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Analysis of the runaway in an industrial heterocatalytic reactor

Tamás Varga[a], Ferenc Szeifert[a], József Réti[b], János Abonyi[a]

[a]*University of Pannonia, Egyetem street 10.,Veszprém H-8201, Hungary, vargat@fmt.uni- pannon.hu*
[b]*Borsochem Ltd., Bolyai tér 6., Kazincbarcika H-3700, Hungary*

Abstract

This work focuses on runaway behaviour of industrial catalytic tube-reactor and presents how decision trees can be used for forecasting the runaway. The steady-state simulator of the reactor and runaway criterion based on Ljapunov's indirect stability analysis have been used to generate the database used by the decision tree induction algorithm. The extracted logical rules can be used in an operator support system (OSS), and are useful for working out safe operating strategies.

Keywords

Reactor runaway, forecast, stability analysis, decision tree.

1. Introduction

Reactor runaway means a sudden and considerable change in the process variables that is a serious problem in many chemical industrial technologies, like oxidation processes and polymerization technologies [1-3]. For example in case of a highly exothermic thermal runaway occurs when the reaction rate increases due to an increase in temperature, causing a further increase in temperature and hence a further increase in the reaction rate. It has contributed to industrial chemical accidents, most notably the 1984 explosion of a Union

Carbide plant in Bhopal, India that produced methyl isocyanate. Thermal runaway is also a concern in hydrocracking, an oil refinery process.

Detection of runaway has two main important aspects. On one hand runaway forecast has a safety aspect, since it is important for avoiding the damage of reactor's constructional material or reactor explosion; on the other hand it has a technology aspect, since the forecast of the runaway can be used for avoiding the development of hot spots in catalytic bed, which speed up the ageing of catalyst. A control system which is able to modify accordingly the operating conditions of reactor in time decreases the costs and increases the safety of operation. The first step to develop such control system is the generation of a reliable runaway criterion.

Most of runaway criteria found in literature are data- or model-based criteria [4-6]. To apply data-based criterion it is necessary to have some measured data that means restrictions on the forecasting the development of runaway. Other problem with data-based methods is found in measurement conditions, e.g. measurement noise can result in false forecast. The model-based criteria require parameter sensitivity and/or stability analysis, so for the application of these kinds of criteria it is necessary to have exact process model with correct model parameters.

This work presents a novel approach of runaway criteria based on data-mining technique. To generate the necessary learning samples for inducting the decision tree, the steady-state model of reactor is worked out and Ljapunov's indirect method is applied to study the model stability under a set of pre-defined operating conditions. The obtained tool is suitable for forecasting reactor runaway based on measured feed parameters.

In addition to development of steady-state simulator of reactor, the work also proposes a detailed dynamic model to make possible further investigations of runaway. For the solution of dynamic model the kinetic constants of material transfer processes and reaction which takes place in solid phase are also needed. The identification of these parameters are based on process data collected during the operation of the technology. It will be shown that the developed dynamic simulator and runaway criteria are applicable for the sophisticated analysis of the runaway behaviour of the studied industrial reactor.

2. Mathematical model of the reactor

The studied vertically build up reactor contains a great number of tubes with catalyst as shown in Fig. 1a. The second order reaction $\mathrm{A}+\mathrm{B}\rightarrow\mathrm{C}$ occurs as the reactants rise up the tube pass the fixed bed of catalyst particles and the heat generated by the reaction escapes through the tube walls into the cooling water.

Our purpose is to obtain an easily comprehensible runaway criterion by using data mining technique such as decision tree method. The necessary learning samples for applying this technique are generated by stability analysis of steady-state model. Generation of the Jacobian-matrix of this model is the first

