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Fluid Dynamics Simulation of Two-Phase Flow in a Separator Vessel through CFD

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ABSTRACT

The poly (ethylene-co-vinyl acetate) - is an EVA polymer produced that has an important role in the National petrochemical industry chain. Understanding the fluid dynamic behavior during processing in pots separators is of fundamental interest for operational continuity. The drag of polymer melt to the top of the vase, is a source of interest to understand the behavior of the flow inside the machine and reduce contamination. The objective of this work is to study the phenomena the fluid dynamic behavior of EVA during processing inside the separator vessel, to propose a modification of the process. We performed numerical simulations of two-phase flow (gas and ethylene polymer melt), using the commercial computational fluid dynamics package CFX 5.5. The turbulence model used was the k-ε for the fluid phase and a model with an Eulerian approach. The modeling used was satisfactory, because during the simulations, we studied the velocity profiles, concentration and trajectory of the biphasic mixture of fluids.

Keywords: *Fluid dynamics, simulation, CFD, EVA.*

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I. INTRODUCTION

In plants producing poly (ethylene-co-vinyl acetate) EVA, a recurring problem is the formation of gels during and after synthesis of polymerization. According to Henk (2015), the gels are any visible imperfection in polyethylene film. According to Barbosa (2013), this defect can be characterized at the polyethylene film, due to the appearance of high molar mass molecules or other contaminants that do not melt, during processing of the product. Contamination in polyolefin film by the formation of gels is a phenomenon that is difficult to predict, reproduce and resolve. According to Adorno (2004), petrochemical plants have characteristics of constructive technology with interconnected equipment, where occur physical and/or chemical reactions, that are unique to the application of the intended production. In the production process of EVA, the production thereof takes place in tubular reactors, through gas compression of ethylene at high pressures and temperatures, in a process of polyaddition and polymerization of monomers (Caliani, 2005).

Figure 01 shows a partial representation of the flowchart of the manufacturing process of EVA at high pressure and temperature. According to Barbosa (2010), the polymer plus unreacted gas leaving the tubular reactor and follow the direction of the primary separator vessel where they are separated into two flows of fluids. At the top of the vessel leaves the gas and the other part, bottom of the vesselgas and molten polymer leaves. The resin and gasunreacted follow to the secondary separator vessel, where it again separates the gas from the polymer melt. The separated gas leaves by the top of the vessel, forming a flow of ethylene feeding the compressor that reintroducesin the gas stream of the process to be reacted again and the melt polymer follows by the bottom of the vessel feeding an extruder. Coupled to the extruder, a granulator cuts the spaghetti resulting pellets that are dragged by a flow of water to the centrifugal separator. Thereafter, the pellets pass through a sieve system and weighing of the product, which is discharged into a hopper which has coupled a mechanical system, collecting samples of the pellets continuously in a time interval of production.

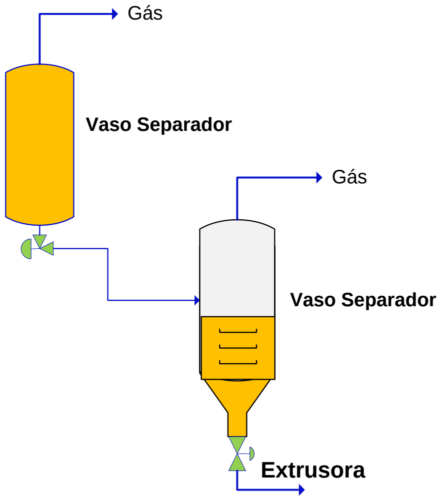

Figure 01: Partial flowchart of the manufacturing process of EVA.
Source: Adapted from Chien et al, 2006 and Wan 2012.

During the production processes of LDPE and/or EVA these materials undergo by pressure vessels with the purpose of separating the liquid and gas phases, which are derived from the polymerization process that occurs earlier in the reactor. In the process containing polymeric fluids, occurs phenomena such as formation of stalactites that appear trapped in the top of the vessel, and over time cause problems in the product quality.
The condition of fluid dynamic of the process allows part of melt is entrained by the flow velocity of the gas to the top of the separator vessel, forming polymer stalactites, which over time cause product contamination. Fluid dynamics analysis is important because, enable to understand the behavior of the fluid flows and propose changes in the current pattern, to reduce the drag of polymer melts, which can influence the formation and the growth of stalactites.

