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The role of dynamic process models for the detection of safe operating regions of process systems

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ABSTRACT

Determining safe regions of operations is important at the design, control and optimization of process systems. E.g. process alarms and safety systems should be designed based on such knowledge. In classical control systems these regions are represented as independent values (constraints) on process variables. This representation is does not consider the interaction of the process variables, and moreover it gives a static view of the process. The paper reviews the importance of the representation of the safe operating regions from an industrial application point of view and the recent tools developed for model-based alarm management. The importance of the application of dynamical analysis of process models is highlighted. A detailed case study is given where this dynamical approach has been applied to determine boundaries of operating regions of a catalytic tube reactor.
(Keywords: operating region, process model, stability analysis, safety)

ÖSSZEFOGLALÁS

A dinamikus folyamatmodellek szerepe a biztonságos üzemeltetési tartományok feltárásában

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A termelő technológiák biztonságos üzemeltetési tartományainak ismerete mind a technológia tervezése, mind irányítása és optimalizálása során egyaránt fontos szempont. Például a technológia alarm rendszerét a folyamat biztonságos üzemeltetési tartományainak feltárása során szerzett tudáson alapulva kellene megtervezni. A klasszikus irányító rendszerekben a biztonságos üzemeltetési tartományok leírása az állapotváltozókra megfogalmazott egymástól független korlátokkal történt. A tartományoknak ez a fajta bemutatása nem veszi figyelembe az állapotváltozók közötti összefüggéseket, vagyis azokat, mint független változókat kezeli, illetve csak egy statikus képet ad a folyamatról. A cikk a biztonságos üzemeltetési tartományok leírásának fontosságát egy ipari alkalmazás kapcsán mutatja be, illetve az utóbbi időben a modellbázisú alarm-kezelés támogatására kifejlesztett eszközökről ad egy rövid leírást. A folyamat modellek dinamikus analízisének fontosságát szem előtt tartva egy esettanulmányon keresztül mutatja be a cikk a kidolgozott dinamikus megközelítésmód alkalmazását egy állóágyas csőreaktor üzemeltetési tartományainak meghatározása során.
(Kulcsszavak: üzemeltetési tartományok, folyamat modellek, dinamikus analízis, biztonság, stabilitás vizsgálat)

INTRODUCTION

Nowadays beside the improvement of the overall process performance, the maintenance of the safe operation conditions is the key element in the development of process control systems. To improve the product quality, to reduce energy and materials waste, and to increase the flexibility of production, the process operators require more insight in the dynamical behavior of the process. In the rush to take advantage of computer-based automation, many companies in the processing industries worldwide have overlooked one of the most important individuals in their business value chain – the plant operator. The plant operator is the forgotten knowledge worker. He is on the frontline of real-time operations, making decisions that directly impact plant safety, reliability, profitability, and ultimately shareholder value. Operators – like other knowledge workers – analyze information, diagnose situations, predict outcomes, and take action to deliver value. While the optimal operating conditions of production processes are getting closer and closer to physical constraints, more and more important is the development of knowledge based expert systems for supporting the operators to keep the operation conditions in this narrow range. Next to this requirement it is necessary that an expert system is able to detect failures, discover the sources of faults and forecast the false operations to prevent from the development of production breakdowns (*Adler and Enig*, 1964; *Barkelew*, 1959).

A process alarm is a mechanism for informing an operator of an abnormal process condition for which an operator action is required. The operator is alerted in order to prevent or mitigate process upsets and disturbances. A poor functioning alarm system is often noted as contributing factor to the seriousness of upsets, incidents, and major accidents. Significant alarm system improvement is needed in most industries that utilize computer based distributed control systems; it is massively common and serious problem. Most of companies have become aware that they need to thoroughly investigate and understand their alarm system performance. Alarm management is a fast growing, high profile topic in the process industries.

