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

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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 by the reaction was applied. Deposition of solid particles and a non-homogeneous flow distribution over the lower reactor walls were founded. Based on the hypothesis that adhesion phenomena is 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 crakings. The polymerization is catalysed by traces of water and AlCl₃. The polybutene reactor under study is a tri-phase tank. 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 phase. 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 which after a few seconds will be hardly adhered to the walls. Once deposits are formed they are very difficult to remove, reducing the operative capacity of the reactor. Adhesion process is continuous and deposits only can be removed by chemical or mechanical techniques. In the reactor under study, the rate of adhesion is faster enough to reduce a very important part of the overall reactor volume after a few years. This fact forces to stop the plant frequently in order to clean the reactor walls, with the consequent high economical impact.

The reactor analyzed does not have any impeller and its charge is only mixed by continuous recirculation forced by pumping the emulsion from the reactor outlet located upwards and introducing again through the reactor entrance located 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, catalyst particles concentration among others. With such information it is possible to image how should be the possible scenario of polymer adhesion.

In this work a finite element CFD analysis of the flow patterns inside the reactor is presented. Inspired about these computational results feasible operative and constructive modifications are proposed, based on the assumption that adhesion is closely related to a combination of catalyst particle deposition (precipitation) and low enough wall shear stresses. In general CFD results are nowadays being used as a very useful design tool. In the reactor design area this technology has not been massively employed being this contribution an example about how this methodology serves to the designer to improve the process productivity.

II. METHODS

A. Problem definition. Constructive and operative features

Polybutene (PIB) reactor is a cylindrical vessel with a total height of 9.5 m, a diameter of 3.3 m and an approximate volume of 60 m³. In Fig. 1 the main constructive data of the reactor are showed. Fig. 1 also shows the dimensions and locations of the inlet and outlet ducts. It is remarkable the sharp curvature of the inlet duct located at the bottom of the vessel.

Reactor is made of carbon steel and has a thermal insulating layer on its outer side. Reactor has not any mechanical impeller, so in order to enhance the reaction process the emulsion is continuously re-circulated. During the catalytic reaction the isobutylene is polymerized producing molecular weights depending on process temperature catalysts concentration and reaction mixture composition.

Fig. 2 is part of a flow sheet and it is useful to clarify the main fluxes involved on the process. Re-circulation
is done by pumping the charge from the Outlet A to the Inlet A at the bottom side. At the same time, a vapor stream is collected through the Outlet B at the top of the PIB reactor and the liquid charge, formed by the polymer diluted in the C4 mixture, is extracted through two small ducts at the Outlet C. Small quantities of catalyst are drifted through the outlet C. Therefore, both compounds must be made up through an auxiliary inlet B.

As it is sketched in Fig. 2 three phases are present, the emulsion formed by the reaction solution (liquid phase), small vapor bubbles (gaseous phase) and small catalyst particles (solid phase). C4 mixture bubbles are generated by an exothermic reaction consuming isobutylene. Due to the necessity to control polymer molecular weight, the temperature and pressure conditions should be strictly controlled, varying from -1ºC and 1.21 atm to 25ºC and 3 atm respectively. Besides, an average catalyst concentration of 0.3 kg per m³ of emulsion 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. Since overall operation temperature needs to be kept almost constant, an isothermal hypothesis is adopted for modeling the process, so only the transport properties of phases are relevant.

Catalyst particle sizes vary from less than 50 microns (20% of the total amount of particle) 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.

Table 1. Rheological properties of the three phases.

<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/</td>
<td>Spheres</td>
</tr>
<tr>
<td>for modeling</td>
<td></td>
<td>bubbles</td>
<td></td>
</tr>
<tr>
<td>Characteristic size</td>
<td>--</td>
<td>1 mm to 2 mm</td>
<td>50 μ to 140 μ</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>690(A)</td>
<td>3.15(A)</td>
<td>2440</td>
</tr>
<tr>
<td>Viscosity (centistokes)</td>
<td>2,0705(B) - 2,2459(C)</td>
<td>1,64(A)</td>
<td>--</td>
</tr>
</tbody>
</table>

As regard the gaseous phase, it is generated during the polymerization reaction in the vicinity of catalyst particles. As was observed in an experimental reactor, the reaction produces small bubbles of C4 of about 1 to 2 mm, which move upward reaching the emulsion free surface.