II. LITERATURE REVIEW

The LDPE and EVA production system includes three sections in the process: the compression unit, the reactor and schemes product separation. The process consists in compressing ethylene gas with high purity to the tubular reactor under high pressure (1000 to 3000 atm) and heat until the reaction initiation temperature and to control in 140-330 °C range. In the reactor is where begin the polymerization reactions by free radicals. Polyaddition reaction of monomers in the reactor, can be initiated by the injection in compounds initiators such as, oxygen and or organic peroxides or through the physical conditions such as radiation or heat (Kiparissides, et al., 1993; Kwag and Choi, 1994; Peacock, 2000; Neumann, 2001; Chien et al., 2007; Asteasuain and Brandolin, 2009).
In accordance with Palma (2009), the finite elements analysis is a method for numerical solution for differential equation, where each element represents a small part of structure or environment to be represented. The net is the arrangement of elements connected by their nodes. The amounts of fields introduced in the elements through their nodes and within each element the field is approximated by an interpolation function, usually polynomial, whose degree depends on the number of element nodes.
The project analysis of prototypes through computational technology simulation allows to effect complex tests to analyze the physical behavior of a product or process obtaining information quickly and accurately via computer. With project analysis can minimize or even eliminate the need for physical prototyping and testing. The technology is used worldwide as a computational tool to developing products. The project analysis employs the method of finite element analysis (FEA) to simulate the product physical behavior. This method is currently one of the most important numerical methods used to obtain approximate solutions to physical problems modeled by partial differential equations, being used for boundary value problems in physics, mathematics, and engineering, for example, (Gois, 2002; Santos e Medronho, 2007).
The project analysis emerged in the 1990s based on the technology of computer-aided design (CAD) (Solid works 2007). Physical prototypes are obstacles to the development of successful products, causing impediments that increase costs and prolong the life of the project, without resulting in the best possible product. Faced with competitive pressures for more innovative designs and optimized, as well as safer and more reliable products, many manufactures have employed the technology of computer-aided engineering (CAE) to simulate repetitions of prototypes-test and optimize designs based on the physical behavior of virtual prototype. Thus, the design analysis presents the advantage to improve the design of products on the computer without the need to build

prototypes for testing. In the highly competitive and globalized world nowadays, to keep themselves in a favorable position, companies must provide not only high productivity but also must offer products and services of the highest possible quality with competitive prices. In this context the maintenance of equipment and machines becomes a crucial factor to achieve these demands for quality and productivity. Equipment often degraded imply reducing product quality or unexpected downtime due to breakage or failure and negatively impact a number of indicators of productivity and quality of the companies.

The fluid dynamics analysis using the Computational Fluid Dynamics – CFD is the area of knowledge is applied to Fluid Mechanics to solve problems related to fluid flows. Covers phenomena of flow, aerodynamic, chemical reactions, combustions, etc. It uses mathematical methods algorithms based on the laws of conservation of mass, momentum and energy together with predefined conditions of the environment, generating values of its variables such as pressure, speed and temperature, within a field or dominion, in stationary regimes or transient (Queiroz, 2008).

ANSYS has developed a complete package for analysis by finite element method, used by engineers around the world, in virtually all fields of engineering. One of these is the computational fluid dynamic analysis, to determine where the flow and temperature distribution in a fluid, ANSYS can simulate flows: laminar and turbulent, compressible and incompressible. How applications may be cited areas aerospace, automotive design and manufacturing processes in general. The variables of interest are typical velocities, pressures, temperatures and surface coefficients (ANSYS Advantage, 2008).

III. METHODOLOGY

3.1 Fluid Dynamic Simulation

The problem to be analyzed comprises the mathematical modeling and numerical simulation of the two layers of polymeric material and the ethylene gas in a separator vessel, by passing these substances for a dispenser inside a separator vessel. A tetrahedral mesh was created in commercial software ANSYS ICEM version 13 and the simulation performed in commercial software ANSYS CFX version 5.5. The initial and boundary conditions were set according to the actual values of the process.

During simulation by the finite element technique with ANSYS CFX version 5.5, was examined the influence of the position of the distributor located within the vessel to describe the flow of ethylene polymer and inside the separator vessel. The simulation was performed based on the process variables using flow distributor at the entrance vessel disposed at an angle of 45 degrees to the inlet axis as shown in Figure 02.

