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Analysis of controlled CSTR models with fluctuating parameters and uncertain parameters

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Abstract

In this paper, a detailed stability analysis of PI controlled CSTRs has been studied, accounting for both fluctuating parameters (i.e. noise) and uncertain parameters to be present in the model. Noise has been considered in the inlet temperature and in the temperature measurement made by the controller, while uncertainty has been taken into account for kinetic parameters, imperfect mixing and bias in the temperature measurement made by the controller. As far as uncertain parameters are concerned, a recently presented methodology to detect the most probable stability regions in the control gains plane has been applied. Such results are combined with the noise analysis (implemented by applying the Fokker–Planck theory of stochastic differential equations), to obtain global criteria for the choice of control gains which guarantee both the stability of the steady state with a given confidence and low fluctuations in the reactor induced by noise in the inlet temperature and in the temperature measurement made by the controller. Furthermore, attention has been given to how to obtain results minimising the computational effort. In this way, it will be shown that the presented techniques, which allow a rigorous analysis of reacting systems, accounting for both uncertain and fluctuating parameters, can be very efficient. © 2000 Elsevier Science S.A. All rights reserved.

Keywords: CSTR model; Noise; PI controlled CSTR; Monte Carlo method

1. Introduction

Physico-mathematical models are always characterised by a certain degree of uncertainty: uncertainty is present in physico-chemical parameters (due to errors in the experimental measurements and in the estimation procedure) and in the models themselves (some secondary effects are neglected, some constitutive equations are used instead of others, etc.). Furthermore, fluctuations are always present in real systems and can be seen as another kind of uncertainty in models, which can be represented by introducing time-dependent stochastic variables in them.

In the applied disciplines, physico-mathematical models are used for the description, interpretation and design of real systems. The effectiveness of models to give realistic predictions is a fundamental requirement, also considering that safety, economical and environmental constraints become more and more binding in the design and operation of process engineering systems. Model effectiveness is, therefore, strictly correlated to model uncertainty, and methodologies designed to obtain safe predictions in terms of confidence values are often applied.

The problem of uncertainty can be critical when the analysed models are highly non-linear [1]. Instability behaviour is often detected in non-linear systems: controlled CSTRs, as an example, can present a very complex dynamic behaviour, ranging from periodic to chaotic oscillations [2–5]. Obviously, in concrete reactor operation, such complex dynamic behaviour must be avoided, increasing the need for reliable model predictions.

Recently [6,7], the uncertainty analysis of PI controlled CSTRs has been performed applying Monte Carlo methods: such an approach allows the identification of safe control gains, which assure the stability of the steady state with a given confidence. In another recent work [8], the noise analysis of PI controlled CSTRs has been presented, applying the Fokker–Planck theory of stochastic differential equations, in order to study the effect of fluctuations during reactor steady state operation. In the present study, a synthesis is performed, in order to identify criteria for the safe choice of control gains, accounting for both constant imperfectly known parameters and fluctuating parameters.

To do so, the same methodologies of the previous works have been applied, but more attention was given to minimis-

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ing the computational effort. This fact is important in view of the application of these methodologies to more complex cases and it will be shown how highly reliable results can be obtained, without the analysis becoming time-consuming.

The analysis presented in this paper consists, therefore, of the following two steps:

- to obtain the most probable stability region in the control gains plane, the first Hopf bifurcation locus has been studied by considering uncertainty in the reaction kinetics, in the non-perfect mixing and in the bias in the temperature measurement made by the controller;
- to point out additional constraints so that control gains are also robust against noise, fluctuations are considered in the inlet temperature and in the temperature measurement made by the controller.

2. Constant imperfectly known parameters: robust stability analysis of non-ideal PI controlled CSTRs

In this section, the methodology proposed in previous works [6,7] is briefly summarised and then results, relevant for the aims of this paper, are presented. Assuming also that model uncertainty can be represented through a set of parameters (such as the bypass coefficient n, in the non-ideal Lo–Cholette CSTR model [9]), any mathematical model can be seen, independently of the complexity of the computation (mainly a numerical simulation), as a function of the following type:

$$y = f(x_1, \dots, x_n) \tag{1}$$

where y is the model output (e.g. a design parameter), whose calculated value depends on the $x_1, \dots, x_n$ uncertain parameters. Since uncertain parameters are stochastic variables, characterised by a given probability distribution, also the prediction y has a statistical characterisation: the uncertainty analysis aims to quantify the probability distribution of the model output y.

The most simple non-ideal PI controlled CSTR model has been analysed: the Lo–Cholette model [9] where an exothermic liquid phase first order reaction $A \to B$ takes place. This very simple model is described, in dimensionless form, by the following system of ordinary differential equations [5]:

$$\begin{aligned}
\frac{d\xi}{dt} &= -\frac{n}{m}\xi + (n-\xi)\mathrm{Da}(\vartheta,\varphi),\\
\frac{d\vartheta}{dt} &= \frac{n}{m}\left(1+\frac{N}{n}-N\right)[\vartheta_{0s} - k_p(\vartheta_M - \vartheta_s) - k_1\tau\varphi]\\
&\quad + \frac{n}{m}N\vartheta_e - \frac{n}{m}\left(1+\frac{N}{n}\right)\vartheta + (n-\xi)\mathrm{Da}(\vartheta,\varphi),\\
\frac{d\varphi}{dt} &= \vartheta - \vartheta_s
\end{aligned} \tag{2}$$