As for the liquid phase, a sample was extracted from the reactor in order to characterize its transport properties. The emulsion kinematic viscosity for two temperatures was measured at laboratory (see table 1) and the corresponding values at process temperatures were estimated by logarithmical extrapolation using the following expression:
\[ \mu = \frac{\rho}{1000} \left[ a \ln(T) + b \right], \]  

being \( a \) and \( b \) obtained by fitting as -8.96 and 51.84 respectively.

**B. Mathematical model**

The unsteady multi-fluid formulation was employed for simulation. In this formulation, Navier-Stokes equations are modified in order to introduce the volume fraction of each phase in the mixture along with appropriate terms considering the mass, momentum and energy transferred through the interface among phases. The continuity equation for each \( \alpha \) phase is the following:

\[
\frac{\partial (\delta_\alpha \rho_\alpha)}{\partial t} + \nabla \cdot (\delta_\alpha \rho_\alpha \vec{U}_\alpha) = S_\alpha + \Gamma_{Sa} \tag{2}
\]

where \( \delta_\alpha \), \( \rho_\alpha \) and \( \vec{U}_\alpha \) are the volume fraction, density and velocity vector of the \( \alpha \) phase. \( S_\alpha \) are volumetric mass sources or sinks and \( \Gamma_{Sa} \) are mass flows through the interfaces between \( \alpha \) and the others phases. It is important to note the role of the constraint Eq. (2).

Momentum equation for \( \alpha \) phase was written as:

\[
\frac{\partial (\delta_\alpha \rho_\alpha \vec{U}_\alpha)}{\partial t} + \nabla \cdot (\delta_\alpha \rho_\alpha \vec{U}_\alpha \otimes \vec{U}_\alpha) = -\delta_\alpha \nabla P + \nabla \cdot \tau_\alpha + \varphi_\alpha + M_\alpha + \Gamma_{Ma}, \tag{3}
\]

where \( P \) is the static pressure shared by all the phases (one pressure model), \( \tau_\alpha \) is the shear stress tensor, \( M_\alpha \) are the volumetric external momentum sources (potential force fields, e.g. gravity), \( \Gamma_{Ma} \) are interface forces caused by the presence of others phases (e.g. drag and lift) and \( \varphi_\alpha \) are the net momentum quantities transferred at the \( \alpha \) phase by mass transfer through its interface. Although Eq. (2) and (3) have been formulated for fluid continuous phases, they can also be employed to describe solid and gas dispersed phases as in this case for catalyst particles and C4 bubbles. The assumption that dispersed particle phases behave like fluids continuous is valid only for low phase volume fractions. In these cases, the shear stress tensor \( \tau_\alpha \) for dispersed phases gets negligible in relation with interface forces \( \Gamma_{Ma} \). Otherwise for solid dispersed phases with high solid volume fractions (upper than 0.1) kinetic and granular theories must be incorporated in order to modeled the shear stress tensor \( \tau_\alpha \). Besides, an additional solid pressure must be considered (Ranade, 2002; Enwald et al., 1996; Srivastava and Sundaresan, 2003; Makkawi and Ocone, 2003; Gidaspow et al., 2004). For the liquid continuous phase the stress tensor is defined as:

\[ \tau_{RM} = \mu_{RM}^{eff} \left( \nabla \vec{U}_{RM} + \nabla \vec{U}_{RM}^T \right), \tag{4} \]

with \( \mu_{RM}^{eff} \) the effective dynamic viscosity of the reaction mixture, it means the molecular one modified by the turbulence contribution. Large eddy simulation with a simple Smagorinsky model (Smagorinsky, 1963; Wilcox, 1998) is employed to model the turbulence effects. This eddy viscosity model is defined as:

\[
\mu_{RM}^{eff} = \rho_{RM} \nu_{RM}^{eff}, \tag{5}
\]

\[
\nu_{RM}^{eff} = (C_s h)^2 D \sqrt{\epsilon} : \epsilon, \tag{6}
\]

with \( \rho_{RM} \) the reaction mixture density, \( C_s = 0.18 \) the Smagorinsky constant, \( h \) the spatial discretization size, \( D \) a Van-Driest damping factor to correct the influence of the wall proximity and \( \epsilon \) the deformation rate tensor.