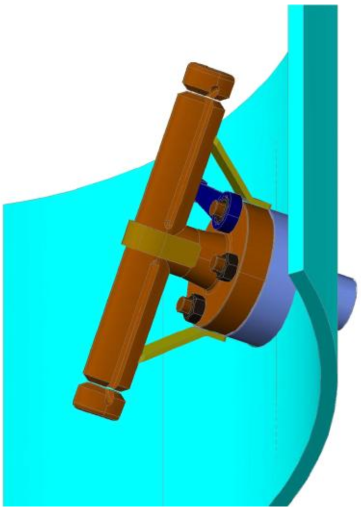

Figure 02: Drawing of the layout of the flow distributor separator vessel.
Source: Operator's Manual PE6 (2010).

The secondary separator vessel's main function is to separate the gas from the polymer at low pressure and feed the extruder. The vessel is made of carbon steel and has a volume of V m³, total height Lm, an inner diameter of 16/3L m and L/16 m diameter manhole. Other construction features are: (i) an entry side L/160 m, (ii) an outlet through the bottom of polymer L/20 m (connected to a level control valve to the vessel), (iii) and an outlet gas from the top of L/42 m.

The vessel is coated with thermal insulating and has a thermal oil heating up to the height H/2, the region of the inlet fluids. The heating oil is provided with a temperature control device which can be adjusted from 40°C to 260°C.

3.2 Mathematical Modeling

The mathematical model used in this work was the model of two fluids with a velocity field solved for each phase. Under this approach, even when dispersed phases are considered continuous and interpenetrating according to Euleriana-Euleriana vision. The hypotheses were two-phased flow, both continuous phases formed by Newtonian fluids; exchange between the amount of movement phases given by the mixture model; isothermal flow and no mass transfer between the phases; presence of buoyant force; dimensionality; turbulent flow, buoyancy and steady. Figure 03 shows the values of certain physical properties of the two fluids and some constants used.

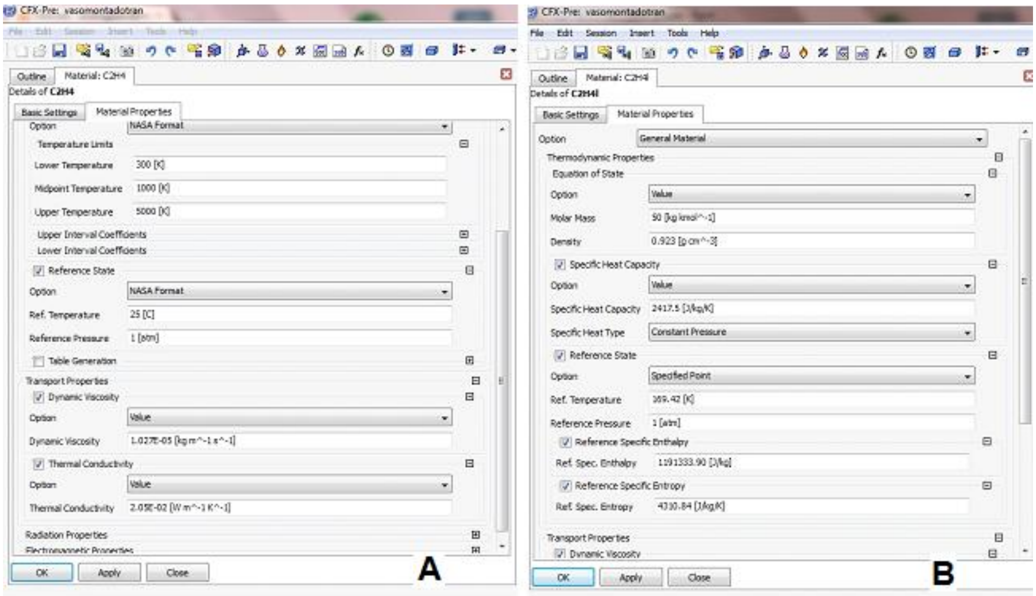

Figure 03: Screenshot of the software with the physical properties of the fluids and constants: The gaseous ethylene and LDPE liquid B.

The mumbers of elements and nodes of the mesh used for the simulation are shown in Table 01. For meshing software was used ICEM 13.0 CFD ® contructing a tetrahedral mesh unstructed and nonuniform formed by elements 3,357,312. The mesh and different regions of the domain where are the boundary conditions are illustrated in Figure 04

Table 01: Number of mesh nodes and elements.