where

$$\begin{aligned}
&\xi = \frac{c_{A0}-c_A}{c_{A0}}, \quad \vartheta = \frac{T-T_{ref}}{\Delta T_a}, \quad \tau = \frac{\mathrm{vol}}{Q},\\
&t = \frac{\bar{t}}{\tau}, \quad \varphi = \int_0^t (\vartheta_M - \vartheta_s)\,d\tilde{t}, \quad \vartheta_M = \vartheta + b,\\
&\Delta T_a = \frac{-\Delta H_r c_{A0}}{\rho c_p}, \quad N = \frac{UA}{Q\rho c_p}
\end{aligned} \tag{3}$$

$$\mathrm{Da}(\vartheta,\varphi) = k_0\tau \exp\left\{\frac{-nE}{R[nT_{ref} + \Delta T_a(n-1)(\vartheta_{0s} - k_p(\vartheta_M - \vartheta_s) - k_I\tau\varphi) + \Delta T_a\vartheta]}\right\} \tag{4}$$

When the two non-ideality parameters n and m equal 1, Eq. (2) degenerate into the ideal model. The operating conditions of the present study are

$$\begin{aligned}
&k_0\tau = 4.807908\times 10^8, \quad \frac{E}{R} = 8000\,\mathrm{K}, \quad N = 0.5,\\
&T_e = 373.16\,\mathrm{K}, \quad T_{0s} = 298.42\,\mathrm{K}, \quad \Delta T_a = 200\,\mathrm{K},\\
&T_{ref} = 430\,\mathrm{K}
\end{aligned} \tag{5}$$

while the chosen steady state conditions for the corresponding ideal model are

$$\theta_s = 0, \quad \xi_s = 0.8, \quad \varphi_s = 0 \tag{6}$$

The main goal of the design of this very simple system is to assure the stability of the steady state. This means that we have to analyse the Hopf bifurcation locus in the control gains plane, where the steady state loses stability and limit cycles arise [2,3].

Considering the uncertainty in the model (parameter n), in the kinetic parameters (k_0, E) and in the bias in the temperature measurement by the controller (parameter b), the true values of the control gains at the bifurcation are unknown. Maintaining the general form of uncertainty analysis of Eq. (1), our problem can be synthesised in the calculation of the value of the proportional control gain k_p at the Hopf bifurcation $(k_p)_H$ as a function of the four uncertain parameters, the integral control gain $k_I\tau$ being a constant parameter, which can be arbitrarily set by the designer

$$(k_p)_H = f(n, k_0, E, b)|_{k_I\tau} \tag{7}$$

Paladino and Ratto [6] proposed a technique, based on Monte Carlo methods [10,11], for the analysis of this system, considering the uncertainty for n, k_0, E only. The Monte Carlo analysis, whose details are presented in [7], consists of the following steps:

1. Identification of the probability distributions of the parameters (in this case n, k_0, E, b);
2. Generation of a sample of the parameters;
3. Iterative evaluation of the function f in Eq. (7) for each element of the sample, in order to obtain a sample of $(k_p)_H$;
4. From the obtained sample, the probability distribution $(k_p)_H$ can be evaluated and confidence values quantified.

Furthermore, this procedure also allows the performance of a global sensitivity analysis of the system, but this aspect is beyond the objectives of the present paper. The critical aspect for this kind of analysis is the number of iterations, which has to be minimised in order to maintain the computational effort at acceptable levels. The 'classical' Monte Carlo approach consists of doing a huge number of iterations (as many as possible) and then get results. A typical example of this is the computation of definite integrals, where the large number of iterations is the 'fee' to pay for the application of a very simple method of computation, which allows one to get correct results without worrying about the shape of the functions, discontinuities, etc. Nevertheless, when dealing with uncertainty analysis of model outputs, the complexity of the models often impedes the rough application of the Monte Carlo approach. However, it is possible to minimise the costs of the Monte Carlo analysis, by applying refined sampling techniques, such as the Latin Hypercube sampling [10], which allows the use of very small sample dimensions without affecting the reliability of results. It can be shown that, by applying the Latin Hypercube sampling technique to sample parameters from their probability distributions, a sample dimension equal to 200 is sufficient to obtain reliable values of k_p which guarantee reactor stability with a confidence of 99% [7]. With such a sample dimension the computational effort would be acceptable also in the case of much more complex models.

So, in the present work the Latin Hypercube sampling technique with sample dimension 200 has been applied and the computation of Eq. (7) for different constant values of $k_I\tau$ (1, 10, 100, 1000) has been iterated. The four parameters k_0, E, n and b have been sampled from the probability distributions shown in Table 1.

In Fig. 1, results are synthesised: owing to uncertainty, stability and instability regions are no longer separated by a line, but by a 'band' (the uncertainty region). The width of the uncertainty region can be obtained by plotting the upper and lower limits of the probability distribution of $(k_p)_H$. This is shown in Fig. 1, where the limits of the uncertainty bands have been obtained by plotting the $(k_p)_H$ values corresponding to the 99% (upper limit) and 1% (lower limit) of confidence. In Fig. 1, the uncertainty region calculated for the present work is also compared with the uncertainty region calculated by neglecting bias. Obviously, the uncertainty region accounting for bias is wider, owing to the fact that a larger number of uncertain parameters was considered. Since the stability region of the steady state is above the Hopf locus, for sufficiently high values of k_p the steady state will be stable. Hence, in Fig. 1, the upper limit of the uncertainty region is represented by the minimum k_p values assuring reactor stability with a confidence of 99%. Such values are shown in Table 2, together with the bifurcation values of the ideal model k_p^{id} calculated for the mean values of the uncertain parameters and with the values computed by neglecting bias.

