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Enhancement of a Semi-Batch Chemical Reactor Efficiency through its Dimensions Optimization

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Abstract

Efficiency of manufacturing processes is very important in today's competitive world with hard economic rules. In chemical engineering area the efficiency depends on the production heart, which is often a chemical reactor. In this paper authors describe process of optimal semi-batch exothermic reactor dimensions finding. The task is to find reactor dimensions which lead to process efficiency improving, i.e. to processing the greater chemicals amount in the same or shorter time. The optimizing process uses an objective function which includes also the reactor mathematical model. The objective function is modified here to find better results and necessary limitations and penalizations are used to improve the dimensions searching. An evolutionary approach represented by the Self-Organizing Migrating Algorithm (SOMA) was used to minimize the defined function. A suitability of the reactor with newly found dimensions was then verified by the process control simulations.

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Keywords: Temperature control; Online identification; Semi-batch reactor; Exothermic process; SOMA

1. Introduction

Even if the problem of the chemical reactors efficiency is quite important and is connected with the reactor dimensions, there are not many studies published about the reactor dimensions optimization these days. Usually, the process is placed to existing vessel and then the authors try to control the process with different control techniques. But, the process is often not suitable for the given reactor geometry. Here, the authors are trying different way – to suite the reactor geometry to the exact process – to achieve the best control results.

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Some published papers which describe an effect of a reactor size on the process control are mentioned further. The „performance“ of three bubble column reactors with the same volume but varied geometry (height to diameter ratios – 0.93; 2.04; 3.98) was investigated in [1]. It was demonstrated, that larger height-to-diameter ratio could enhance CO_2 capture efficiency. Paper [2] tries to observe more efficient membrane reactor setups in order to improve production yield. Optimization has been carried out by a differential evolution considering 40 decision variables including dimensions of membrane reactor. The authors concluded that the obtained variables improved the „performance“ of the continuous catalyst regeneration reformer process. Park et al. [3] developed a 2D mathematical model of a pilot-scale fixed-bed reactor for a Fe-based Fischer-Tropsch synthesis. The developed model clearly showed the effects of the tube diameter on the temperature profiles, in terms of the radial heat transfer area. Varga et al. [4] tried to find optimal feeding profile of fed-batch chemical reactor. The optimal feeding profile was generated with sequential quadratic programming, classical evolutionary strategy and the advanced version of evolutionary strategy based on covariance matrix adaptation. Any publications dealing with a semi-batch reactor dimensions optimization to compare it with here presented results were not found unfortunately.

Our paper is organized as follows: In section 2, the semi-batch reactor, its structure, mathematical model and the process control are described; section 3 presents simulation results and section 4 concludes the current work and suggests new areas for investigation.

2. Methods section

2.1. Current situation

In past different control techniques have been applied on fed-batch reactor presented in this paper [5,6,7]. The goal was to optimize the reactor temperature using two manipulated variables (the reactor feeding and the cooling water temperature) to achieve the shortest possible one batch cycle time.

Nomenclature

A [s^{-1}]	Pre-exponential factor
$a_{FK}(t)$ [-]	Mass concentration of the chromium sludge
c_{FK} [$J.kg^{-1}.K^{-1}$]	Chromium sludge specific heat capacity
c_R [$J.kg^{-1}.K^{-1}$]	Reactor content specific heat capacity
c_v [$J.kg^{-1}.K^{-1}$]	Coolant specific heat capacity
E [$J.mol^{-1}$]	Activation energy
ΔH_r [$J.kg^{-1}$]	Reaction heat
K [$J.m^{-2}.K^{-1}.s^{-1}$]	Conduction coefficient
k [s^{-1}]	The reaction rate constant
$m(t)$ [kg]	Weight of the reaction components in the system
$\dot{m}_{FK}$ [$kg.s^{-1}$]	Mass flow of the entering chromium sludge
$\dot{m}_v$ [$kg.s^{-1}$]	Coolant mass flow
m_{vR} [kg]	Coolant mass weight in the reactor double wall
R [$J.mol^{-1}.K^{-1}$]	Gas constant
S [m^2]	Heat transfer surface
$T(t)$ [K]	Temperature of reaction components in the reactor
T_{FK} [K]	Chromium sludge temperature
$T_v(t)$ [K]	Temperature of coolant in the reactor double wall
T_{vp} [K]	Input coolant temperature