Domínio	Nós	Elementos
Fluído	538121	3051770
Solido	62824	305542
Todos Domínios	600945	3357312

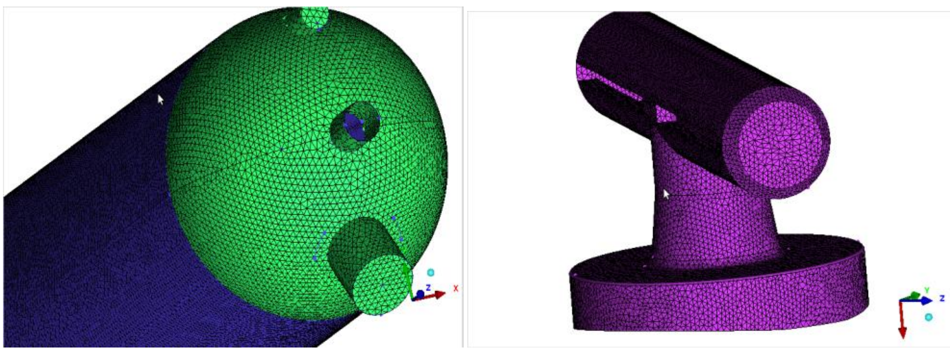

Figure04: Tetrahedral mesh used in the numerical solution (separator vessel in distributor A and B).

The initial conditions are described in Table 02 and boundary conditions listed in Table 03.

Condições Iniciais	
Fluído inicial	Eteno gasoso presente como 100 % em todo tanque
Pressão	1 atm
Velocidade	Nula em todos os domínios
Temperatura	Constante de 200 °C

Table 02: Initial Conditions.

Condições de Contorno	
Entrada dos materiais no distribuidor	Eteno gasoso 24 % e PEBD fundido 76 % com vazão mássica de 3.6528e+00 [kg s^-1]
Condição de parede	não deslizante nas superfícies do tanque e do distribuidor
Pressão manométrica na região de abertura	0 atm nas regiões de baixo e cima do tanque
Modelo de turbulência empregado	K-Epsylon
Temperatura dos fluidos	200 °C

Table 03: Boundary Conditions.

IV. RESULTS AND DISCUSSION

The mathematical model was solved numerically using the commercial simulator Ansys CFX 5.5. More details on the numerical method used can be found in Burns, Ansys Inc. Maliska. The convergence criterion was the residual mean square (RMS) of the conservation equations smaller than 10-4. The simulation contained 600 interactions and was scheduled to stop of there was convergence of less than 10-4. The processing time and the graph showing the results of the convergence of moments of mass correnponding coordinates can be viewed in Figure 05.

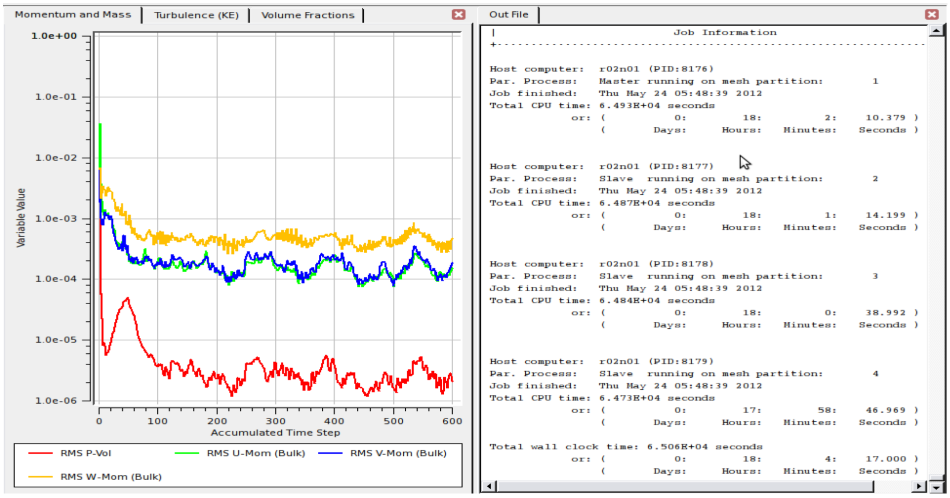

Figure 05: Convergence results for the moments of mass coordinates and corresponding processing time.