Focusing on the system, it is composed by the reaction mixture (continuous fluid), vapor (dispersed fluid bubbles) and catalyst (dispersed solid particles). For low particle volume fractions the bubble-particle contact is negligible thus shear stress term in Eq. (3) is not taken into account. C4-bubble generation can be incorporated either as a transferred mass quantity through interfaces (from reaction mixture to dispersed fluid bubbles) or as a volumetric mass source (for dispersed fluid bubbles) along with a volumetric mass sink (for reaction mixture). Taking into account the relationship between vapor generation and catalyst particles, implementing the second option seems to be easier than the first one. Therefore, \( \Gamma_{Ma} = 0 \) in Eq. (2) and the following local expressions for the mass source \( S_{vapor}(x) \) and the mass sink \( S_{RM}(x) \) were used:

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

\[
S_{RM}(x) = -S_{vapor}(x).
\]

In Eq. (6) \( \varphi_{OB} \) is the total mass flow of C4 through Outlet B, \( V_{emul} \) is the total emulsion volume and \( \delta_{cat}^{\text{cat}} \) and \( \delta_{cat}^{\text{cat}} \) are the local and averaged catalyst volume fractions.

As for the momentum equation, momentum transfer due to mass exchange through interfaces was taken null \( (\Gamma_{Ma} = 0) \) and interface forces \( M_\alpha \) were only given...
by drag efforts. Because of the low volume concentration of solid particles the Schiller-Naumann model was suitable to estimate their drag coefficient \( C_D \). As for the C4 bubbles, the volume fraction of this phase was a priori unknown so the same drag model was implemented for its. \( C_D \) expressed as a function of the particle Reynolds number \( Re_p \) as:

\[
C_D = \begin{cases} 
24 \quad \text{if} \quad Re_p < 1000 \\
0.44 \quad \text{if} \quad 1000 < Re_p < 2 \times 10^5 
\end{cases} \tag{7}
\]

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:

\[
\begin{align*}
S_h^\alpha & = \{ v^h \mid v^h \in H^{1,h} \}, \quad v^h \equiv v_D^h \text{ in } \Gamma_D \\
S_h^p & = \{ q^h \mid q^h \in H^{1,h} \} \\
S_h^\delta & = \{ r^h \mid r^h \in H^{1,h} \}, \quad r^h \equiv r_D^h \text{ in } \Gamma_D \\
V_h^\alpha & = \{ N_v^h \mid N_v^h \in (H^{1,h})^{nd}, N_v^h \equiv 0 \text{ in } \Gamma_D \} \\
V_h^p & = S_h^p \\
V_h^\delta & = \{ N_\delta^h \mid N_\delta^h \in (H^{1,h})^{nd}, N_\delta^h \equiv 0 \text{ in } \Gamma_D \} \\
H^{1,h} & = \{ \phi^h \mid \phi^h \in C^0(\overline{\Omega}) \} \\
\end{align*}
\]

with \( H^{1,h} \) the Sobolev space of order one, \( \Omega \) the mesh partition, \( \Gamma \) the computational domain, \( \Gamma_D \) its boundary and \( \overline{\Omega} \) its closure, \( \Gamma_D \) the part of the boundary with Dirichlet boundary conditions and \( nd \) the number of spatial coordinates. \( S \) is used for the trial functions (interpolation) and \( V \) for the weight functions. The finite element problem is defined as:

\[
\text{find } \delta_\beta^h, \bar{u}_\beta^h \in S_v^h, \quad p^h \in S_p^h, \quad \bar{u}_\delta^h \in S_v^h \quad \text{ with } \beta \text{ an index over the dispersed phases and } C \text{ the index of the continuous phase such that}
\]

\[
\begin{align*}
\sum_{\alpha} [W_{cont}^\alpha] \left[ \frac{d(\rho_\alpha)}{dt} + \nabla \cdot (\rho_\alpha \mathbf{U}_\alpha) - (S_\alpha + \Gamma_m) \right] \text{d}V \\
+ \sum_{\alpha} [W_{mom}^\alpha] \left[ \frac{d}{dt} \rho_\alpha \mathbf{U}_\alpha + \nabla \cdot (\rho_\alpha \mathbf{U}_\alpha \otimes \mathbf{U}_\alpha) \right] \\
\end{align*}
\]

