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Implementation of the Dynamic Modeling for Development of Chemical Processes

Liz Mabel Ríos Hidalgo[1]*, Ronaldo Santos Herrero[2], Belkis Guerra Valdés[1]
Luis Manuel Peralta[2], Guillermo Esperanza[1]

[1]Study Centre of Applied Chemistry. Central University of Las Villas, Highway to Camajuani km $5^{1}/_{2,}$ Santa Clara. Villa Clara, Cuba. CP: 54830
lizrh@uclv.edu.cu

[2]Department of Chemical Engineering. Central University of Las Villas

In this work we study the behaviour of reactants systems highly complex through the modeling of the dynamic process of synthesis, by means of the obtaining of a phenomenological dynamic model that can simulate the behaviour of these systems, which involves multiple reactions in liquid phase.
Its objective is develop methods and mathematical procedures for evaluating and predict the behaviour of complex reactions and highly dangerous, achieving integrated design semi continuous stirred tank type reactors while minimizing the consumption of material resources, reducing the dumping of waste into the environment and adding more security working with hazardous products.
The methodology proposed for the integral design of the reactor involves the main geometric parameters of the reactor design, as they relate to the main variables of the technological process, considering the efficiency, controllability and process safety. To be scheduled on a dynamic simulation system allows not only a comprehensive analysis itself, but also the simultaneity of the fundamental calculations of the reactor design. By optimizing the overall design of the reactor can find the best values for the geometric design parameters, considered in the sensitivity analysis, based on technical economic indexes of the process and its controllability.
With programs developed on PSI, was able to obtain profiles of these variables, consistent with the values taken in the experimental runs developed convincingly validated phenomenological models made in the development of programs. The models obtained allow us to assess the sensitivity of the processes against different failures and / or accidents, especially for the synthetic processes of hazardous substances, which is achieved by predicting the course of the reactions (usually exothermic systems) of safely. The simulated various types of process, achieving adequate results, allowing the design of plants with a high degree of reliability. The integrated design, that includes the optimization of operating parameters and fundamental geometric dimensions of semi continuous stirred tank reactors with heat transfer, to minimize material

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consumption in the manufacturing process and reactor. There are no known histories of design methodologies integral reactor, as proposed here.

1. Introduction

The increased complexity faced by the reactor dynamics simulation lies in the need for kinetic models can describe the desired accuracy, variations in the concentrations of reactants and products during the course of the reactions (Goya and Peralta, 2004). For the specific cases before us are not performed experimental kinetic studies since there are no applicable methods, so it is assumed kinetic mechanisms based on the literature.
In the chemical reactor design is necessary with several different specialists; the leading role belongs to the chemical engineers, mechanical and automatic control. The choice of normal construction and reactor principal dimensions and materials of construction and the determination of operating parameters and other data necessary for design, does a chemical engineer, based on the production process chosen to calculate chemical-specific technology and the environment they work. The mechanical engineer chooses the standard equipment and prepares the non-standard equipment in this selection process and / or design is guided by technical and regulatory elements set out in existing codes in each country. The automatic control engineer designs the system ensures automatic control and process safety. It follows, then, that success depends on the design efficiency is achieved with the combination or integration of efforts of different specialists involved in it. This comprehensive approach to design was raised (Dickey, 1991), there are other references, he discusses deeply the fundamentals of technical design a chemical reactor, made a brief reference to process control, and defends the view that the design full and proper to consider also the consequences of mechanical design, in this respect, refers only to calculate the minimum diameter tree agitation system and the thickness of the walls of reactor. However, theoretical analysis on the design of chemical reactors does not address real possibility and necessity of integral design, methodology or provides a solution to this problem (Dickey, 1991). Some authors like, (Viera, 1991), indicated some mechanical aspects, in addition to the technical design, as is the calculation of the thickness of the walls of the reactor, but not proposing an integrating link for the design of reactor. Other works, like technological design integrated with process control, using mathematical modelling and dynamic simulation, in these cases is not designed the reactor, including all basic dimensions (Luyben and Floudas, 1994). All this results in that in the practical design of reactors, chemical and technological aspects of process control, and mechanical design, remain separate branches, with their characteristics and specific problems.
The proposed mathematical modelling and dynamic simulation is effective to achieve this connection. These techniques have evolved as a prime tool for efficient design of reactors, to determine optimum operating conditions and evaluate the sensitivity of the process against various types of failure, providing a considerable benefit, since it guarantees the control of enhances the security of the production process and product.

2. Methods used and experimental conditions

For the development of phenomenological models were taken as base complete-differential equations posed by (Rios and Peralta, 2004), related to the design of mathematical modeling. Definition of the physical - chemical and basic data of the system studied by the literature or experimental studies, coming to define the stoichiometric equations and kinetic mechanisms proposed. On this basis, we performed mass balance unsteady state of each element involved in the process and energy balances required for the processes under study.

Software were implemented in the equations obtained above, in this case was used the PSI. For the approach, in the phenomenological model of differential equations of the balance of elements in the reactor in semi-continuous operation, were considered the terms of input, output and accumulation of mass and energy.