The numerical solution was performed on Parallel Cluster Environment Sun Fire X containing in total 38 and interconnected, we called that compose it "Newton" and are part of the wrapper arranged to process and resolve problems on high-performance computing. It is noteworthy that each node can operate as a standalone computer, but its connectivity makes that the work can be divided and resolved faster. The final processing time was 18 hours and 4 minutes, and there was no convergence results, in part by the mesh size which may have been too coarse to the problem inquestion and/ or because the number of steps that may has been inadequate. But, can actually be cridited to the mesh size, because it is perceived that the solution is oscillating and it indicates that you'd find some post convergence.

Figure 05 shows most clearly the results obtained when one sees the biphasic separation of the two materials, where the molten polymer is represented with blue color and ethylene is gaseous blank. You can observe the exitence of the drag of the process as it contributes to the genaration os stalactites equipment. Another important fact during the simulation was the representation of level of the molten resin in the vessel, which can compare with the values shown on the controller level, as shown in Figure 06.

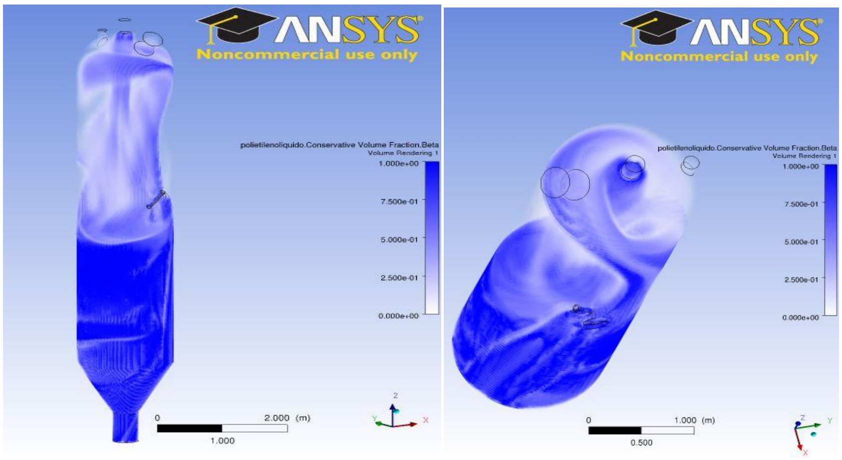

Figure 05: Map of separation of the two materials in the fluid in its liquid form is represented with blue color and gaseous blank. In the front view, and B in perspective showing the manhole and higher output.

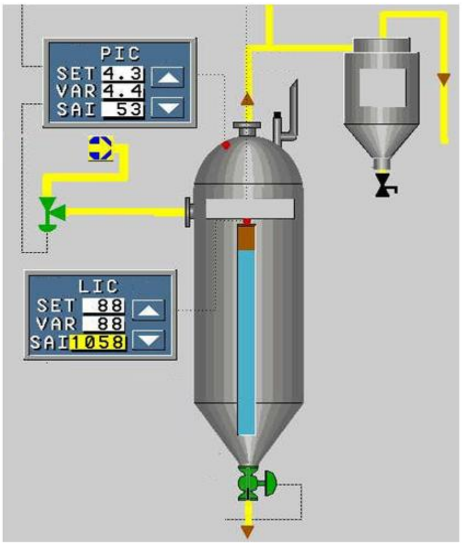

Figure 06: Indication of level control on the screen of DCS.

In Figure 07, you can see the separation of the two biphasic material toward the bottom outlet of the separator vessel. This amount of occluded gas entrained in the polymer chain does not couse quality problems such as generation of infused, but generates a loss in efficiency because it ceases to be reused in the process.

