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Concurrent Engineering Reactor Design

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Abstract

A system of softwares was developed in order to aid chemical reactor operation and design, as a tool to define operational policies and support process engineers. A C++ software, using artificial intelligence techniques, acts as an Expert System, guiding the user throughout reactor simulation and providing results in an easily comprehensible form. A Fortran software was used to simulate a reactor, including a neural network algorithm to estimate the rate of reaction. The C++ environment works together with the Fortran reactor simulator and a Fortran neural training software. This linked structure is considered part of the "concurrent engineering" study area. As a case study, the Expert System was applied to a fixed bed reactor for ethanol oxidation to acetaldehyde, over a Fe-Mo catalyst.

Keywords: Artificial intelligence, Concurrent engineering, Computer Aided Design, CAD, Neural networks.

1. Introduction

In modern chemical plants, process is controlled by a digital distributed system (DCS), under operator supervision. Recently, the role of these operators have shifted from direct responsibility for control to a supervision status, including identifying abnormal situations and determining the necessary actions to be taken when the process is not stable (like inevitable feedstock changes). For that, simulation tools are effective to help them modify rapidly and safely the process to the proper condition. Even when the system is normal (that is, operating at nominal conditions), a fail can occur, resulting in a shutdown or a risky situation. Early detection of such situations and quick diagnosis of faults require insight into the operational performance and anything that assists this task is clearly a competitive advantage and a useful tool.

Quantitative and qualitative techniques (such as property databases, optimisation procedures, steady state and dynamic simulation, operation training) have been available for some time. Recently, techniques from artificial intelligence field have been adapted to help in using these packages cooperatively and have been especially effective in speeding up the response time of operators (Wang et al., 1994).

This has encouraged the development of diagnostic expert systems for process evaluation: the computer acts as a specialist, analyzing data and showing conclusions

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about the simulation and the operation. This technique is part of the Artificial Intelligence field (Bugaeva et al., 1996).
A neural network was used in this work to predict the rate of reaction. It is an important tool for process simulation in cases where deterministic models are not available. The net must be trained for the first time, introducing it to a set of pairs [input, output]. An iterative adjustment of the *weights* occurs, trying to minimize the difference between calculated outputs and the actual outputs. Once the optimal weights were obtained, it is possible to predict outputs from new inputs (Bhagat, 1990; Wasserman, 1989).

2. Architecture of the Environment

The software tools developed for carrying out the simulation and its analysis include:
1. Neural network training software (Fortran);
2. Reactor simulator (Fortran);
3. Expert system (C++), responsible for the analysis of the simulation.

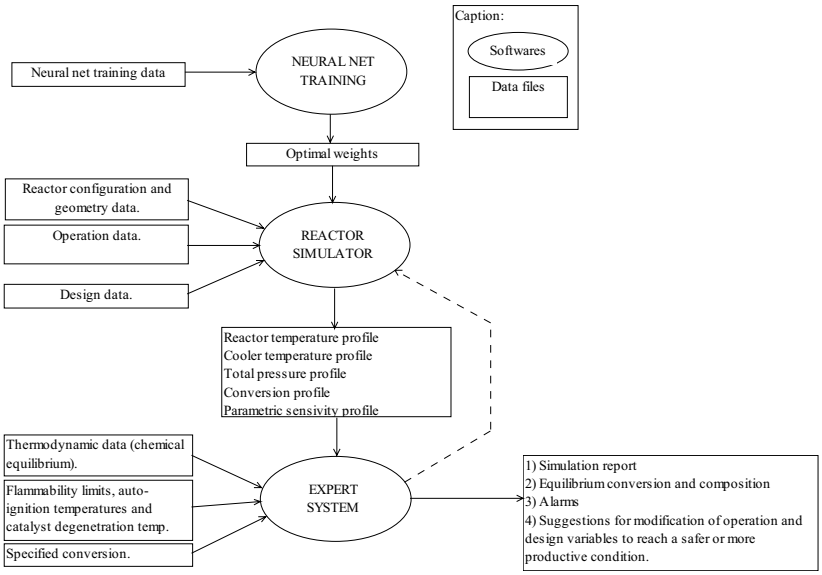

Figure 1. The environment structure

Figure 1 shows the linked system of softwares, and the information stream between them (the dashed line means that the expert system controls the reactor simulator). This crosslinked architecture allows an efficient execution of all softwares in order to simulate the system, including concepts of concurrent engineering. The techniques discussed on this paper can be applied to any system or equipment, but for computing ends, it was necessary to choose a case study to be implemented: the ethanol oxidation to acetaldehyde, under air stream, in a fixed-bed tubular reactor filled with Fe-Mo catalyst. The chemical equation is showed in Eq.1:

