Brazilian Journal
of Chemical
Engineering

ISSN 0104-6632
Printed in Brazil
www.abeq.org.br/bjche

Vol. 27, No. 04, pp. 627 - 642, October - December, 2010

OPTIMAL MEASUREMENT LOCATIONS FOR PARAMETER ESTIMATION OF NON LINEAR DISTRIBUTED PARAMETER SYSTEMS

J. E. Alaña

Universidad Del Zulia, Facultad de Ingeniería, Escuela de Ingeniería Química,
Maracaibo, Venezuela.
School of Chemical Engineering and Analytical Science, Fax: +58 261 7598100,
The University of Manchester, Manchester, UK.
E-mail: joalana@luz.edu.ve

(Submitted: April 8, 2009 ; Revised: April 26, 2010 ; Accepted: May 10, 2010)

Abstract - A sensor placement approach for the purpose of accurately estimating unknown parameters of a distributed parameter system is discussed. The idea is to convert the sensor location problem to a classical experimental design. The technique consists of analysing the extrema values of the sensitivity coefficients derived from the system and their corresponding spatial positions. This information is used to formulate an efficient computational optimum experiment design on discrete domains. The scheme studied is verified by a numerical example regarding the chemical reaction in a tubular reactor for two possible scenarios; stable and unstable operation conditions. The resulting approach is easy to implement and good estimates for the parameters of the system are obtained. This study shows that the measurement location plays an essential role in the parameter estimation procedure.
Keywords: Sensor placement; Distributed parameter system; Parameter estimation; Sensitivity coefficients.

INTRODUCTION

An essential problem in parameter estimation is the selection of the experimental measurement locations. This problem consists of an arrangement of a limited number of measurements over the spatial domain that guarantees the best estimates of the system parameters.

The allocation of sensors is a task not necessarily dictated by physical considerations or by intuition and, therefore, some systematic approaches should still be developed to reduce the cost of instrumentation and to increase the efficiency of the parameter estimation procedures. Although the parameter estimation accuracy in a distributed parameter system depends significantly on the selection of sensor positions, only a few contributions to the experimental designs for such systems have been reported. The effects of either number or spatial allocation of measurements for the parameter estimation problem were considered by Kubrusly (1980), Carotenuto and Raiconi (1980), Kitamura and Taniguchi (1981), Courdesses et al. (1981), Courdesses and Amouroux (1982), and Nakagiri (1983).

Le Pourhiet and Le Letty (1976) offered two algorithms, as an optimal sensor location for parameter estimation applied to a deterministic distributed parameter system. The main idea is to maximise the identification error sensitivity with respect to the location of a new sensor. The first algorithm concerns the enhancement in the sensitivity criterion by adding a new sensor to the set of all sensors allocated in preceding iterations. The second takes into account the position of the new sensor at the previous iteration. Both algorithms stop when the assignment of a new sensor adds no

*To whom correspondence should be addressed

substantial improvement as far as the identification error sensitivity is concerned.

Sokollik (1976) considered the number and position of sensors, as well as the measurement times, to solve the parameter estimation problem of a distributed parameter system. The model was approximated by a lumped system using finite-differences. In this method both time and space domains were discretized with invariable sampling intervals. The optimal set of space-time was given by minimising the parameter estimate covariance.

Qureshi et al. (1980) presented a technique for scheming optimal experiments for distributed parameter system identification with observations contaminated with noise. The boundary perturbations were considered. The optimisation criterion to be maximised was the determinant of the Fisher Index Matrix (FIM) associated to the parameters to be identified, which depends on both boundary perturbations and spatial positions of the measurements. This method was developed for hyperbolic and parabolic partial differential equations.

Carotenuto and Raiconi (1981) considered the parameter identification of the one-dimensional static diffusion equation. The effects of an additional measurement point in terms of a potential improvement in the parameter estimate were analysed, and a criterion for selecting the location was presented. Rafajlowicz (1981) presented a method for optimal experiment of a distributed parameter system identification problem, which comprises sensor location and determination of classes of random inputs. A searching of an optimal probability measure corresponding to the position of the sensors was studied. This approach is equivalent to that considered in Qureshi et al. (1980), where the determinant of the information matrix is maximised. However, the information matrix was correlated to the system eigenvalues rather than to the system parameters. The conditions for optimality of the experimental design were derived, including an upper bound for the number of sensors (Rafajlowicz, 1983, Singh and Hahn, 2005, 2006, Zamprohna et al., 2005, Papadimitriou, 2004).

More recently, a number of computational approaches were introduced. (Kubrously and Malebranche 1985, Uciński 1992, 2000a, 2000b, 2003, 2005, Uciński and Bogacka, 2002, Uciński and Demetriou, 2004). The central idea is to define a design criterion to be minimised as a scalar measure of the FIM associated to the estimated parameters. This is followed by methods of optimum experimental design for nonlinear models to solve the sensor location problem at hand or, alternatively, by employing standard nonlinear programming procedures. Olanrewaju and Al-Arfaj (2006) presented a state estimation scheme based on Kalman filters for reactive distillation systems without extensively addressing the sensor selection problem. Nahor et al. (2003) minimised the ratio of the largest to the smaller eigenvalue of the FIM to compute optimal temperature sensor positions for food processes. To the best of our knowledge, these techniques have not been applied yet to systems described by partial differential equations, in spite of their resolute advantages (Uciński, 1999, Löhner and Camelli, 2005, Waterhouse et al., 2009, Vande, 2000, Venkateswarlu and Kumar, 2006, Punithakumar et al., 2006, Peng, 2005, Cotae et al., 2008, Balsa-Canto et al., 2008).