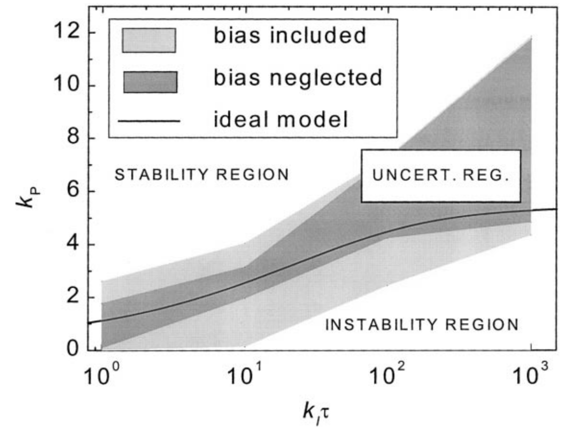

Fig. 1. Uncertainty region for the Hopf locus obtained with the Monte Carlo methodology.

Table 1
Probability distributions of the uncertain parameters

Kinetic parameters	
Bivariate normal distribution with	
Average estimates	k_0*=142361 s^{-1}
	(E/R)*=8005.8 K
S.D.	$\sigma(k_0)\cong 49500\equiv 35\%$
	$\sigma(E/R)\cong 141\equiv 2\%$
Correlation	$\chi\cong 0.96$
Bypass coefficient	
Asymmetrical normal distribution with	
Maximum	n=1 (ideal model)
S.D.	$\sigma(n)$=0.02
Constraints	n<1, n>0.92
Bias	
Normal distribution with	
Mean	0°C
S.D.	10°C

So, with the presented approach, it is possible to quantify, in a statistically rigorous way, uncertainty of model expectations, also in the presence of non-linear dynamics. Furthermore, the application of the Latin Hypercube sampling reduces the computational effort to the minimum, allowing its application also for complex models. A stability criterion can be identified for the choice of control gains in terms of *confidence* values. For any given $k_I\tau$, the robust stability criterion is

$$k_p|_{k_I\tau} > k_p^{99} \quad (8)$$

Table 2
Confidence values of $(k_p)_H$

$k_I\tau$	k_p^{id}	k_p^{99} (bias included)	k_p^{99} (bias neglected)
1	1.12	2.62	1.79
10	2.56	4.06	3.17
100	4.487	7.3	7.25
1000	5.29	11.9	11.8

3. Fluctuating parameters: noise analysis of ideal PI controlled CSTRs

Other kinds of uncertainties are present in models: parameters which fluctuate continuously with time (i.e. noise). So, after identifying control gains assuring reactor stability also in the presence of model and parameter uncertainty, the effectiveness of the control system in reducing fluctuations in the reactor has to be verified. In the noise analysis, the goal is to quantify the amplitude of the fluctuation of the output, given the fluctuations of the input parameters. Recently, a noise analysis (both theoretical and numerical) has been performed [8] for PI controlled ideal CSTRs, where the reactor temperature was the output and the noise in the temperature measurement made by the controller was the input. If the noise in the inlet temperature is also considered, the following relationship between inputs and output has to be studied

$$\vartheta = f(\vartheta_0, \vartheta_M) \tag{9}$$

The fluctuations in the inlet temperature $\varepsilon_0(t)$ and in the temperature measurement $\varepsilon_M(t)$ are assumed additive coloured noises, with time averages given by

$$\langle\varepsilon_j(t)\rangle = 0, \qquad \langle\varepsilon_j(t)\varepsilon_j(s)\rangle = D\alpha_j \exp(-\alpha_j|t-s|), \quad j = 0, \mathrm{M} \tag{10}$$

where the latter expression defines the exponential correlation of the coloured noise, the dimensionless auto-correlation time (normalised with respect to τ) is $t_c=\alpha^{-1}$ and the variance is

$$\langle(\varepsilon_j(t)-\overline{\varepsilon}_j)(\varepsilon_j(t)-\overline{\varepsilon}_j)\rangle = \langle\varepsilon_j(t)\varepsilon_j(t)\rangle = \sigma_j^2 = D_j\alpha_j, \quad j = 0, \mathrm{M} \tag{11}$$

The model under consideration for the noise analysis is, therefore, (n=1 and m=1)

$$\begin{aligned}\frac{d\xi}{dt} &= -\xi + \mathrm{Da}(\vartheta)(1-\xi),\\ \frac{d\vartheta}{dt} &= \vartheta_{0s} - k_p(\vartheta-\vartheta_s) - k_1\tau\varphi + N\vartheta_e - (1+N)\vartheta\\ &\quad +\mathrm{Da}(\vartheta)(1-\xi) - k_p\varepsilon_M(t) + \varepsilon_0(t),\\ \frac{d\varphi}{dt} &= \vartheta - \vartheta_s + \varepsilon_M(t)\end{aligned} \tag{12}$$

with the additional differential equations describing the time evolution of the coloured noises

$$\frac{d\varepsilon_j}{dt} = -\alpha\varepsilon_j - \alpha_j\sqrt{D_j}\,\Gamma(t), \quad j = 0, \mathrm{M} \tag{13}$$

The function $\Gamma(t)$ is the Langevin force, with time averages

$$\langle\Gamma(t)\rangle = 0, \qquad \langle\Gamma(t)\Gamma(s)\rangle = 2\delta(t-s) \tag{14}$$

where $\delta(t)$ is the Dirac function. The Langevin force is a gaussian white noise and is the limit of a coloured noise for α (and σ) tending to infinity (and for t_c tending to 0). A white noise will never occur in practice and is an ideal limit, but can be a very useful conservative approximation since, for gaussian white noises, we could simply define

$$\varepsilon_j(t) = \sqrt{D_j}\,\Gamma(t), \quad j = 0, \mathrm{M} \tag{15}$$

in the system (12), without the necessity of the additional differential Eq. (13).