\[
\begin{align*}
\forall W_{cont}^\alpha \in V_{cont}^\alpha, \forall W_{mom}^\alpha \in V_{mom}^\alpha \quad \forall \alpha 
\end{align*}
\]

with \( \alpha \) each phase (continuous and dispersed) in the system. The weight residual formulation (9) uses different weight functions for each equation (CONT: for continuity equations and MOM: for momentum equations) according to numerical stabilization requirements (Tezduyar et al., 1992; García-Cascales and Paillère, 2006; Zanotti, 2007). As regard the continuity equations, the continuous phase (\( \alpha = C \)) uses \( V_{cont}^C = V_h^C \) and each dispersed phase (\( \alpha = \delta \)) uses \( V_{cont}^\delta = V_h^\delta \). As for the momentum equations, both the continuous phase and each dispersed one use \( V_{mom}^\alpha = V_h^\alpha \).

D. Numerical model

In order to gain some insight about the role of the free surface located between the reaction mixture and the vapor existing in the upper part of the reactor the first simulation was done using the overall reactor geometry (see Fig. 1). These preliminary results showed that emulsion free surface had a motion negligible. Hence for the rest simulations only a fraction of the reactor above the normal level of the emulsion free surface (around 0.4 m) was taken into account, reducing the mesh size in 20%. Regarding to 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 small temperature variations the problem was considered as isothermal and simulations were performed at two operation temperatures corresponding to the operation extreme conditions of -1ºC and 25ºC respectively, considering the corresponding reaction mixture viscosities. Regarding to the time integration a first order backward Euler scheme was applied. For each analyzed case a time period of 200 seconds with a constant time step of 0.01 seconds was simulated. The problem was solved using distributed computing over several processors in a Beowulf cluster (Storti et al.; Sonzogni et al., 2002). Each simulation (20,000 time steps) demanded around 5 days in a Beowulf Cluster with 10 processors.

Boundary conditions. Fully developed velocities were imposed to Inlet A, Outlet A and Outlet B while a constant pressure equal to the operation pressure was employed at Outlet C. In order to modeling re-circulation flow from Outlet A to Inlet A the volume fraction for each phase at Inlet A must be linked to the outgoing mass flow at Outlet A. It means that the instantaneous mass flow rate of each phase at Outlet A along with the corresponding reaction mixture viscosities, considering the corresponding reaction mixture viscosities. Fully developed velocities were imposed to Inlet A, Outlet A and Outlet B while a constant pressure equal to the operation pressure was employed at Outlet C. In order to modeling re-circulation flow from Outlet A to Inlet A the volume fraction for each phase at Inlet A must be linked to the outgoing mass flow at Outlet A. It means that the instantaneous mass flow rate of each phase at Outlet A along the corresponding from Inlet B (constant volume fractions of \( \delta_{dat} = 1.24e-4 \), \( \delta_{tip} = 0 \) and \( \delta_{HM} = 0.999876 \)) were added in order to estimate the composition of the entering flow. Moreover, mass flow rate at each boundary were monitored during the whole simulation time interval, guarantying the reactor global mass conservation, focusing the effort in fitting the vapor generation with the volumetric flow rate data measured at Outlet C. The velocity for each particle at walls was considered as non slip.

E. Results and discussion

As it was before mentioned two operation conditions were simulated. The first one corresponding to a con-
stant temperature of -1ºC and a pressure of 1.21 atmos-
pheres at the top part of the reactor, and the second one
for 25ºC of temperature and 3 atmospheres of pressure.
In the following paragraphs the results for the first op-
eration condition are extensively discussed. A steady
state solution was assumed after the global mass balance
was verified. As it was previously mentioned, adhesion
problem was assumed to be related to the catalyst con-
centration at the reactor walls as well as to local low
wall-shear stresses. Attending 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.

Fig. 3. CVF (scale range from 0 to 8x10^-4) and WSE
(scale range from 0 to 1.0) at t = 200 seconds. From left
to right: a) CVF at mean plane x-y. b) CVF at mean
plane y-z. c) CVF at reactor walls from -x view. d)
WSE at reactor walls from -x view. e) CVF at reactor
walls from x view. f) WSE at reactor walls from x view.