step in application of Ljapunov's indirect method to investigate stability of model. It is followed by the examination of eigenvalues of the Jacobian-matrix. In case all of eigenvalues are negative than the model is stable but if one of eigenvalues is over zero than model is unstable in the investigated part of reactor. To further investigate the development of runaway in the reactor a detailed dynamic model is needed. To make clear what the detailed word means let us show the structure of dynamic model on Fig. 1b. with notation of the connection at each hierarchy level. A more detailed presentation of models and the developed simulators based on these models can be found on http://fmt.uni-pannon.hu/softcomp. Both of the models are solved by using MATLAB®.
The dynamic behavior of reactor can be obtained by solving the mass and heat balances partial differential equations at both of solid and gas phases in tubes and the cooling water in jacket. The steady-state model can be obtained from dynamic model by elimination of that part of equations which is differentiated with respect to time. Past this elimination the following simplification is made: the reaction takes place in gas phase; temperature distribution of the solid and gas phase are equal; temperature distribution of jacket is constant.
An experimentally measured reaction rate is applied in the steady-state model [7]. The calculated and measured temperature profiles give a good correspondence.

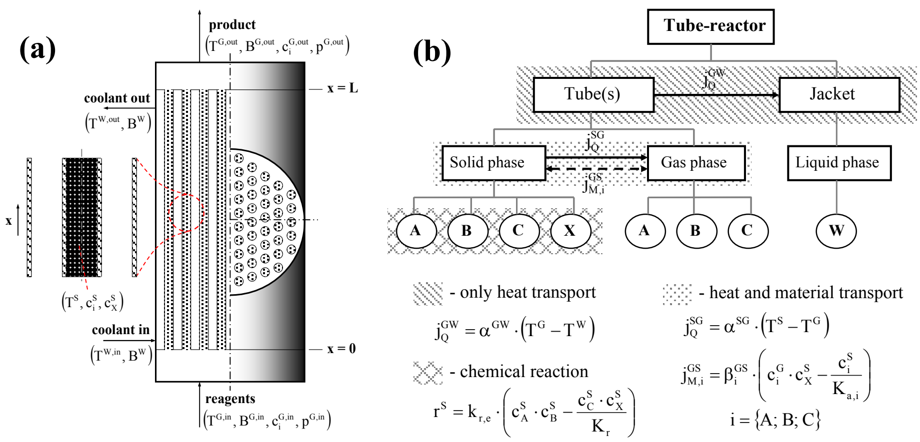

Fig. 1. (a) Scheme of the reactor. (b) Structure of detailed dynamic model: X means the active spots on the surface of the catalyst. In expressions *j* means the heat (*Q* in sub script) or component (*M*) flux density between the 2 phases noted in sup script. *α* and *β* mean the heat and component transport coefficient while *K* signs the reaction (*r* in sub script) and adsorption (*a*) balances.

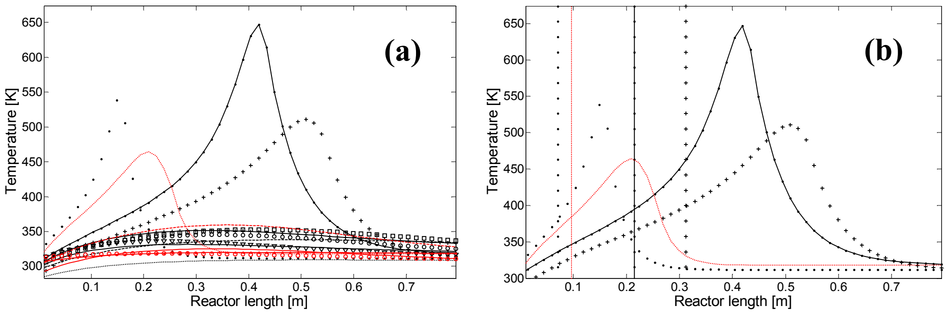

Fig. 2. (a) The calculated steady-state temperature profiles at every generated inlet conditions and (b) the profiles when runaway occurs by using stability analysis. The vertical lines on (b) show the first unstable point at each case.

3. Decision tree based runaway forecast

Learning from examples, i.e. concepts acquisition, is one of the most important branches of machine learning that has been generally regarded as the bottle-neck of expert system development. For this purpose a wide range of models and identification algorithms have been developed. Among them, through the paper binary decision trees are applied to create rule-based of the classifier. A binary decision tree consists of two type of nodes: (i) internal nodes having two children, and (ii) terminal nodes without children. Each internal node is associated with a decision function to indicate which node to visit next. Each terminal node represents the output of a given input that leads to this node, i.e. in classification problems each terminal node contains the label of the predicted class [8]. An illustrative example for a decision tree is given in Fig. 3. As this figure illustrates such model is easily interpretable, so it can be easily integrated into an operator support system.