Applying the Fokker–Planck theory to the linearisation of the system of stochastic differential Eqs. (12)–(13) at the steady state, it has been shown that quick and correct results can be obtained, both for coloured and white noises [8]. Typical plots of the amplitude ratio AR versus α are shown in Figs. 2 and 3, in the case of noise in the inlet temperature. Similar figures have been obtained in previous work [8] for noise in the temperature measurement.

Given any pair of control gains, the AR-curve has a maximum (the stochastic resonance). In the case of noise in the inlet temperature, by increasing $k_I\tau$, α_0 at stochastic resonance (α_0^{res}) increases, but AR_0^{res} decreases, while in the case of noise in the temperature measurement, both α_M^{res} and AR_M^{res} increase [8]. On the other hand, at constant $k_I\tau$, by

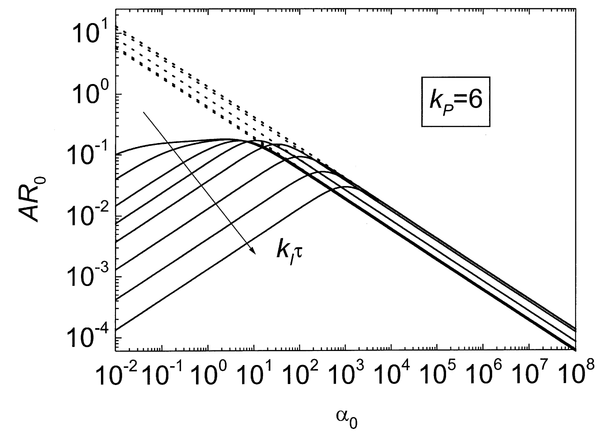

Fig. 2. Noise in the inlet temperature. AR_0 vs. α_0 varying $k_I\tau$ (k_p=6): $k_I\tau$=0.1, 1, 10, 10^2, 10^3, 10^4, 10^5, 10^6.

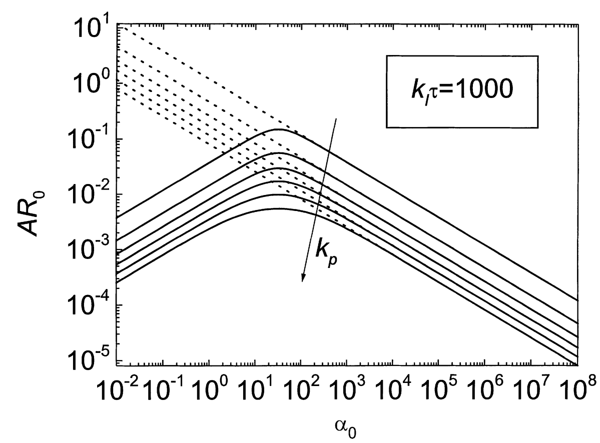

Fig. 3. Noise in the inlet temperature. AR_0 vs. α_0 varying k_p ($k_I\tau=10^3$): k_p=6, 10, 20, 40, 80, 160.

increasing k_p for both types of fluctuations, α_0^{res} and α_M^{res} remain (almost) unchanged, while AR_0^{res} and AR_M^{res} decrease [8]. So, it comes out that, for constant $k_I\tau$ values, the higher k_p, the lower the amplitude ratio becomes at resonance, implying that, in analogy with the stability analysis, a minimum constraint for k_p can be identified for the noise analysis.

4. Combined analysis of imperfectly known parameters and fluctuating parameters

Once the uncertainty analysis and the noise analysis have been carried out, the synthesis has to be performed, in order to obtain criteria, coupling both classes of uncertainty: constant imperfectly known physico-chemical parameters and fluctuating parameters. A robustness criterion can be defined for this purpose: assuming a reference safety value for the reactor temperature standard deviation σ^{safe}, the k_p confidence value is robust if, given the standard deviations σ_M and σ_0 for the noise in the measure and in the inlet, respectively, the following condition holds:

$$k_p > k_p^{99} \Rightarrow AR < AR^{safe} \quad (16)$$

In order to assess robustness, the curves of the amplitude ratio at resonance AR^{res} versus k_p, for constant $k_I\tau$, have been studied (see Figs. 4 and 5 for the case of noise in the temperature measurement).

In Fig. 4, α_M-values at resonance (α_M^{res}) for the different $k_I\tau$ are determined, when $k_p = k_p^{99}$, while in Fig. 5, the curves of the amplitude ratio at resonance AR_M^{res} versus k_p are plotted. These curves are monotone decreasing and it is evident that the constraint $k_p > k_p^{99}$ defines a maximum limit for the amplitude ratio at resonance, called AR^{MAX}. This means that, for each $k_I\tau$ and for each type of noise, if we select $k_p > k_p^{99}$, we will be sure that $AR_j < AR_j^{MAX}$, j=0, M. As a consequence of this, it is clear that, the lower AR_j^{MAX} is, the more robust k_p confidence values are.