As an example of application of mathematical modeling and dynamic simulation of the reactor design shown in working for a technology viable in the conditions of the country, for the treatment of wastewater contaminated with nitro aromatic compound (TNR) using hypochlorite sodium. This compound is dissolved in the wastewater from the production process can form metal salts and very sensitive compounds that accumulate can lead to accidents, hazardous to human health and the environment, which is why it is vitally important disposal. The role of treatment is to achieve the destruction and elimination of aromatic nitro compound wastewater from the synthesis, purification and washing of this product.

First, it conducted a detailed study to establish the optimal process conditions for the treatment of wastewater aromatic nitro compound, carrying out experiments that different designs, from the study of the influence on the % removal of the concentration aromatic nitro compound in the reaction with sodium hypochlorite (NaClO) are: pH, concentration ratio TNR: Sodium hypochlorite: r c (TNR) / c (NaClO), sodium hypochlorite concentration: C (NaClO), agitation speed: Vag., Response Time: treac. Temperature: T. The proposed technology consists of the following steps: addition of hypochlorite, aeration, dechlorination, neutralization and sedimentation. The wastewater will undergo a filtration process, from where they will spend a reactor (Reactor 1) equipped with agitation to contact sodium hypochlorite (NaClO) arriving from a feeder tank. During this stage there is an oxidation reaction occurring total bleaching wastewater. After treatment with hypochlorite are a number of gases dissolved in these waters as $Cl_{2\ (g)}$, so is the aeration process in another type stirred tank reactor (Reactor 2), in order that these gases dissolved in move wastewater to dissolve into the air and can be evacuated (for this was studied in air flow l/h and the aeration time needed). In the same reactor, subsequently passed to the dechlorination process which removes dissolved chlorite and chlorate to make them react with sodium thiosulfate ($Na_2S_2O_3$) to 10% to be reduced to chloride.

To facilitate and expedite the calculations related to the technological design of tanks equipped with agitation was used the computer program "PSI", which allowed scaling, model and simulate the stages with chemical reaction, in addition, given its configuration, can be used in other projects that require such equipment design. Below is an example of the use of digital simulation for the design of these stages, developed by Rios and Peralta (2004).

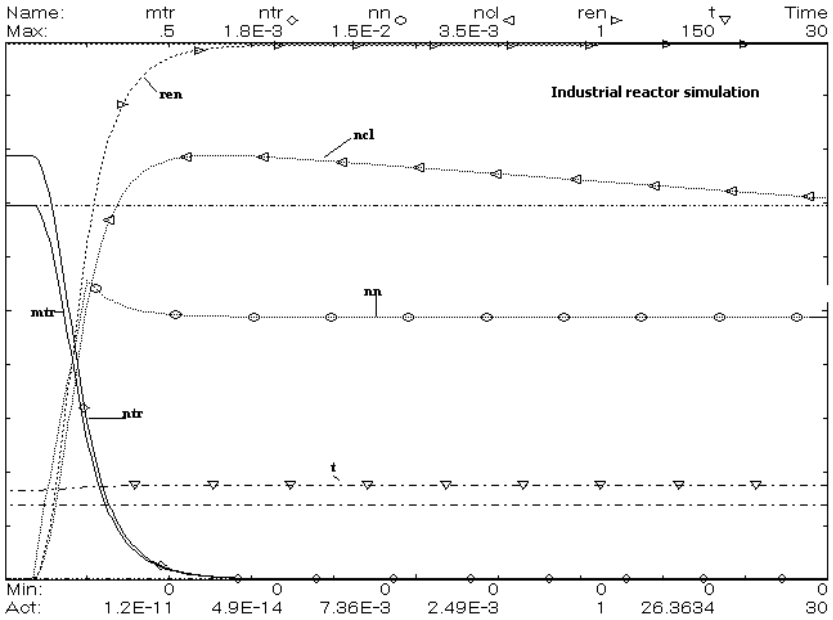

Figure 1: Performance of the different variables in the simulation of reactor number one industrial scale.

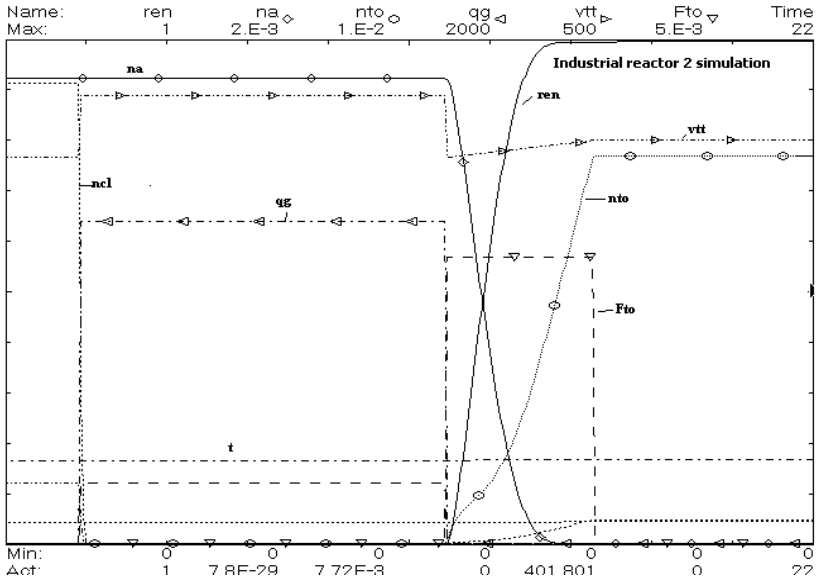

Figure 2: Performance of the different variables in the simulation of two industrial-scale reactor.