The BP Upstream Technology Group proposed five-level scale using the following nomenclature: Overloaded, Reactive, Stable, Robust, and Predictive. Technology to fully achieve the Predictive performance level is still experimental and “bleeding edge”. In ideal case, Predictive performance will involve the following kinds of techniques:

- *Early fault detection*: The early detection of the deviation of the process or equipment from its normal operation by monitoring a set of process variables. Deviations can be detected even when all the process variables are individually within their operating and alarm limits.
- *Early fault diagnosis and advice:* The operator is advised within specific actions needed to prevent the upset from occurring.
- *Procedual automation*: The automation of standard and emergency operating procedures associated with both normal plant transitions (e.g. start-up, shutdown, product change, and so forth) as well as critical corrective actions to recurring disturbances. {procedual automation allows for both on-line sequence execution and monitoring of steps in procedure as well as collaboration between field and control room board operators.
- *Extensive uses of operator support systems* involving pattern recognition, adaptive graphics, artificial intelligence, and other new experimental methodologies.

Predictive alarm management is important goal since the operator’s ability to respond to an alarm in a timely fashion determines the degree of success in preventing loss. The consequences if an uncorrected alarm generally worsens with the passage time. During an abnormal condition, the board operator is confronted with making of decisions on numerous tasks that must be performed in an appropriate sequence. The timing and the order of executing these tasks determines the outcome of the operator's effort. For example, if two process variables deviating from the normal and can potentially cause the same significant loss, the operator must quickly decide which variable to address first. In such a case, the operator must take an action to address the variable that is more volatile or can reach the point of loss in the shortest time. Therefore, the shorter the time available to respond, the higher the priority of the alarm will be, assuming equal consequences can result.

This problem is most relevant at the early detection of reactor runaway. 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. For example in case of a highly exothermic reaction 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 while the reactants are depleted. In case of less complex systems the stable and unstable operating regimes of a reactor can be analytically determined. The stability analysis is a powerful tool to determine the boundary of stable operation conditions. Such investigation can be based on the analysis of the mathematical of the reactor model with Ljapunov's indirect stability analysis method. This method is based on the analysis of eigenvalues of Jacobian matrix which contains the first-order partial derivatives of the model with respect to state-variables.

In this paper it will be shown that the possible (thermal) runaway of reactors should be forecasted till the time instant the runaway can be avoided by the optimal control of the process. This requires predictive stability analysis (for predictive alarm management). For this purpose in this work a model based technique is worked out, where the Ljapunov's indirect stability analysis of the state variables along simulated trajectories are used to detect the boundary of the controllable region of the process. In this paper the term controllability means that at given state of the process it is possible to find a future control trajectory to maintain the safe operation and to avoid of the reactor runaway, i.e. a command signal is need to be obtained to keep the state-variables of the system in the stable region. In case of a state is not controllable there is not any signal will ever be able to control the state. In this article the boundary of controllability represents states of reactor and if state-variables of the reactor cross this limit during the operation the operator cannot do anything to avoid the development of reactor runaway.

As it has been mentioned predictive alarm management systems should be able not only to the early detection of the alarm, but also to give advice to the operators. As it has been suggested, such system should apply artificial intelligence and pattern recognition for this purpose. For this reason, in this work decision tree induction techniques are applied to form the interpretable boundaries of the safe operating regions. To introduce this novel approach of controllability a heterocatalytic tube reactor is analyzed and the temperature of the reactor is controlled by the heat removing through the jacket.

After the long introduction about the investigated problem and the possible solutions the most important features of classical and predictive stability analysis are collected. It is followed by the introduction of the developed algorithm to determine the boundary of controllability and the investigated case study is shortly presented. Finally the obtained results and some important conclusions are summarized.

MATERIAL AND METHOD

With a control system which is able to forecast and perform some modifications in operating conditions to avoid the development of reactor runaway the operating costs can be decreased while the safety of production is improved. The first step in the development of such control system is the generation of a reliable runaway criterion. Most of runaway criteria found in literature can be classified as data- or model based (*Adler and Enig*, 1964; *Barkelew,* 1959; *Lacey,* 1983). To apply data-based criterion it is necessary to have some measured data that makes impossible to apply a data-based criterion to forecast the development of runaway. Other problem with data-based methods is found in measurement conditions, e.g. measurement noise can result false detections. Model-based criteria require parametric 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.

In advanced model based techniques the reactor runaway is detected through the stability analysis of the process model, e.g. by Ljapunov's indirect method (*Sastry*, 1999). Generation of the Jacobian-matrix of reactor model is the first step in application of Ljapunov's indirect method to investigate stability of reactor. 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 at the investigated operating point.

