).

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Received: July 26, 2007.
Accepted: February 12, 2008.
Recommended by Subject Editor: José Pinto.