Fig. 3 contains six pictures, the first two of them are two
cut planes, one an x-y cut plane where the entrance duct
and the outlet ducts are cut in halves. The other one is
perpendicular to the first one and it is placed on the y-z
plane. This view is called the front view while the oppo-
site one is called the rear view. The four remaining pic-
tures show the front (third and fourth pictures) and rear
side walls (the fifth and sixth ones). These figures show
the conical part of the reactor receiving the fluid flow
from the entrance duct and due to its inclination of
about sixty degree, this part is prone to particle adhe-
sion. Therefore, most of the attention will be given to
this part of the reactor geometry.

In Fig. 3-a it is clearly noted how the entrance flow jet
has a strong tangential velocity component, sweeping
the cone right wall and allowing the decantation of solid
particles at the opposite wall. A particle concentration
larger than the averaged one (1.24x10^-4) is visualized
over most of the reactor cone, whereas a small part of
this region that is directly affected by the entrance flow
jet holds lower particle concentrations. In Fig. 4 both
CVF and WSE over the conical reactor walls are drawn
at three different simulation times. It is useful to see
how the entrance jet comes into the reactor sweeping a
fraction of the conical wall with a period of around 30
seconds. Results in Fig. 4 show that decantation of solid
particles over the reactor lower walls increases catalyst
concentration above 3 times respect to the averaged
concentration. Lower catalyst concentrations are
founded at the entrance-jet core, while regions with vol-
ume fractions greater than 4x10^-4 are located in the vic-
inicity of it.

Results showed a periodic behavior of the flow jet like a
wandering effect. 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 fact, more than 150 mesh sampling points over the
reactor cone were selected and 140 solutions at different
time steps were considered. In Fig. 5 the minimum,
maximum and time-averaged values for CVF and WSE
at four radial distances from the entrance are drawn (see
sketch in figure 8 for radial coordinate definition). Polar
diagrams in Fig. 5 underline the zone directly influ-
enced by the entrance flow. The increment in CVF on
the opposite conical wall is also evidenced. As it can be
seen, close to the entrance (radius = 0.25 m), CVF
reaches 6x10^-4 on the left-middle conical wall while
minimum values are around 4x10^-4. WSE exceeds 6 Pa
in a direction aligned with the jet (0 degrees at polar
diagram) and close to the entrance orifice, but it quickly
diminishes along the radial coordinate. Both CVF and
WSE become more homogeneous while radius grows.
Furthermore, maximum CVF decreases, although the
averaged one holds close to 4x10^-4. WSE quickly dimin-
ishes far away from the entrance and the efforts hardly
ever exceed 1 Pa for radius larger than 1.42 m.
By changing the operation conditions from -1°C to 25°C of temperature the viscosity was reduced from 1.112 centistokes to 0.547 centistokes. Viscosity reduction affects directly wall shear efforts as well as drag forces, lessening both of them. This fact increases decantation over the conical reactor walls indicating that higher operation temperatures would promote higher adhesion rates.

**F. Studied modifications**

Three operative and constructive modifications are discussed and they are assessed in terms of particle decantation reduction and wall shear stresses increment.

**First case: an increased re-circulation flow.** The first case analyzed is defined in terms of an increment of the recirculation flow from 288 m³/h to 400 m³/h holding the original constructive geometry. In this case flow-pattern results are similar to those founded for the lower recirculation flow. This means that the entering flow jet comes into the reactor producing the same non-homogeneous flow distribution over the conical walls. Fig. 6 shows the maximum (roof limit) and minimum (floor limit) extreme values of CVF and WSE over the conical reactor walls for different radius. Min roof refers to the maximum value (roof limit) of the minimum CVF while Min floor refers to the minimum one (floor limit). This means that any minimum CVF value is bounded between Min floor and Min roof curves. As it can be noted, minimum CVF values are reduced as recirculation flow increases. On the other hand, maximum CVF values do not show any significant difference for both analyzed flows. Fig. 7 displays the same analysis for WSE. Minimum and maximum WSE quickly fall down along the radius. There are not significant differences in floor limits for maximum and minimum WSE by increasing the re-circulation flow. As regard the roof-limit of minimum WSE, it is strongly increased near the entrance but differences become negligible beyond radius of about 0.7 m. On the other hand, significant differences are founded for the roof-limit of maximum WSE at every radius.