4. Results

4.1. Applicability of stability analysis

The first step of the implementation of the decision tree based runaway forecasting system is to check the applicability of the stability analysis for detecting runaway development at a set of randomly selected inlet conditions. As Fig. 2. illustrates the analysis of the eigenvalues of the Jacobian-matrix at the operating points calculated by the steady-sate simulator gives reliable results. However, it is quite difficult to implement this approach in an industrial environment.

4.2. The novel method for detecting reactor runaway

The results of the previously presented stability analysis performed in case of a great amount of randomly generated inlet conditions are proper for gathering learning samples to obtain a decision tree that is suitable for forecasting the reactor runaway based on only the measured feed parameters. On Fig 3. from left to right can get from root to the leaves of the tree. In a decision tree the leaves contain the answer of the investigation in this case 1 means runaway doesn't occur while 2 means the opposite. The algorithm found the cooling water inlet temperature has the main effect and reagent inlet temperature has the least impact in development of runaway.

$T^{W,in} <= 306.59$:
| $T^{W,in} <= 296.333$: 1 (384.0/8.2)
| $T^{W,in} > 296.333$:
| | $p^{G,in} <= 1.37308$:
| | | $n^{A,in} > 4.25926$: 1 (138.0/9.4)
| | | $n^{A,in} <= 4.25926$:
| | | | $n^{B,in} > 2.52618$: 1 (19.0/4.6)
| | | | $n^{B,in} <= 2.52618$:
| | | | | $p^{G,in} <= 1.24615$: 1 (13.0/6.5)
| | | | | $p^{G,in} > 1.24615$: 2 (11.0/4.2)

Fig. 3. A part of the inducted decision tree where $n^{i,in}$ is $B^{G,in} \cdot c_i^{G,in}$. The first value in the brackets gives the amount of the learning samples which can be sorted using the previous conditions. The learning algorithm depends on information gain, the algorithm counts this value at each of the inlet parameters in a nodes of the tree and chooses one of these parameters with the highest value. The second number in the brackets means the numeric value of information gain.

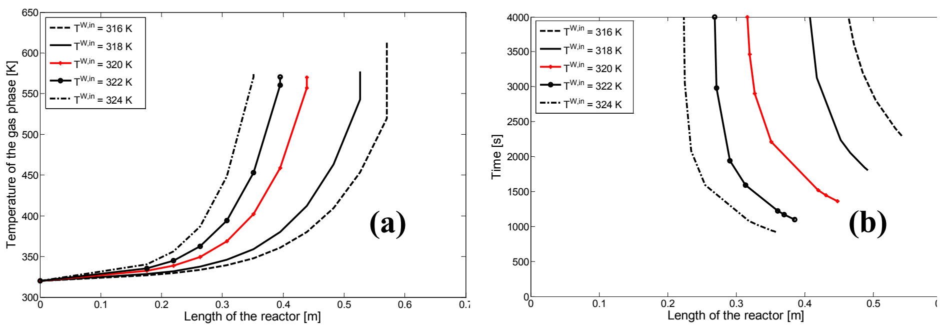

Fig. 4. The movement of maxima (a) and the unstable point (b) along the catalyst bed at different cooling water inlet temperatures.

4.3. Movement of the boundary of the stability

To investigate the development of runaway in geometric space the detailed dynamic model must be solved and the stability analysis must be applied at every time step. It is presented earlier that the cooling water inlet temperature has the main impact in development of reactor runaway. The obtained results shown in Fig. 4 have a good correspondence with this conclusion. Due to the increase of the temperature the boundary of the stability is coming closer and closer to the front of the reactor and it develops earlier in time too.

5. Conclusions and future work

This work demonstrated a new method using a data mining technique to detect runaway in a heterocatalytic reactor. The results show that the proposed decision tree based approach is able to distinguish between runaway and non-runaway situations based on a set of linguistic rules extracted from data obtained by the analysis of the steady state model of the process. The result of this analysis can be easily incorporated into an operating support system and can be applied for the selection of the critical operating variables.

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