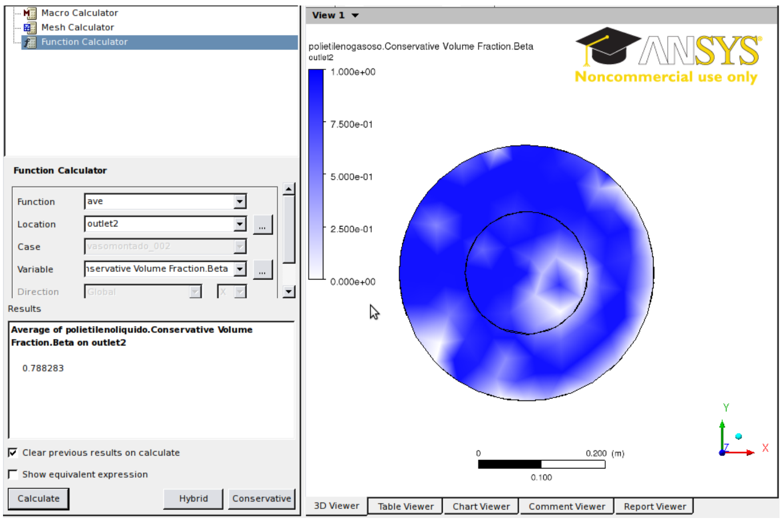

Figure 06: Calculation% of resin (blue) in the bottom outlet of the vessel.

Figure 07 shows the flow lines of the fluid velocity inside the separator vessel. The results of higher speeds than occur in the inlet and outlet nozzles of the machine shown to be consisten with the reality of the process. The speed value found in this simulation very close calculated according to the average flos. The speed found in the simulator was around 0.025 m/s calculated 0.0299 m/s.

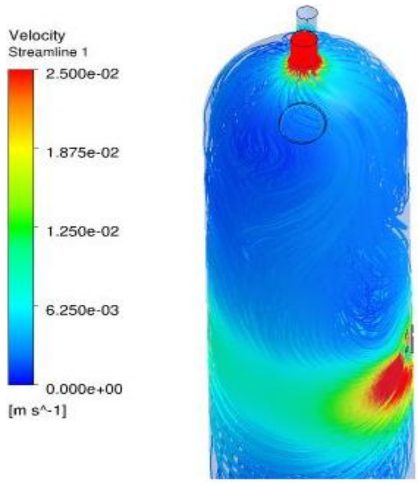

Figure 07: Lines of flow velocity of the fluid at the top of the vessel.

V. CONCLUSIONS

The simulation results were consistent with expectations for the velocities, the fluid path inside the machine. The model allowed to demostrate a constant level of polymer in the vessel which allows to conclude that the solution became with values in reality. The concentration of ethylene occluded in the polymer melt which is dragged onto the bottoms stream is an important factor on the point of view of process losses. This issue is very complicated since it refers to changes in process variables that increase or dimensional expansion of the gas inside the machine. As future work, we intend to apply the method to new distrubutors flow inside the separator vessel, in order to reduce the drag of polymer to the top of vessel, applying the approach Ansys simulation in order to compare resulsts.

REFERENCES

[1]. ADORNO, Laurence Ricardo. Levantamentos de demandas ergonômicas em dez plantas petroquímicas brasileiras: Dissertação de Mestrado de Engenharia Ênfase em Ergonomia, Universidade Federal do Rio Grande do Sul, Porto Alegre 2004. Disponível em: <http://www.producao.ufrgs.br/arquivos/publicacoes/laurence_ricardo_adorno.pdf>. Acessoem 24/01/10.

[2]. ANSYS INC. Advantage Excellence in Engineering Simulation. Volume II, Issue 2, 2008.

[3]. ANSYS INC. ANSYS CFX 11.0 ® Manual. 2008.

[4]. ASTEASUAIN, M.; TONELLI, S.M., BRANDOLIN, A.; BANDONI, J.A.. Dynamic simulation and optimisation of tubular polymerization reactors in gPROMS. Computers and Chemical Engineering, Volume 25, Issues 4–6, 1 May 2001, Pages 509–515.

[5]. BARBOSA, Luiz Antonio. Método aplicado à otimização da fabricação de polietileno de baixa densidade após produção de EVA: um estudo de caso. Trabalho de Conclusão do Curso de Engenharia de Produção das Faculdades Integradas de Taquara – Faccat, Taquara, 2010.

[6]. BARBOSA, L. A. Estudo da geração de crosslinking durante a fabricação de EVA/PEBD. Dissertação de Mestrado em Tecnologia de Materiais e Processos Industriais. Universidade Feevale, Novo Hamburgo, Rio Grande do Sul, Brasil, março 2013. Available in: <http://biblioteca.feevale.br/Dissertacao/DissertacaoLuizBarbosa.pdf>. Access, 19/12/2013.