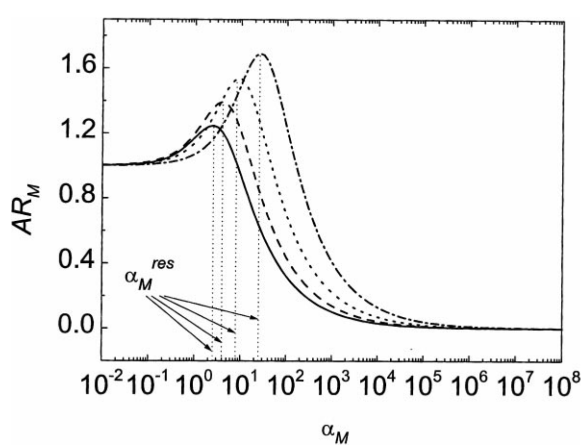

Fig. 4. AR_M vs. α_M for the confidence values of k_p. (—) $k_I\tau$=1, k_p^{99}=2.62; (– – –) $k_I\tau$=10, k_p^{99}=4.06; (· · ·) $k_I\tau$=100, k_p^{99}=7.3; (–·–·–) $k_I\tau$=1000, k_p^{99}=11.9.

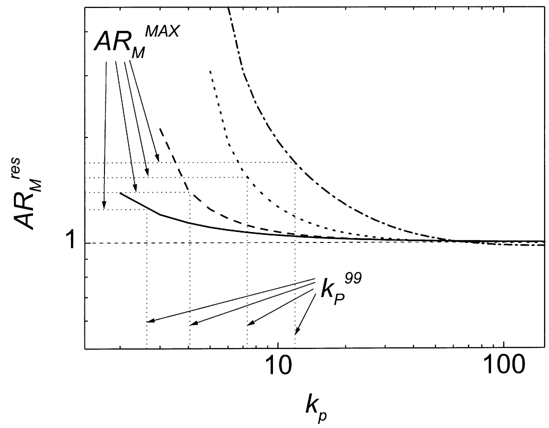

Fig. 5. AR_M at resonance vs. k_p and determination of AR_M^{MAX}. (—) $k_I\tau$=1, α_M^{res}=2.5; (– – –) $k_I\tau$=10, α_M^{res}=4.0; (· · ·) $k_I\tau$=100, α_M^{res}=7.9; (–·–·–) $k_I\tau$=1000, α_M^{res}=25.1.

The approach presented in Fig. 5 is conceptually quite simple. Nevertheless, to consider coloured noise (i.e. a realistic description of fluctuations) implies additional differential equations to be introduced in the model, with subsequent complications during computations. Moreover, similarly to the Hopf bifurcation locus, the values of AR_j^{MAX} may be affected by uncertainty and a Monte Carlo analysis would be also required in this case. Nevertheless, since the identification of techniques characterised by the lowest computational effort ranked among the goals of the present paper, in the following a simplified approach to verify the robustness of the control gains is presented. As far as the stochastic model is concerned, the simplified approach is based on the white noise approximation: it allows easier calculations and is conservative (i.e. safe), so matching requirements for a rapid and reliable analysis. As far as the effects of uncertainties on the stochastic model are concerned, the following argumentations are taken into account:

1. Fluctuations in the inlet temperature and in the temperature measurement by the controller are additive noises; therefore they do not affect the stability of the system, the Hopf locus is not altered by fluctuations and the stability analysis here presented is consistent also in the presence of noise.
2. The effect of noise consists in letting the reactor temperature fluctuate under the stable steady state conditions: hence the noise analysis has do be intended in series and not in parallel to the stability analysis.
3. Since such fluctuations are highly amplified in the neighbourhood of the Hopf bifurcations [8], the noise analysis should give the designer useful information on how distant from the Hopf locus should the control gains be chosen, to guarantee good performance also in the presence of noise: this means that the objective of the present study should be to determine the distance Δk_p from the Hopf locus to be added to the k_p^{99} confidence value

assuring stability; robustness of k_p^{99} can be stated if Δk_p is very small with respect to k_p^{99}.

4. The distance Δk_p is only slightly affected by uncertainty, allowing the ignoring of the uncertainty analysis for the stochastic model.

5. Combined analysis: simplified approach

The simplified approach is based on the white noise approximation. A coloured noise is characterised by a variance σ^2 and by a time-correlation α^{-1}. If the corresponding white noise is analysed, having the same intensity D, but $\alpha\to\infty$, the approximation of AR can be defined as

$$(\mathrm{AR}^{\mathrm{app}})^2 = \left(\frac{V_\theta}{D}\right)_{\mathrm{white}} \alpha^{-1} \tag{17}$$

where V_θ is the variance of the reactor temperature fluctuations induced by the white noise. In Figs. 2 and 3, straight dotted lines are the plots of $\mathrm{AR}^{\mathrm{app}}$, compared to the true amplitude ratio of the coloured noise. The simplified approach is exact if $\alpha>\alpha^{\mathrm{res}}$, otherwise, it is a conservative approximation. Exactly the same behaviour is observed for the noise in the temperature measurement. So, for each pair of control gains *(k_p, $k_I\tau$)*, it is sufficient to calculate one single value of (V_θ/D) with the Fokker–Planck theory, and then obtain $\mathrm{AR}^{\mathrm{app}}$ by simply applying the algebraic Eq. (17) for any desired value of α. So, it is evident that the use of the white noise approximation represents a major simplification and it is sufficient to calculate, e.g. the curves (V_θ/D) versus k_p for different values of $k_I\tau$ to obtain a complete portrait of the reactor behaviour in the control gains plane.