Ljapunov's stability analysis is suitable in detection of the development of runaway and the algorithm based on this stability analysis can separate cases whether the runaway occurs in the reactor or not. However, it is quite difficult to implement this criterion in an industrial environment. Furthermore, it is applicable to detect when the runaway has been occurred, which is interesting from the analysis of historical process data point of view, but it is not usable for on-line process monitoring and control, where the operator is interested in the region of the safe operation and the last time instant when the runaway can be avoided by the control system.

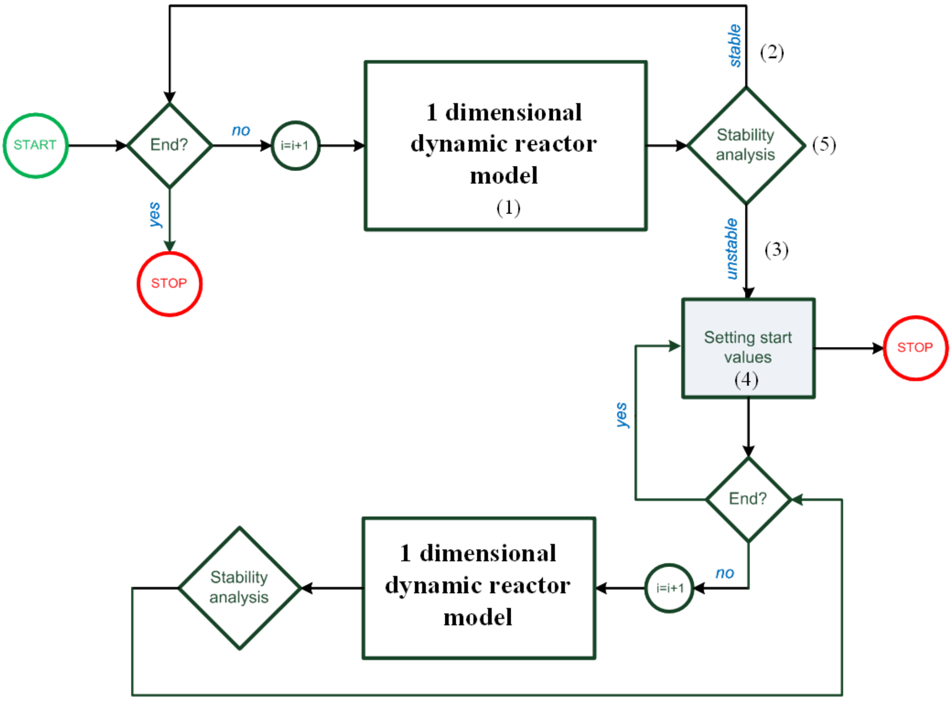
For the predictive analysis of the process not only a detailed (accurate) process model is needed, but also a process simulator that is able to estimate the trajectories of the process variables in case of normal and abnormal operations. This simulator should be also able to model the dynamical behavior of controlled system, including its safety elements. The extracted knowledge from the process model is extremely important since these elements of the system define and sometimes "enlarge" the region of safe operation.

To allow the industrial implementation of the proposed approach an algorithm was worked out to detect the boundary of stability and controllability of the process in the space of the most important process variables. Such knowledge is extremely useful, since it can be interpret as (multivariate) constraints defined on process variables that can be given to operators of the process, built into the control system, or into an optimization algorithm used for the optimization of the operation. In the next part of this section the developed algorithm will be described.

As *Figure 1* illustrates the first step of the proposed methodology is the application of the classical Ljapunov's stability analysis to detect the stability of the reactor model. In our previous works we introduce that Ljapunov's indirect method gives reliable results in forecast of reactor runaway (*Varga et al.*, 2006; *Varga et al.*, 2007). The dynamic reactor model is applied to calculate all profiles of state-variables in every time step and in every calculated point along the reactor the choosing stability analysis method is applied to check the stability. In case instability is detected at least in one point of reactor then the investigated inlet condition is labeled as runaway occurs, but if the applied criterion does not sign the inlet condition is labeled as runaway does not occur.