The graphs represent some of the most representative variables of the programs, and their values were taken at the end of reaction time, with the dynamic model can be

represented graphically and find the resulting values at any instant of time, either programmed variables.

The design method of the reactors was based on designs of experiments performed at laboratory scale and with this data model was conceived on an industrial scale using the scaling method to obtain background information on the level of mixing, ensuring the actual conditions obtaining mixing at the industrial level.

An analysis of the graph showing the results of the simulation of one industrial scale reactor we can conclude that both the mass of the product TNR (mtr), as the number of moles (ntr) become zero at about six minutes of chemical reaction. In turn, the performance (ren) in this time interval is very close to 100 %. The number of moles of sodium hypochlorite (nn) increases to the extent that the same be added and finally reaches a stable value. The number of moles of chlorine (ncl) increases progressively until the sixth minute and on that slowly decreases progressively. The heat of reaction was determined experimentally and found that there are no problems with heat transfer. The temperature remains fairly constant, showing that a value exceeding 20 % does not create problems or raising the temperature or heat transfer.

An analysis of the graph showing the results of the simulation of two industrial-scale reactor can be concluded that in the first stage of treatment shows that the number of moles of chlorine (ncl) is zero as air is added with a flow value constant, during a time of 12 min. The number of moles of chlorate (na) remains constant until it begins the second stage of treatment in which the addition of sodium thiosulfate chlorate makes disappear about 16 minutes after the start of the reaction. The number of moles of sodium thiosulfate (nto) will increase as it adds up that takes a constant value at the end of the reaction. Likewise, the power flow of sodium thiosulfate (Fto) increases rapidly at first takes a constant value and decreases to zero when it completes its addition. The total volume of wastewater (vtt) undergoes an increase, which takes a constant value, with bubbling air, then takes the initial value during the second phase will increase as will adding sodium thiosulfate to reach a constant value. The gas flow (qg) ensures total dispersion of gas in the vessel and was determined experimentally and industrial scale at which we calculated the dimensions and parameters of an air bubble in a ring. The modelling and simulation studies of chemical reaction steps showed that there are no problems with heat transfer and the temperature remains almost constant throughout the interval, reaching the end of treatment a yield 100 %, approximately 16 minutes, which confirms the accuracy and reliability of the experimental results.

2.1 Integral Design

Comprehensive design stirred tank type reactors semi involves consideration of several factors, among which are: agitation system design, heat transfer requirements and requirements for process control and safety. This methodology involves the main geometric parameters of the reactor design, as they relate to the main variables of the technological process, considering the efficiency, controllability and process safety. To be scheduled on a dynamic simulation system allows not only a comprehensive analysis itself, but also the simultaneity of the fundamental calculations of the reactor design. The technological design of the reactor is referred to the mass and energy balances of each of the components involved in the reactions, both of which have already been addressed by developing mathematical models of the processes.

The scaling should be considered as part of the comprehensive methodology. Is recommended to apply a scaling procedure, with a fundamental approach for dynamic modeling, from understanding the process in sufficient detail, by studying at smaller scales. The combination of scaling itself with the dynamic modeling allows a correct prediction and integral operation in the reactor on a larger scale.

3. Conclusions

• With programs developed on PSI, was able to obtain profiles of these variables, consistent with the values taken in the experimental runs developed convincingly validated phenomenological models made in the development of programs. The models obtained allow us to assess the sensitivity of the processes against different failures and/or accidents, especially for the synthetic processes of hazardous substances, which is achieved by predicting the course of the reactions of safely.

• The methodology proposed for the integral design of the reactor involves the main geometric parameters of the reactor design, as they relate to the main variables of the technological process, considering the efficiency, controllability and process safety. To be scheduled on a dynamic simulation system allows not only a comprehensive analysis itself, but also the simultaneity of the fundamental calculations of the reactor design. By optimizing the overall design of the reactor can find the best values for the geometric design parameters, considered in the sensitivity analysis, based on technical economic indexes of the process and its controllability.

• The simulated various types of process, achieving adequate results, allowing the design of plants with a high degree of reliability. The integrated design, that includes the optimization of operating parameters and fundamental geometric dimensions of semi continuous stirred tank reactors with heat transfer, to minimize material consumption in the manufacturing process and reactor. There are no known histories of design methodologies integral reactor, as proposed here.

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