5.1. Noise in the temperature measurement

Comparison of the curves $(\mathrm{AR_M}-k_p)$ and $(\mathrm{AR_M^{app}}-k_p)$ is shown in Fig. 6 for $\alpha_M=10$ and 1000. As expected, the $\mathrm{AR_M^{app}}$ curves for $\alpha_M=10$ are significantly higher than the true ones, while for $\alpha_M=1000$, the approximated approach is almost indistinguishable from the complete one.

So, when α_M is sufficiently large, the approximated Eq. (17) is exhaustive and allows a correct evaluation of $\mathrm{AR_M}$, while for low values of α_M the approximation seems to be too conservative. However, remembering the following facts [8]:

1. It is a general result that, for a coloured noise,

$$\lim_{k_p\to+\infty} \mathrm{AR_M} = 1, \quad \forall k_I\tau, \alpha_M; \tag{18}$$

2. In the worst cases, $\mathrm{AR_M}$ versus k_p curves are monotone decreasing functions from $+\infty$ to the horizontal asymptote $\mathrm{AR_M}=1$, or, in other words, in the worst cases, it is not possible to reduce $\mathrm{AR_M}$ to values smaller than 1, but, for k_p sufficiently high, $\mathrm{AR_M}$ can be reduced at most to 1;
3. Signals measured by control devices are mainly filtered and therefore the amplitude of the noise in the measurement is usually small: this implies that the only thing to do, in most cases, is to avoid the noise in the measurement being too amplified;
4. Since α_M is the ratio between the residence time in the CSTR τ and the auto-correlation time t_c, values of α_M smaller than 10 are unlikely and, therefore, the case of $\alpha_M=10$ is the worst possible situation for the approximated approach;

to obtain useful results, it is sufficient to do a very simple correction to the $\mathrm{AR_M^{app}}$ values of Fig. 6 for $\alpha_M=10$. Such a correction simply consists of interrupting the $\mathrm{AR_M^{app}}$ versus k_p curves at their minimum and replacing the increasing branch of curve in Fig. 6 with a horizontal line (see Fig. 7).

With the slight modification of Fig. 7, the approximated approach can be used to find additional constraints for the choice of control gains. Remembering items 1 through 4 above in this paragraph, the most natural constraint is to guarantee $\mathrm{AR_M}<1$ or, in the worst case of item 2, to guarantee $\mathrm{AR_M}\cong 1$ (i.e. $\mathrm{AR_M}$ slightly larger that 1). In particular,

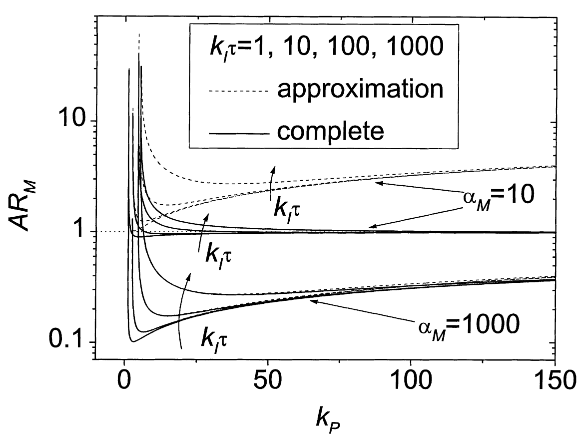

Fig. 6. Comparison between the approximated approach ($\mathrm{AR_M^{app}}$) and the complete study of coloured noise in the temperature measurement (α_M=10 and 1000).

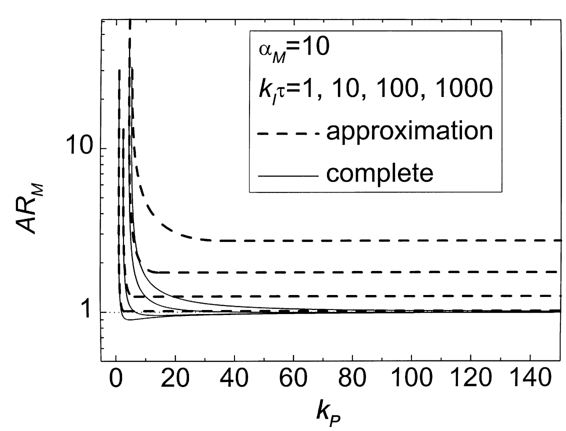

Fig. 7. Correction of ($\mathrm{AR_M^{app}}$) for noise in the temperature measurement (α_M =10).

Table 3
Minimum values for k_p, Δk_p and $k_p^{99}+\Delta k_p$ — noise in the temperature measurement

	$\alpha_M=10$			$\alpha_M=1000$		
$k_I\tau$	k_p^{min}	Δk_p	$k_p^{99}+\Delta k_p$	k_p^{min}	Δk_p	$k_p^{99}+\Delta k_p$
1	3.1	1.98	4.6	1.13	0.01	2.63
10	6.4	3.84	7.9	2.58	0.02	4.08
100	14.8	10.3	17.6	4.6	0.11	7.41
1000	37	31.7	43.6	6.3	1	12.91

- when $\alpha_M=1000$ (and in every other case, when the AR_M^{app} curves intercept the horizontal line $AR_M=1$), it is possible to guarantee $AR_M<1$ by simply choosing a k_p larger than the value at the interception with $AR_M=1$ (k_p^{min}, see Table 3);
- when $\alpha_M=10$ (and in every other similar case), one can choose a k_p larger than the value at the minimum of the AR_M^{app} curve (i.e. at the beginning of the straight line in Fig. 7): in this way, in the most conservative possibility, it is assured that AR_M will remain smaller than the minimum of the AR_M^{app} curve, but, if we observe Fig. 7, such a minimum constraint for k_p implies that, in practice, the true AR_M curve has reached the acceptable values $AR_M\cong 1$ (k_p^{min} values are shown in Table 3).