Figure 1

Flow sheet of the developed algorithm



1. ábra: A kidolgozott algoritmus folyamatábrája

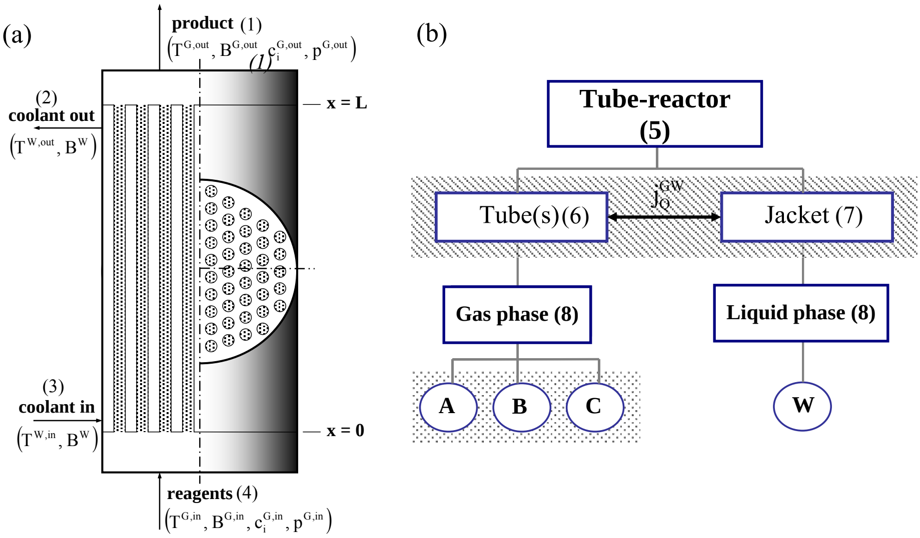
1 dimenziós dinamikus reaktor modell(1), Stabil(2), Instabil(3), A keresés kezdeti értékének rögzítése(4), Stabilitás vizsgálat(5)

In case of the algorithm cannot find at least one unstable state during the whole operation then the algorithm stops and trajectories of state-variables are plotted. Otherwise it starts to search for the last controllable operating point. In a reactor with a highly exothermic reaction the development of reactor runaway cannot be avoided in every case by performing the most dramatically manipulations such as closing down the reagent dosing because of the accumulation of the reagent(s). Hence, it is important to recognize the last controllable state of the reactor and immediately perform necessary control actions (manipulations) to avoid the runaway. In this step the algorithm checks which determined manipulations can be capable and when it needs to be performed. The algorithm makes one step back in time and investigates the stability of the modified model. If it is stable the analyzed state is labeled as the last controllable state. Otherwise the algorithm makes another step while it finds a stable state. To speed up searching for the last controllable state the secant method is applied in the algorithm.

To introduce the worked out algorithm a vertically build up reactor contains a great number of tubes with catalyst as shown on *Figure 2a* was studied. A highly exothermic reaction occurs as the reactants rising 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. Due to the exothermic reaction it has a great chance to develop hot spots somewhere in catalyst bed which increase the rate of catalyst ageing. The selection of operating conditions is important to avoid the development of reactor runaway and to increase the lifetime of catalyst. The dynamic simulator of the reactor was worked out to analyze the development of runaway phenomenon and it was built into the introduced algorithm to calculate profiles of state-variables.

Figure 2

Scheme of the investigated heterocatalytic reactor(a) and the structure of dynamic reactor model(b)



2. ábra: Az ipari reaktor sémája(a) és a kidolgozott dinamikus modell struktúrája(b)

Termék(1), Hűtőközeg ki(2), Hűtőközeg be(3), Reagensek(4), Csőreaktor(5), Csövek(6), Köpenytér(7), Gázfázis(8), Folyadék fázis(9)

As it can be seen in model structure in *Figure 2b*, process variables calculated only in the gas phase in the worked out one dimensional model but in the heat balance of tubes the heat capacity of catalyst bed is also considered. Before model equations are presented some assumptions must be performed. These assumptions are summarized as follows:

- only the gas phase is considered in tubes;
- reaction takes place in the gas phase;
- to calculate the rate of reaction the Langmuir-Hinselwood kinetic is modified with the term which is considered the reaction equilibrium;.
- the temperature of the gas and solid phase are equal;
- to calculate the pressure drop in the reactor a modified Ergun-equation is applied.