As it can be noted from Fig. 6 and 7, re-circulation-flow enlargement has a positive effect in both CVF and WSE. Nevertheless, since entrance flow keeps strongly channeled over a fraction of the overall conical reactor wall, the inlet elbow must be modified in order to promote the angular homogenization of the entrance mass flow rate. In the next analyzed case, the inlet elbow is removed and a deflector is incorporated inside the reactor in order to get a more homogeneous distribution of the entering flow over the conical reactor walls.

**Second case: removal of the inlet elbow and incorporation of a flow deflector.** Fig. 8 shows the constructive modifications implemented around the flow-entrance zone. The inlet elbow was replaced by a straight duct. Furthermore, 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 conical reactor walls avoiding obstructions during the reactor normal operation. According to information about the maximum catalyst particle size two positions were considered, the first one with a gap of 30 mm and a second one with a gap of 20 mm. Simulations were performed considering a re-circulation flow of 400 m³/h.

The results obtained allow conclude that the included modifications strongly affect the entering flow jet producing a more homogeneous CVF and WSE distribution over the conical reactor wall. In Fig. 9 and 10 the maximum and minimum limits for CVF and WSE are drawn for both deflector positions. In Fig. 9 the roof and floor limits for maximum and minimum CVF are drastically reduced around the gap zone. Once the flow leaves this region, CVF increases...
meaningfully. Furthermore, differences between roof and floor limits for maximum and minimum CVF become smaller.

In fact, hence flow distribution gets more homogeneous the maximum and minimum limits approach themselves. WSE and CVF have an opposite behavior along gap zone. This means that WSE diminishes while CVF increases for the first 0.7 m, after that, both become roughly constants.

As regard the wall shear efforts, both minimum and maximum WSE are strongly increased by reducing the gap but WSE quickly diminishes far away from the gap zone. By comparing Fig. 7 and 10 differences between the roof and floor limits get smaller for the second case, as a consequence of the more homogeneous flow pattern around the entrance.

As it was pointed out, removing the inlet elbow clearly improves the inlet-flow distribution. Therefore, several constructive modifications for the inlet duct were studied in order to promote this behavior. Due to the actual constructive characteristics of the PIB reactor all possible modifications were constrained to have a limit height from the ground level to the reactor entrance equal to 1.0 m. Four inlet configurations were considered; the first one by lowering the duct 0.6 m, the second and third ones by incorporating stagnation deposits of lengths $H = 0.7$ m and 0.8 m, respectively, and the last one using a cyclonic configuration in order to get a rotational flow. Fig. 11 shows the original elbow along with the first, second and third configurations while Fig. 12 shows several views of the fourth model.

In order to find the best elbow model a fully developed turbulent velocity was introduced through the inlet while a constant pressure was considered at outlet. Once stationary conditions were reached the velocity field at outlet was analyzed. Fig. 13 shows the vertical velocity for all the considered models. As can be seen, the original elbow geometry produces a non homogeneous flow distribution at the downstream. The flow pattern does not become more homogeneous by extending the duct upstream. Of course, the latest is expected because the development length for this kind of flows is larger than the admissible duct extension (three times the duct diameter). As for the modified elbows involving a stagnation deposit, some improvement is obtained with the biggest one. Although the flow pattern is not homogeneous it seems to be more isotropic than the others.
As can be seen the results above showed not complete solve the current non-homogeneous flow distribution. On the other hand, as is displayed in Fig. 14 the fourth proposed elbow introduces a non-stationary rotational flow pattern wandering the overall duct cross area with a rotational period rounding 2 seconds.

Third case: incorporation of a gyratory spout for injecting the inlet flow. As it was mentioned for the previous cases, WSE strongly diminishes along the radius. For this reason, it was incorporated a gyratory spout spinning over the y-coordinate axis in order to inject the re-circulation flow. The object of it is producing a high velocity jet that sweeps the whole conical reactor wall during its rotation. In such a way, the inlet duct was removed from the model and the re-circulation mass flow rate was introduced into the reactor by a local mass and momentum source located at the bottommost point of the reactor cone.

