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# Modelling and simulation of inhibition-injection systems applied to polymerization reactors

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**Abstract**

The most critical aspect of polymerization reactors is the agitator's stop and becomes more serious when this occurs exactly at the removal of the heat load, which is generated by the reaction (exothermic). This phenomenon is typical in power-failure situations of the energy supply or because of other related problems at the plant. The objective of this work is to compare the performance of two configurations for the inhibition-injection system for vinyl chloride monomer (VCM) polymerization reactors. To determine the injection time a rigorous mathematical model was developed. From the results of this work one of the configurations was implemented in an industrial plant.


*Keywords:* Injection system; Inhibition; Reactors; Polymerization; Modelling; Simulation

## 1. Introduction

Uncontrolled reactions during polymerization processes are the cause of most incidents (McIntosh & Nolan, 2001). In particular, the vinyl chloride monomer (VCM) polymerization can lead to enormous catastrophes in the reactor and release VCM to the environmental (AIChE, 1993; Papp, 1990). However, unlike the pressure-relief systems, there are very few papers on the inhibition system projects, especially on the inhibition-injection method and its efficiency (McIntosh & Nolan, 2001).

The critical aspects of the projects involving inhibition-injection systems are (McIntosh & Nolan, 2001):

- Detection method of an uncontrolled reaction or with tendencies to runaway;
- Definition of the performance method of the inhibition system;
- Difficulty of homogenization of a small amount of the inhibitor in the reaction mass;
- Location and number of injectors;
- Timing and duration of the injection.

The time interval between the agitator's stop and the injection of the inhibitor solution should be as small as possible; usually, less than 2 min. However, considering monomer removal as a tool to be used during the inhibition, some industrial plants have established a limit of 5 min as an efficient injection (AIChE, 1993; McIntosh & Nolan, 2001; Papp, 1990).

According to Papp (1990), in a study including producers of poly vinyl chloride (PVC), 7 of the 25 plants considered confirmed the application of an automatic system for injection of the polymerization inhibitor. However, almost all the big producers of PVC have an automatic system. The most important objective is to have a plant without any kind of interference by the operational

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**Nomenclature**

| | |
|---|---|
| $A_p$ | area of the discharge pipe, $m^2$ |
| $A_V$ | area of the vessel, $m^2$ |
| $d$ | diameter of the discharge pipe, m |
| $F_w$ | force of the walls on the fluid, N |
| $F_N$ | normal force on the wall at the bottom of the vessel, N |
| $F_A$ | friction force on the fluid, N |
| $f_D$ | Darcy friction factor |
| $f_F$ | Fanning friction factor |
| $g$ | gravitational acceleration, $m/s^2$ |
| $H_V$ | liquid vessel height, m |
| $H_p$ | liquid pipe height, m |
| $L_{Eq}$ | equivalent length of the liquid in the pipe, m |
| $m_{tot}$ | total mass of inhibitor (holdup in the vessel and discharge pipes), kg |
| $M_{tot}$ | global momentum of the volume element, kg m/s |
| $P_R$ | pressure in reactor (outlet discharge pipe), atm |
| $P_g$ | gas pressure, atm |
| $Re$ | Reynolds number |
| $t$ | time, s |
| $v_p$ | average velocity of the inhibitor at the outlet discharge pipe, m/s |
| $v_v$ | average velocity of the inhibitor at the vessel, m/s |
| $V_{tot}$ | total liquid volume, $m^3$ |
| $V_g$ | occupied volume by the gas, $m^3$ |
| $V_i$ | initial volume of gas in the vessel, $m^3$ |
| $V_s$ | initial volume of inhibitor in the vessel and pipe, $m^3$ |

*Greek letters*

| | |
|---|---|
| $\varepsilon$ | roughness of the discharge pipe, m |
| $\rho$ | density of the inhibitor, $kg/m^3$ |

team, to maintain the safety of the plant (Fitzpatrick, 2001), considering the fact that a dependence of the operator's action may become a critical factor in emergency situations.

Usually, the inhibitor for each reactor is previously prepared and stocked in a special vessel, under a pressure of nitrogen ($N_2$). Some plants have 2 vessels, allowing a double dosage. Other plants use 2 types of inhibitors: a moderate one, for regular control, and a more active one, for emergency cases. Nevertheless, according to Papp (1990), there are two approaches for the pressure of $N_2$: high continuous pressure and increasing pressure when necessary.

Due to the importance of the inhibition system to control runaway reactions, interlocks are used to guarantee the reserve of the inhibitor, for example, no permission for the load of VCM if the level in the inhibitor vessel is low or if the pressure of $N_2$ is low (AIChE, 1993).

The objective of this work is to compare the performance of two configurations of inhibition systems for VCM polymerization reactors. The rigorous mathematical model developed was used to determine the total time of injection of the inhibitor for both configurations, as well as for the condition where the injection occurs by gravity. The validation of the developed model was accomplished by the implementation of one of the configurations at an industrial plant.

## 2. Injection system

Fig. 1 displays an outline of the proposed injection system, which consists basically of a pressurized vessel with $N_2$ to inject inhibitor in the bulk of the mixture, through a valve that is installed in the wall of the polymerization reactor. Two alternatives are considered, but most parts of the equipment and instrumentation are common. The basic difference between them is the means of pressurization.

For alternative I, once the vessel is filled with the inhibitor solution, it is pressurized with high-pressure $N_2$ and kept like this during the normal operation of the reactor. The total volume and pressure of the vessel are calculated to inject all the mass of inhibitor into the reactor. At the moment when the injection begins, the

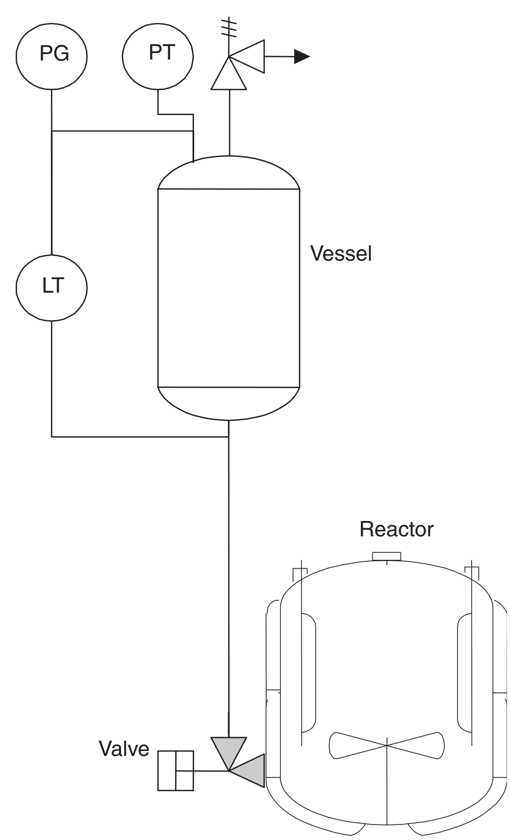


Fig. 1. Inhibitor reaction injection system.