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Use of a two-dimensional pseudo-homogeneous model for the study of temperature and conversion profiles during a polymerization reaction in a tubular chemical reactor

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Abstract:

A two-dimensional pseudo- homogeneous model is used to study temperature and conversion profiles during the polymerization reaction of low density polyethylene (LDPE) in a tubular chemical reactor. This model is integrated by the Runge-Kutta 4th order semi implicit method, using orthogonal collocation to transform the system of equations, describing the heat and mass transfers involved, into ordinary differential equations.

Ethylene polymerization has been simulated, over a range of temperature and pressure, according to the mechanisms of radical polymerization. The results of several tests, under conditions similar to those of an industrial scale polymerization, are presented. The influences of the initial temperature, $\mathbf{T_0}$, the total pressure $\mathbf{P_t}$ and the ratio **L/D** (main dimensions of the reactor), on the profiles of temperature and conversion rates, are tested and analyzed to predict the behavior and performance of the tubular chemical reactor considered.

A peculiar attention was given to the effect of an increase of the initial temperature $\mathbf{T_0}$ since such a raise will result in a decrease of $\mathbf{T_c}$ (hot spot) appearing at the entrance of the reactor on one hand, and in an improved conversion on the other hand. An opposite effect is observed for $\mathbf{P_t}$ since a pressure increase will result in a rapid raise of $\mathbf{T_c}$ and a decrease in the conversion. The range of pressure and temperature is thus limited by the system performance: excessive pressures must be avoided and working temperatures must be chosen in the range where the polymerization reaction is very fast; such conditions allow not only a good conversion but also a resulting polymer with a low crystallinity and, thus, a low density.

In the present work, the effect of the ratio **L/D** was also studied in order to find the most suitable ratio that permits the best evacuation of the heat released during polymerization.

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