The mean of model parameters and variables are summarized in the notation list. Based on the introduced model assumptions the balance of each component mass is the following:

$$V^G \cdot \frac{\partial c_i^G}{\partial t} + \frac{d\left(B^G \cdot c_i^G\right)}{dx} = \upsilon_i \cdot V^S \cdot r^G \ , \tag{1}$$

where i = {A; B; C}. The temperature of reactor and jacket are calculated with the next correlations:

$$V^G \cdot \rho^G \cdot c_p^G \cdot \frac{dT^G}{dt} + B^G \cdot \rho^G \cdot c_p^G \cdot \frac{dT^G}{dx} = V^S \cdot r^G \cdot \left(-\Delta H_r\right) - A^{GW} \cdot j_Q^{GW} \tag{2}$$

$$V^W \cdot \rho^W \cdot c_p^W \cdot \frac{dT^W}{dt} + B^W \cdot \rho^W \cdot c_p^W \cdot \frac{dT^W}{dx} = A^{GW} \cdot j_Q^{GW} \ . \tag{3}$$

The reaction rate is calculated based on Langmuir-Hinselwood expression:

$$r^G = k_0 \cdot \exp\left(-\frac{E_A}{R \cdot T^G}\right) \cdot \frac{\left(p_A^G\right)^{n_a} \cdot \left(p_B^G\right)^{n_B} - \dfrac{p_C^G}{K \cdot \left(p_A^G\right)^{1-n_A} \cdot \left(p_B^G\right)^{1-n_B}}}{1 + \left(p_C^G\right)^{n_C}} \ , \tag{4}$$

where the reaction equilibrium constant is the function of temperature:

$$K = \exp\left(A - \frac{B}{R \cdot T^G}\right) \ . \tag{5}$$

As it mentioned in the assumptions the pressure drop on catalyst bed is calculated by a modified Ergun-equation:

$$\frac{dp^G}{dx} = -2 \cdot f_c \cdot \frac{\rho^G \cdot \left(B^G\right)^2}{d_p \cdot (A)^2} \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot \left(1.75 + 150 \cdot \frac{1-\varepsilon}{Re}\right) \ , \tag{6}$$

The worked out model has been implemented into MATLAB. The developed dynamic simulator is built into the earlier introduced algorithm to simulate the dynamic behavior of reactor.

RESULTS AND DISCUSSION

The aim of this work to investigate a tube reactor with a highly exothermic reaction when must be manipulations performed to keep the reactor in controllable region and which manipulate variable must be modified. To solve this problem a searching algorithm was developed based on reactor model and Ljapunov's indirect stability analysis. Stability analysis of the process model is used to detect unstable operating points. The algorithm was introduced in more detail in the previous section. The development of temperature profiles in case of reactor runaway occurs can be seen in *Figure 3a*. The temperature maximum is moving in front of the flow it is important because there is no need to investigate the stability of the model after the temperature maximum so as the maximum is moving towards to the feeding point the boundary of the unstable region is moving in the same way. The result of stability analysis can be seen in *Figure 3b*. As it can be seen the first unstable operating point is detected at 128 s, so the reactor runaway occurs in this operation and there is need some modification to be performed before this time. The boundary of unstable region is moving as we predicted in the reactor.

The goal is to choose and perform a manipulation to avoid the development of runaway. The proposed algorithm can be applied to determine the boundary of controllability of reactor but to apply the algorithm the possible manipulations need to be determined. In this case study 5 possible manipulations are considered and summarized in *Table 1.*

Table 1

Investigated manipulations

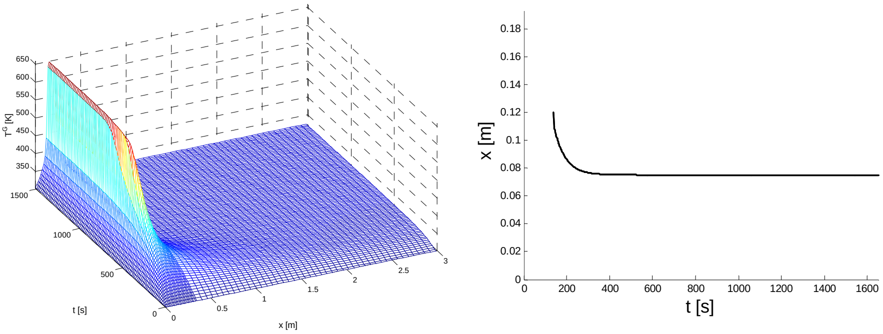
	c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Original (1)	52.8	18.1	1.80	320	320
Modified (2)	0	0	1.25	290	290