So, given the actual operating conditions, the k_p^{min} values can be easily calculated, and subsequently Δk_p can be directly obtained

$$\Delta k_p = k_p^{min} - (k_p)_H \tag{19}$$

where the Hopf bifurcation value $(k_p)_H$ is represented, in Figs. 6 and 7, by the value at the vertical asymptote. As already discussed, if uncertainty is accounted, the value of $(k_p)_H$ is affected, as well as k_p^{min} but it has been verified that Δk_p is insensitive to uncertainty. This can be explained by the fact that the noise analysis is a linear analysis, and is not influenced by the non-linearity of the system. So, Δk_p can be easily computed by applying $(k_p)_H$ and k_p^{min} values of the ideal model without uncertainty (i.e. $(k_p)_H = k_p^{id}$). Furthermore, it is important to remember that such a value Δk_P has to be added to the confidence value k_p^{99}. Since such a confidence value is already an approximation in excess of the Hopf bifurcation value in the 99% of cases, the robustness criterion

$$k_p^{safe} = k_p^{99} + \Delta k_p \tag{20}$$

seems to be reasonably safe, without the necessity to introduce the uncertainty analysis for Δk_p, too.

5.2. Noise in the inlet temperature

Comparison of the curves (AR_0-k_p) and ($AR_0^{amp} - k_p$) is shown in Fig. 8 for $\alpha_0=10$ and 1000. As before, in the case $\alpha_0=10$, the approximated approach predicts AR_0 values larger than in the true case, but, since for a coloured noise in the inlet temperature

$$\lim_{k_p\to+\infty} AR_0 = 0, \quad \forall k_I\tau, \alpha_0, \tag{21}$$

this does not represent a problem, since the approximated curves remain effective in predicting the minimum values of Δk_p assuring $AR_0<1$. In the case $\alpha_0=1000$, the approximated approach cannot be distinguished from the complete approach.

So, in the case of noise in the inlet, it is very easy to identify (for each $k_I\tau$) the values of k_p^{min} and Δk_p. Such values are shown in Table 4. With the same motivations as before, the uncertainty analysis for Δk_p can be ignored in this case, too.

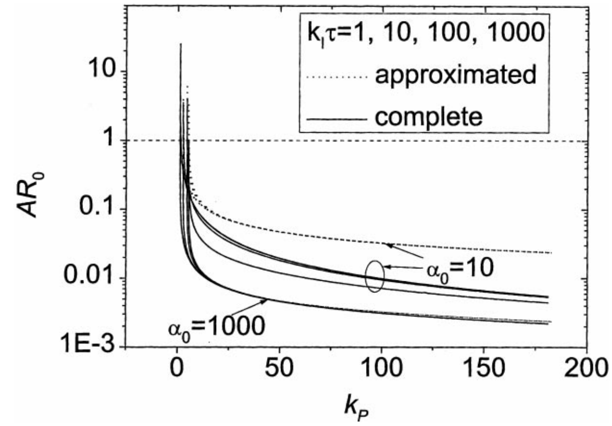

Fig. 8. Comparison between the approximated approach (AR_M^{app}) and the complete study of coloured noise in the inlet temperature (α_0=10 and 1000).

5.3. Global constraint for control gains (combined analysis)

In Figs. 9 and 10, confidence values obtained with the uncertainty analysis of the Hopf locus (Table 2) are plotted together with the k_p^{safe} values in Eq. (20) obtained with the noise analysis (Tables 3 and 4), for noise in the temperature measurement and in the inlet temperature, respectively. In the particular case studied in this paper, noise in the mea-

Table 4
Minimum values for k_p, Δk_p and $k_p^{99}+\Delta k_p$ — noise in the inlet temperature

	$\alpha_0=10$			$\alpha_0=1000$		
$k_I\tau$	k_p^{min}	Δk_p	$k_p^{99}+\Delta k_p$	k_p^{min}	Δk_p	$k_p^{99}+\Delta k_p$
1	1.4	0.28	2.9	1.125	0.005	2.63
10	2.7	0.14	4.2	2.563	0.003	4.06
100	4.59	0.1	7.4	4.488	0.001	7.3
1000	5.39	0.1	12	5.292	0.002	1.19

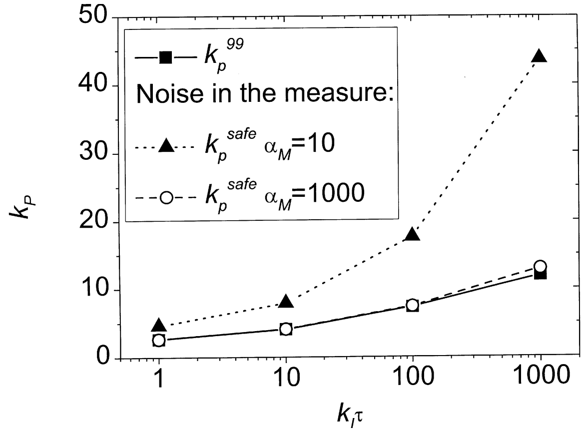

Fig. 9. Constraints for k_p resulting from the uncertainty analysis of the Hopf locus and the noise analysis for the temperature measurement by the controller (α_M=10 and 1000).

surement brings the most restrictive values for k_p, above all for α_M=10, while for noise in the inlet the confidence values k_p^{99} are slightly affected and it can be stated that they are sufficient to guarantee $AR_0<1$ without any adjustment. This means that in this last case k_p^{99} is robust, but in the other cases robustness cannot be assured, so implying that safe criteria for the choice of control gains must consider all classes of uncertainty.