A cylindrical spout of 50 mm of diameter was adopted and three injection velocities of 28, 41.1 and 56 m/s corresponding to entrance flows of 200, 300 and 400 m$^3$/h was considered. For the spout movement a constant rotational velocity of 10 revolutions per minute was applied for all flows.

It must be noted that any constructive modification affecting the original reactor geometry could entail an oversize of the re-circulation pumps. In table 2 the estimation of the pressure lost for each analyzed elbow are included.

Table 2. Pressure lost generated by incorporating the analyzed constructive modifications (re-circulation flow of 400 m$^3$/h).

<table>
<thead>
<tr>
<th>Constructive modification</th>
<th>Pressure lost $\Delta P$ [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original elbow</td>
<td>-811</td>
</tr>
<tr>
<td>Extended elbow</td>
<td>-1169</td>
</tr>
<tr>
<td>Elbow with deposit of H = 0.70 m</td>
<td>-25458</td>
</tr>
<tr>
<td>Elbow with deposit of H = 0.80 m</td>
<td>-26077</td>
</tr>
<tr>
<td>Cyclonic elbow</td>
<td>-14484</td>
</tr>
<tr>
<td>Rhomboidal deflector (gap: 30 mm)</td>
<td>-2479</td>
</tr>
<tr>
<td>Rhomboidal deflector (gap: 20 mm)</td>
<td>-6727</td>
</tr>
</tbody>
</table>

From pressure lost in table 2 it is easy to have a rough estimation of the additional pump overload by adding the pressure lost of each constructive modification as follow:

$$\Delta P_{\text{added}} = \Delta P_{\text{new elbow}} + \Delta P_{\text{deflector}} - \Delta P_{\text{old elbow}}$$ (10)

For instance, considering the incorporation of a cyclonic elbow along with a rhomboidal deflector with a gap of 20 mm, it would produces and additional pressure overload of 21,211 Pa.

Fig. 13. Vertical velocity at outlet for the original, and the first, second and third analyzed elbows.

Fig. 14. Vertical velocity at outlet at four time states for the cyclonic elbow. From left to right: t = 0.5, 1, 1.5 and 2 seconds.

Fig. 15 shows the CVF and WSE for three simulation times. It can be seen how the inlet jet sweeps the whole conical reactor wall, raising the uppermost side of the cone and generating a rotational flow pattern evidenced by a significant wake. As was expected the maximum CVF are found just at the opposite wall respect to the inlet jet direction. However, the particle residence time at cone wall is controlled by the spout rotational speed, being for this case (10 rpm) less than 2 seconds. Graphics in Fig. 16 display the maximum and minimum CVF and WSE over the conical reactor walls for all analyzed re-circulation flows. As regard maximum CVF values, they hold between 3.5x10^{-4} and 5x10^{-4} but, as it was previously mentioned, particles are continuously removed from the cone wall. Moreover minimum CVF are roughly constants along the radius, with values around 2.5x10^{-4}. As for the maximum WSE, a marked increasing is founded. For the highest re-circulation flow maximum WSE upper than 50 Pa are obtained until radius close to 1 m. Even at the uppermost point of the conical reactor wall the maximum WSE values can reach value rounding 10 Pa.
Fig. 16. Maximum and minimum CVF and WSE over the conical reactor walls for the three analyzed flows. 
Left: CVF. Right: WSE.

III. CONCLUSIONS

The numerical analysis carried out in the present study reached to the following conclusions:

- Under actual operation conditions an increase in catalyst particle concentration is evidenced over the conical reactor walls. Moreover, low wall shear efforts are also founded.
- Simulations show that the re-circulated inlet flow is strongly channeled over a small fraction of the overall conical reactor wall. This fact produces lower wall shear efforts over the opposite wall, increasing catalyst concentration. Increasing the re-circulation flow does not modify this flow pattern.
- A remarkable improvement is obtained by removal the inlet elbow, incorporating a rhomboidal flow deflector inside the reactor and increasing the re-circulation flow. This enhancement quickly diminishes far from the deflector zone.
- Finally, higher wall shear efforts and lower catalyst concentrations are obtained by incorporating a gyratory spout to inject the re-circulation flow. It produces a high-velocity inlet jet that sweeps the whole conical reactor wall in each spin.

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