1. táblázat: A vizsgált beavatkozások

Eredeti üzemeltetési paraméterek(1), Módosított üzemeltetési paraméterek (2)

Figure 3

Simulated temperature profiles in gas phase(a) and the result of stability analysis of reactor model(b)



(a) (b)

3. ábra: A gázfázisbeli hőmérsékletprofilok alakulása(a) és a reaktor modell stabilitás vizsgálatának eredménye(b)

The algorithm checks all the considered manipulations at six different operating regimes. The rate of feeding of reagents is modified to generate different operating conditions. Results are summarized in *Table 2.* Reactor runaway develops every investigated operating regions and the time of the first detected operating point based on Ljapunov's indirect stability analysis can be found next to the first unstable term in each case. The last controllable term means that operating point when the investigated manipulations need to be performed to avoid the development of runaway. In the last row the time difference between the first unstable and the last controllable operating points is calculated. In the first experiment 2 of the possible 5 manipulations cannot be used to avoid the runaway, it is represented with infinity sign in the last row and with the concentration of reagent B is the perfect choice in this region to prevent the operation from runaway because there is enough 1 s before the detection to decrease the concentration to 0 to keep the reactor in the stable state. Further analyze the results can be seen that this manipulation does not work in all of investigated regimes (see Exp. III. and V.). There is one operating regime (Exp. III.) in which none of investigated manipulations are capable to avoid runaway only 1 s before the development of runaway is detected. The concentration of reagent A and the inlet temperature of cooling media can be applied in all operating regimes to prevent from runaway.

Table 2

Results of controllability analysis

Exp. I.: original operating conditions (3)						
First unstable: 128 s (1)		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable (2)	**[s]**	90	127	0	0	115
Δt	**[s]**	38	1	∞	∞	13
Exp. II.: the feeding mass of reagent B is increased with 10% (4)						
First unstable: 121 s		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable	**[s]**	89	120	0	0	96
Δt	**[s]**	32	1	∞	∞	25
Exp. III.: the feeding volume of reagent B is increased with 200% (5)						
First unstable: 134 s		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable	**[s]**	109	0	0	0	128
Δt	**[s]**	25	∞	∞	∞	6
Exp. IV.: the feeding volume of reagent B is increased with 190% (6)						
First unstable: 130 s		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable	**[s]**	106	129	0	0	122
Δt	**[s]**	24	1	∞	∞	8
Exp. V.: the feeding volume of reagent A is decreased with 66.7% (7)						
First unstable: 164 s		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable	**[s]**	108	0	163	0	163
Δt	**[s]**	56	∞	1	∞	1
Exp. VI.: the feeding volume of reagent A is decreased with 65% (8)						
First unstable: 158 s		c_A [mol/m^3]	c_B [mol/m^3]	p^G [bar]	T^G [K]	T^W [K]
Last controllable	**[s]**	105	157	0	0	157
Δt	**[s]**	53	1	∞	∞	1

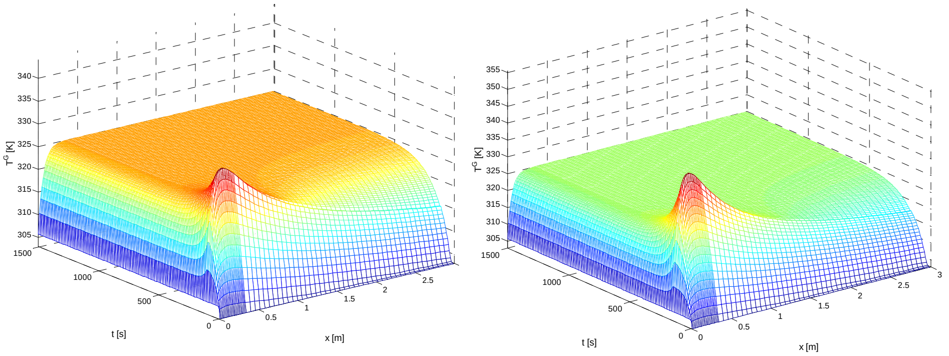
2. táblázat: A reaktor kézben tarthatósági vizsgálatának eredménye

Első instabil munkapont(1), Utolsó kézben tartható munkapont(2), Eredeti üzemeltetési paraméterek(3), B komponens térfogatárama 10 %-kal növelve(4), B komponens térfogatárama 200 %-kal növelve(5), B komponens térfogatárama 190 %-kal növelve(6), A komponens térfogatárama 66.7 %-kal csökkentve(7), A komponens térfogatárama 65 %-kal csökkentve(8)

To check the reliability of results chosen manipulations by the algorithm are tested and the simulated results are plotted in *Figure. 4*. It is well seen that applied manipulations are capable to avoid runaway and keep the reactor in safe operation regime in case there are performed in proper time.