$$C_2H_5OH + \tfrac{1}{2}\, O_2 \rightarrow C_2H_4O + H_2O \qquad (1)$$

3. Reactor Simulator: the core of the system

The reactor simulator is based on mass, energy and momentum balance differential equations, solved simultaneously by fourth-order Runge-Kutta numerical method.
Input data involve operating and design parameters, like inlet feed temperature, inlet cooler temperature, inlet pressure, feed flow, cooler flow, air to ethanol molar ratio, reactor length, tube diameter, type of configuration (concurrent or countercurrent), catalyst particle diameter and catalyst density.
Inlet temperature, cooler temperature, feed flow and cooler flow were chosen as operation variables. Reactor length, tube diameter, particle diameter and inlet pressure were chosen as design variables. Simulation outputs are reactor temperature, coolant temperature, conversion, total pressure and parametric sensitivity profiles.
The parametric sensitivity, as defined by Rodrigues (1994), measures the variation of reactor temperature, as a response for a given variation in a selected inlet variable (coolant inlet temperature). This parameter gives an indication about the stability of the reactor, and allows the detection of unsafe conditions, helping to avoid system runaway.
Reaction rate is calculated by a neural network sub-routine, using the weights determined by the training software. The input variables to the net are: conversion, temperature, pressure and feed composition (air to ethanol molar ratio). The output of the net is the rate of reaction. The neural net approach was used to allow the software to be generic for cases when the operation data are available but the reaction rate is not. The net was trained with data used in previous work (Maciel Filho, 1985). Input data range from 0 to 1.0 for conversion, from 463 to 679 K for temperature and from 1.8 to 2.2 atm for pressure.

4. Expert System

The expert system is a C++ software developed to analyze reactor data simulation and eventually it calls the simulator itself. The reports emitted help the operator in making decisions and previewing dangerous situations.
This software is structured in modules, each one with a particular function:
Chemical equilibrium module: computes equilibrium conversion for the chemical reaction studied, using parameters given by the user: stoichiometric coefficients, enthalpy of formation of the species, Gibbs free energy of species, polynomial equation for heat capacity (Sandler, 1989). Other information is given by simulator, like mean reactor temperature and feed composition. The software calculates the equilibrium conversion and the equilibrium stream composition at the end of reactor. Finally, the system shows how far the reactor is from the maximum conversion.
Operational variables study: carries out a study of the influence of operational variables on process variables. The inlet feed temperature, feed flow and cooler flow were chosen as operational variables. The process variables were maximum reactor temperature (hot spot), mean reactor temperature, final conversion, pressure drop and maximum parametric sensitivity.
Alarms: deals with extreme or risky situations. Some information must be given by user, as specified conversion, catalyst degenerating temperature, flammable species, auto-ignition temperature of species, flammability limits, maximum pressure drop.

Once abnormal situation is detected, the expert system pops an alarm and it suggests a new condition to avoid the problem or risky situation.

Design variable study: performs a study about the influence of design variables on process variables, in order to help designing this type of equipment. The reactor length, tube inside diameter, catalyst particle diameter and inlet total pressure were chosen as design variables. The process variables are: maximum reactor temperature (hot spot), mean reactor temperature, final conversion, pressure drop and maximum parametric sensitivity.

Condition of non-degeneration of catalyst: calculates the values of operational variables to which the catalyst degenerating temperature is not overcome. In this case, the maximum temperature in reactor is below the catalyst degenerating temperature (281 ^{o}C). Process variables at this condition are also calculated.

5. Results and Discussion

The system of softwares was executed for an example condition in order to depict its features and potentialities. At first, the chemical equilibrium module is activated, computing data given in Table 1. Note that acetaldehyde production in the simulated case is very close to equilibrium condition. This is in fact a possible operation condition as shown experimentally by Maciel Filho (1985) and discussed in a scale up of the process studied by Domingues and Maciel Filho (1992).

The next step is to report process variables at simulated condition, showed in Table 2.

Table 1. Chemical equilibrium data

Parameter		Value	Unit
Equilibrium conversion		0.999992	
Specified conversion		0.99	
Simulated conversion		0.9994	
Acetaldehyde production:	Equilibrium condition	2.559	moles/h
	Simulated condition	2.533	moles/h

Table 2. Process variables

Parameter	Value	Unit
Mean temperature	228	^{o}C
Maximum temperature	328	^{o}C
Final conversion	0.9994	
Pressure drop	0.025	Atm
Maximum parametric sensivity	52	

The alarm module is then executed, giving the following warnings:

Alarm 1: auto-ignition temperature of acetaldehyde (130 ^{o}C) was overcome, but there is no explosion risk, once its concentration is outside flammability limits (4,0 - 60,0 %);

Alarm 2: reactor temperature is too high, causing catalyst degeneration. Immediately, the expert system calls the “non-degeneration condition” module, and suggests to lower inlet feed temperature to 198 ^{o}C (maximum possible value), maintaining the original value of the other parameters. The module also advises that at this condition, the reactor

temperature in any point will be smaller than catalyst degeneration temperature, but the final conversion will decrease to 0.92.

Pressure drop at simulated case is smaller than the limit value (0.2 atm), and final conversion is above the specified one (0.99). No alarms are emitted in these cases.

The “operational variables study” module generates 15 graphs, correlating maximum temperature, mean temperature, final conversion, pressure drop and maximum parametric sensitivity to inlet feed temperature, feed flow and cooler flow. Figure 2 shows some of these graphs related to feed flow study.

