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 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 C_4 olefin refinery streams of fluidized catalytic cracking. The polymerization is catalyzed by traces of water and $AlCl_3$. The polymerization mechanism consists in chain polymerization 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 $AlCl_3$ 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 particles 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,