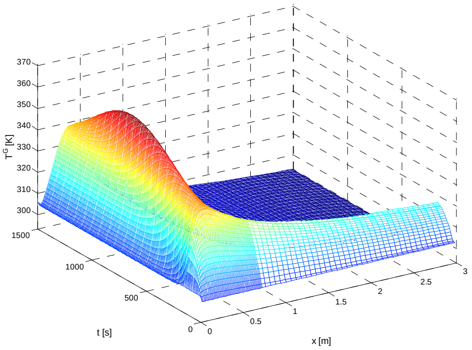
Figure 4

Checking results provided by the developed algorithm in case of the original operating condition



Concentration of reagent A is decreased to 0 at 90 s (1)

Concentration of reagent B is decreased to 0 at 127 s (2)



The inlet temperature of cooling media is decreased to 290 at 115 s (3)

4. ábra: A kidolgozott algoritmussal kapott eredmények ellenőrzése az eredeti üzemeltetési paraméterek esetén

A komponens koncentrációja 0-ra csökkentve a 90. másodpercben(1), B komponens koncentrációja 0-ra csökkentve a 127. másodpercben(2), A hűtőközeg belépő hőmérsékletének csökkentése 290 K-ra a 90. másodpercben(3)

CONCLUSIONS

The operation of complex production processes is one of the most important research and development problems in process engineering. Predictive process alarm management is an important concept that should be continuously researched and developed. This paper showed that the possible (thermal) runaway of reactors should be forecasted to avoid uncontrollability of the process. For this purpose a method for model based predictive stability analysis has been worked out, where the Ljapunov's stability analysis of state variables along simulated trajectories are applied to detect the boundary of the controllable region of process. An algorithm was worked out to test possible manipulations in avoiding the runaway. Applying the developed algorithm in different operating regimes five manipulations were investigated how long before the detection of runaway need to be executed. The algorithm can be used to reveal all the stable operating regimes. These regions can be easily interpreted by operators and process engineers, and can be implemented in real-time process monitoring and/or on-line process optimization algorithms. The developed methodology has been applied to an industrial benchmark problem. Further research will focus on how the extracted knowledge can be transformed into a set of constraints on the process variables and how these constraints can be applied in process optimization and alarm management.

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NOTATION LIST

Notation	**Meaning**	**Unit**
α^-	Heat transfer coefficient	$\frac{W}{m^2 \cdot K}$
A^-	Contact area	m^2
A	The cross-section area of the catalyst bed	m^2
B^-	Volume velocity	$\frac{m^3}{s}$
c_i^-	Concentration, where $i = \{A;B;C\}$	$\frac{mol}{m^3}$
c_p^-	Heat capacity	$\frac{J}{kg \cdot K}$
ΔH_r	Heat of the reaction	$\frac{J}{mol}$
d_p	Diameter of the catalyst particle	m
ε	Ratio of the volume of solid phase and the volume of catalyst bed	-
E_A	Activation energy	$\frac{J}{mol}$
j_Q^-	Heat flux density	$\frac{W}{m^2}$
K	Reaction equilibrium	-
k_0	Pre-exponential factor	$\frac{mol}{m^3 \cdot s}$
υ_i	Stoichometric coefficient	-
p^-	Pressure	Pa
p_i^-	Partial pressure of components	Pa
r^-	Rate of the reaction	$\frac{mol}{kg \cdot s}$
R	Ideal gas constant	$\frac{J}{mol \cdot K}$
Re	Reynold's number	-
ρ^-	Density	$\frac{kg}{m^3}$
T^-	Temperature	K
V^-	Volume	m^3
x	Reactor length	m
Superscipts		
G	Gas phase	
S	Solid phase	
W	Jacket	
GW	Transport between gas phase and the jacket	