Supporting Information

Site count: is a high-pressure quenched-flow reactor suitable for kinetic studies of molecular catalysts in ethylene polymerization?

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Temperatures profiles

One important question concerns the evolution of the temperature in the reactor. The equation below was used to prove that the adiabatic temperature rise is lower than 1°C ($\Delta T = 0.1$-0.5°C), even in case of monomer consumption higher than 10%.

$$\Delta T = \frac{Q \cdot Mw}{(C_p \cdot \rho \cdot V)}$$

(2)

Where

$C_p$ is given by eq. $C_p = C_1 + C_2 T + C_3 T^2$ whit $C_1 = 140140$, $C_2 = -152.3$, $C_3 = 0.695$ for toluene

$\rho$ is the toluene density = 0.87 g·ml$^{-1}$;

$V$ is the volume which was passed through the Teflon tube;

$M_w$ is the molar mass of toluene = 92.14 g·mol$^{-1}$;

The released heat, $Q$, is given by the product between $\Delta H$ of polymerization and the mol of monomer consumed. The value of $\Delta H$ of polymerization is 25 kcal·mol$^{-1}$.

A series of tests were carried out where we measured the temperature in tubular reactor in order to evaluate the difference temperature between inlet and outlet of the reaction tube. The $\Delta T$ during the ethylene polymerization with the catalyst system I/MAO was measured using two K thermocouples. The first thermocouple was positioned in point 3 (see Fig. 1 in the paper), replacing the T-mixer with a cross-mixer; the second one was placed in point 5 at the end of tubular reactor. The temperature profiles in Fig. S1 are relative to runs 4 and 5 carried out using tubular reactor of 2 m and run 1 carried out using tubular reactor of 0.5 m which corresponds to residence times of 0.51, 0.7 and 0.09 s respectively, and ethylene consumption up to 6%.
For tests at short reaction times, the ΔT measured was lower than 0.5°C, furthermore for reactions carried out at long reaction time we observed a maximum of 1°C, which means that even for long reaction time the heat release during the polymerization is negligible.
Fig. S2. SEC profiles of polymers obtained with catalyst II/MAO/tBu$_2$-PhOH (runs 7 (a) and 8 (b))