When all types of uncertainty are accounted for, the superposition the different kinds of noise has also to be considered: since the considered noises are additive and being the noise analysis linear, there is no interaction. This means that the variance of the reactor temperature will be the sum of the variances induced by the two noises singularly, while the amplitude ratios AR_0 and AR_M are not altered. Hence the values of Δk_p for the singular noises are not altered and, combining the noises, the maximum Δk_p has to be selected. So, for each $k_I\tau$, the global constraint for the proportional control gain is

$$k_p^{\mathrm{safe}} = k_p^{99} + \max_{j=0,\mathrm{M}} (\Delta k_p) \tag{22}$$

In the present study, noise in the temperature measurement mainly controls the global constraint: however exceptions can occur, e.g. if α_0=10, α_M=1000 and $k_I\tau$=1, 10. So, the main effect has to be searched case by case.

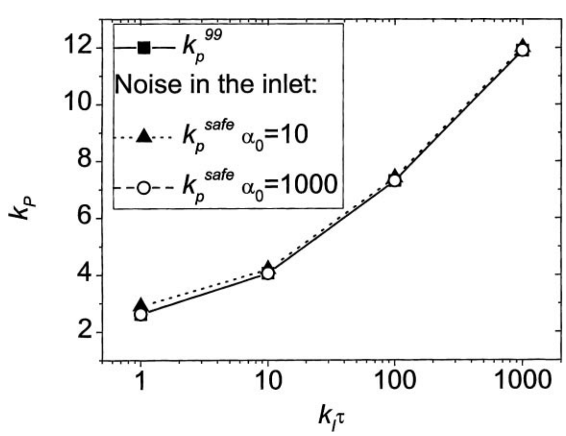

Fig. 10. Constraints for k_p resulting from the uncertainty analysis of the Hopf locus and the noise analysis for the inlet temperature (α_0=10 and 1000).

6. Conclusions

In this work the stability of PI controlled CSTRs is studied, in the presence of uncertainties in the model. Two kinds of uncertainty have been considered: imperfectly known physico-chemical and process parameters and fluctuating parameters (noise). In the first case, a technique based on Monte Carlo methods has been applied [6,7], allowing the obtaining of safe values for control gains, assuring reactor stability with a given confidence. In the second case, the Fokker–Planck theory of stochastic differential equations has been adopted [8] to study fluctuations in the reactor temperature induced by noise in the inlet temperature or in the temperature measurement made by the controller. Subsequently, a synthesis is performed of the two approaches, to obtain global criteria for the choice of control gains.

In the presented analyses, considerable care has been given to minimising the computational effort. A refined sampling technique (Latin Hypercube sampling) has been applied during the Monte Carlo analysis, allowing the obtaining of a correct evaluation of the cumulative distribution of the model output even with very small sample dimensions (e.g. with a sample of 200 elements). Furthermore, a simplified approach has been presented for the noise analysis with the Fokker–Planck theory, based on the white noise approximation: results obtained with the simplified approach are exact or at least conservative with respect to the complete analysis, therefore they are in all cases safe.

Hence, with the presented approaches, techniques for a rigorous analysis of reacting systems, accounting for both uncertain and fluctuating parameters, are very efficient. This result is important for the study of much more complex models, characterised by complex reactions networks, distributed parameter systems, etc.

7. Nomenclature

A	heat transfer area (m^2)
AR	amplitude ratio
b	bias in the temperature measurement by the controller
c_A	reactant concentration (kmol cm^{-3})
D	noise intensity
Da(θ)	Damkoehler number
E	activation energy (J kmol^{-1})
k_0	Arrhenius pre-exponential factor (s^{-1})

k_I integral control gain (s^{-1})
k_p proportional control gain
m dead volume rate in the Cholette model
n bypass coefficient in the Cholette model
N number of transport units
Q flow rate ($m^3\,s^{-1}$)
t dimensionless time, normalised with respect to τ
t_c auto-correlation time
$\bar{t}$ time (s)
T temperature (K)
ΔT_a adiabatic temperature difference (K)
U overall heat transfer coefficient ($J\,s^{-1}\,m^{-2}\,K^{-1}$)
V variance of the noise
vol reactor volume (m^3)

Greek letters

α t_c^{-1}
ε fluctuating variable
θ dimensionless temperature
φ integral control state variable
ξ conversion
ρ density ($kg\,m^{-3}$)
σ standard deviation of the noise
τ residence time (s)

Subscripts

0 inlet
e external
H Hopf bifurcation
M measured
s steady state

Superscripts

app approximated
id ideal model without uncertainty
min minimum value for noise analysis, obtained with the ideal model without uncertainty
res stochastic resonance

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