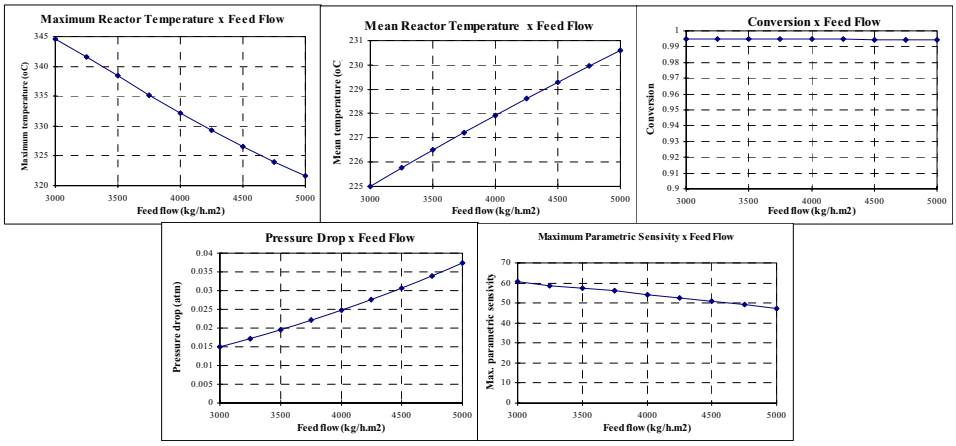

Figure 2. Operational variables study graphs.

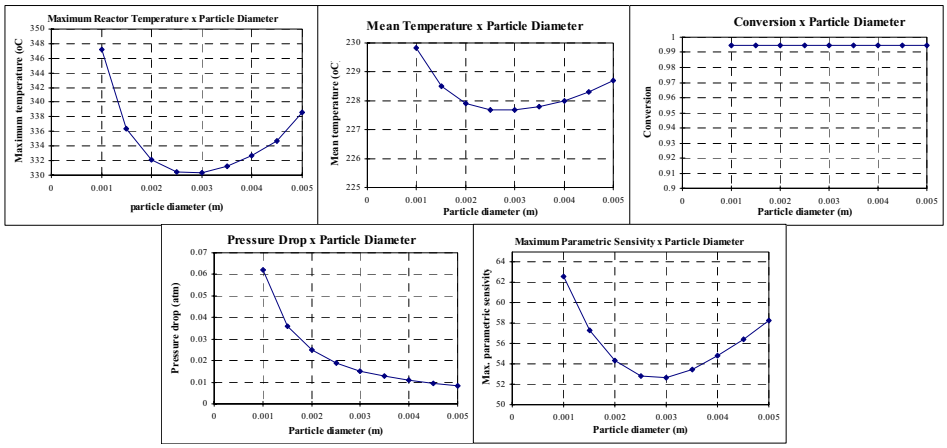

Figure 3. Design variables study graphs

Based on this study, the operator can foresee what is going to happen in case of some change in operational variables and take an action to maintain the process at an optimum condition or avoid an unsafe operation. In this case, the parametric sensitivity will raise from 54 to 60, indicating that reactor temperature will be less stable.

The “design variables study” module generates 17 graphs, correlating maximum temperature, mean temperature, final conversion, pressure drop and maximum parametric sensitivity to tube diameter, catalyst particle diameter, inlet total pressure,

plus a reactor length graph and a partial pressure profile of all compounds in reactor. Figure 3 shows some of these graphs related to particle diameter.
The goal of these graphs is to aid designing this type of equipment, looking for optimal operational conditions. For example, let us suppose that the task is to determine the best catalyst particle diameter to be used in the reactor. After having executed the simulation, studying particle size influence in the range from 1 mm to 5 mm, the graphs in figure 3 are available to take such decision. The maximum reactor temperature, mean reactor temperature and maximum parametric sensitivity graphs show that particle diameter from 2.5 to 3.0 leads to a highest heat transfer and gives the reactor more stability.
Having this information in hand, design engineer does not need to ask for experimental work or may reduce the number of experimental runs in order to decide which is the best particle size to be used.

6. Concluding Remarks

A system of softwares was presented, based on concurrent engineering principles, in order to perform an intelligent simulation of fixed-bed chemical reactors. A C++ environment was developed as a tool for aiding plant operators in making rapid decisions to determine new operating conditions when process is changed and also for supporting engineers to design more effective equipments and determine the best operational policy.
Neural nets algorithms were included in a FORTRAN reactor simulator to estimate the rate of reaction, at given conversion, temperature and pressure. Comparison between neural nets and the rate model showed good agreement (Papes, 1994). The neural training process was carried out by a FORTRAN software also developed in this work.
As an example, the system of softwares was applied to the reaction of ethanol oxidation to acetaldehyde, over Fe-Mo catalyst, in a tubular reactor. Some of the graphs generated by the system were showed, illustrating the benefits of this tool in assisting operation and design of chemical reactors. Limitations of space have not permitted other examples to be given but they were equally successful (Papes, 1999, 2004).

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