[7]. BURNS, A.D. Computational Fluid Dynamics Modeling of Multi-Phase Flows. Lecture Notes: Alpha-BetaNumerics. 2002.

[8]. CALIANI, Erico. Modelagem e simulação de um reator autoclave para a produção de polietileno de baixa densidade (PEBD): Dissertação de Mestrado em Engenharia Química, Universidade Estadual de Campinas, São Paulo, 2005. Disponível em: <http://libdigi.unicamp.br/document/?code=vtls000365855> Acesso em 22/01/09.

[9]. CHIEN, I-Lung, KAN, Tze Wei, CHEN, Bo-Shuo. Dynamic simulation and operation of a high pressure ethylene-vinyl acetate (EVA) copolymerization autoclave reactor. Computers&ChemicalEngineering, volume 31, edição 3, 19 Janeiro 2007, páginas 233–245. Disponível em:<http://www.sciencedirect.com/science/article/pii/S0098135406001906>. Acessoem 10/12/2012.

[10]. HENK L. Gel formation during extrusion of LDPE and LLDPE. Available in: <http://pisa.org.za/files/Henk%20Lourens%20paper.doc>. Access, 15/01/2015.

[11]. GOIS, J. P., PITERI, M. A., Geração Automática de Malhas de Elementos Finitos e a Estrutura de Dados Winged-Edge Modificada. Sociedade Brasileira de Matemática Aplicada e Computacional. Tendências em Matemática Aplicada e Computacional, V. 3, No. 1, 2002, p. 121-130.

[12]. KIPARISSIDES, C., G. VERROS, and J. F. MACGREGOR (1993). Mathematical modeling, optimization, and quality control of high-pressure ethylene polymerization reactors. J. M. S. - Rev. Macromol. Chem. Phys. C33(4), 437-527.

[13]. KWAG, B. G. and CHOI K. Y. (1994). Modeling of a multistage high-pressure ethylene polymerization reactor. Chem. Engng. Sci. 49, 4959-4969.

[14]. NEUMANN, G. A. Modelagem de um reator tubular de alta pressão para produção de PEBD. Dissertação de Mestrado Engenharia, Universidade Federal do Rio Grande do Sul, Porto Alegre 2001. Available in: <http://www.lume.ufrgs.br/bitstream/handle/10183/3180/000333398.pdf?sequence=1>. Access, 20/02/2013.

[15]. PALMA, Diogo Cristiano. Metodologia de simulação por elementos finitos de polias para transportadores de correia de grandes capacidades. Trabalho de Conclusão do Departamento de Engenharia Mecânica da Escola de Engenharia da UFRGS. Porto Alegre, 2009. Disponível em: <http://www.lume.ufrgs.br/bitstream/handle/10183/25826/000753971.pdf?sequence=1>. Acessoem 07/07/2012.

[16]. PEACOCK, A. J. Handbook of polyethylene, strutures, porperties, and aplications. Editado por Marcel Dekker, Inc. New York, 2000.

[17]. QUEIROZ, Natália Ferreira.Simulação com CFD de escoamento de fluxo ao redor de um edifício de 10 andares - Tutorial Ansys Workbench 11.0. Universidade Federal do Rio Grande do Norte, 2008. Disponível em: <http://www.labcon.ct.ufrn.br/arquivos/TutorialAnsysWorkbench.pdf>. Acesso em 10/05/2012.

[18]. SANTOS, Fabio Pereira, MEDRONHO, Ricardo A. Simulação numérica dafluidodinâmica de um riser de craqueamento catalítico. 4º PDPETRO, Campinas, SP 4.2.0389-1, 21-24 de Outubro de 2007. Disponível em: <http://www.portalabpg.org.br/PDPetro/4/resumos/4PDPETRO_4_2_0389-1.pdf>. Acesso em 10/01/2013.

[19]. SOLIDWORKS. Desmistificando a análise de projetos. Disponível em: <http://mkt.solidworks.com/emarketing_enu>. Acesso em: julho de 2007.

[20]. WAN, Victor.ProcessEconomicsProgramReport 155B - ETHYLENE-VINYL ACETATE COPOLYMERS. Santa Clara, Califórnia, Setembro 2012. Disponível em: <http://ric.braskem.com.br/sites/bbc/Acervo Digital/Estudos/PEPs/PEP ethylenevinylacetatecopolymers set2012.pdf>. Acesso em 10/12/2012.