Emulsion polymerization process control

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Abstract **– A dynamic model for the emulsion polymerization of styrene within an emulsion batch reactor has been studied. The model includes the main steps for styrene polymerization, along with the relevant balance equations. The resulting set of differential equations was solved for the temperature profile and monomer consumption as a function of time. Emphasis was put on the reaction temperature, which is controlled by the jacket temperature. The controller loop, which determines the flow rate of the cooling/heating fluid, is also included. Finally, the advantage of having a rigorous control system in order to have the desired properties in the final product was analyzed.**

Index Terms**—Batch reactor; Control; Emulsion; Polymerization, Scale-up.**

I. NOMENCLATURE

A	Heat transfer are (m^2)
C_{Pr}	Heat capacity of reactor contents (J/g°C)
C_{Pj}	Heat capacity of water in the jacket (J/g°C)
F_C	Cold flow water (L/s)
F_H	Hot flow water (L/s)
k_p	Propagation kinetic constant (L/mol s)
M	Monomer (mol)
n	Average number of radicals per particle (-)
N_T	Particle concentration (1/L)
P	Power input by stirred (W)
$Q_{J,Loss}$	Heat losses from jacket (W)
$Q_{R,loss}$	Heat losses from reactor (W)
R_P	Reaction rate (mol/L s)
T_J	Jacket temperature (°C)
T_r	Reactor temperature (°C)
U	Heat transfer coefficient (W/m^2 K)
V	Reactor volume (m^3)
x	Conversion (-)
ΔH	Heat of polymerization (J/mol)
$_V$	Viscous dissipation
ρ	Density (kg/L)

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II. INTRODUCTION

Emulsion polymerization has grown to become one of the major means for the production of synthetic polymers. There are substantial incentives for improved design and control of emulsion polymerization reactors [1, 2]. To achieve these aims the problem of the scale up laboratory data is crucial [3]. Polymerization reactions are very complex reaction systems characterized by a strong change in the viscosity and high exothermicity, which is often accompanied by auto-accelerating kinetics that can lead the system into uncontrollable situations and nonlinearity characterize polymerization processes [4]. Many industrial polymerization reactions are carried out in batch reactors. In emulsion polymerization, monitoring and control of monomer conversion is crucial both for proper process operation and for obtaining products with desired properties (due to the influence of conversion of polymer molecular weight and particle size distributions)[5,6].

Polymer reaction engineering is a discipline that deals with various problems concerning the fundamental nature of chemical and physical phenomena in polymerization processes. Mathematical modeling is a powerful tool for the development of process understanding and advanced reactor technology in the polymer industry [7-9]. The application of process models to the design of model-based reactor optimizations and controls is considered in this paper.

III. GLOBAL ENERGY BALANCE FOR THE BATCH REACTOR.

The global energy balance, performed in the batch reactor, see fig 1., includes the system energy dynamic behavior, which considers the heat generated from the exotermic reaction; as well as the energy loss to the surroundings, the interchange of heat between the jacket and the reaction system, including the heat induced by the stirrer, and the global difference temperature that exists in the reactor, according to its material properties.