Christofides and Antoniades (2000, 2001, 2002) presented new approaches to calculate the optimal actuator/sensor locations of uncertain transport-reaction systems under control. They established that the solution to this problem is near-optimal for the closed-loop infinite-dimensional processes analysed. Similar and other kinds of techniques have been reported by Van den Berg et al. (2000) and Harries et al. (2004). These aspects will be analysed in future works regarding the optimal measurement positions for parameter estimation of distributed parameter systems.

This paper proposes an experimental design for measurement placement of distributed parameter systems. This is done by taking into consideration the spatial locations where the sensitivity coefficients of the system reached theirs extrema values.

THE SYSTEM GOVERNING AND SENSITIVITY EQUATIONS

The system considered is a homogeneous tubular reactor without catalyst packing. An irreversible first–order chemical reaction $A \rightarrow B$ takes place and is described by the concentration rate $C_A(t,z)$ and the temperature $T(t,z)$. This reaction is exothermic and a cooling jacket is used to remove heat from the reactor. A fraction of the products can be recycled, r, and mixed with the reactants at the inlet of the reactor ($z=0$) (Bendersky and Christofides 2000, Li and Chistofides 2007, Alaña, 2010).

Derived from mass and energy balances, and under the standard assumptions of constant density (ρ), heat capacity of the reacting fluid (cp), and constant axial fluid velocity (v), the dynamic behaviour of the reactor is described by a set of partial differential equations defined on a spatial domain $z \in (0,1)$, in dimensionless form,

$$\frac{\partial y_1(t,z)}{\partial t} = -\frac{\partial y_1(t,z)}{\partial z} + \frac{1}{Pe_C}\frac{\partial^2 y_1(t,z)}{\partial z^2} + R_{i3} \quad (1)$$

$$\frac{\partial y_2(t,z)}{\partial t} = -\frac{\partial y_2(t,z)}{\partial z} + \frac{1}{Pe_T}\frac{\partial^2 y_2(t,z)}{\partial z^2} + R_{i1} + R_{i2} \quad (2)$$

In these equations; $y_1(t,z)$, $y_2(t,z)$ are the state variables that represent concentration and temperature, respectively. The control variable u_C represents the cooling water temperature. The terms Pe_C, Pe_T are the Peclet numbers of mass and energy flows, respectively, B_C is the Damkohler number, γ is the activation energy, B_T and β_T are the parameters related to heat of reaction and heat transfer, respectively, and $t \in (t_0, t_f)$, where t_0 and t_f are initial and final times, respectively. The terms R_{ij} correspond to the examples; i=1 stable case with a recycle r=0.00, and i=2 unstable case with a recycle r=0.50, j stands for the following expression,

$$R_{11} = B_T B_C (1 - y_1(t,z)) \exp\left(\frac{y_2(t,z)}{1 + \frac{y_2(t,z)}{\gamma}}\right), \quad (3a)$$

$$R_{21} = B_T B_C (1 + y_1(t,z)) \exp\left(\frac{\gamma y_2(t,z)}{1 + y_2(t,z)}\right)$$

$$R_{12} = R_{22} = -\beta_T (u_C - y_2(t,z)) \quad (3b)$$

$$R_{13} = -B_C (1 - y_1(t,z)) \exp\left(\frac{y_2(t,z)}{1 + \frac{y_2(t,z)}{\gamma}}\right), \quad (3c)$$

$$R_{23} = B_C (1 + y_1(t,z)) \exp\left(\frac{\gamma y_2(t,z)}{1 + y_2(t,z)}\right)$$

The boundary and initial conditions are,

a. Stable case; $t \in (0,5)$

$$z = 0 \quad \begin{aligned} &\frac{\partial y_1(t,0)}{\partial z} = Pe_C y_1(t,0) \rightarrow \\ &\frac{\partial y_2(t,0)}{\partial z} = Pe_T y_2(t,0) \end{aligned} \quad (4a)$$

$$z = 1 \quad \frac{\partial y_1(t,1)}{\partial z} = 0 \quad \frac{\partial y_2(t,1)}{\partial z} = 0 \quad (4b)$$

$$t = 0 \qquad y_{10} = y_{20} = u_C = 0 \quad (4c)$$

b. Unstable case; assuming negligible reaction in the recycle loop and instantaneous mixing of fresh feed and recycle feed at the reactor inlet, the boundary and initial conditions in the interval $t \in (0,25)$ take the form,

$$z = 0 \quad \begin{aligned} &\frac{\partial y_1(t,0)}{\partial z} = Pe_C \left[y_1(t,0) - (1-r) y_{10} - r y_1(t,1) \right] \\ &\frac{\partial y_2(t,0)}{\partial z} = Pe_T \left[y_2(t,0) - (1-r) y_{20} - r y_2(t,1) \right] \end{aligned} \quad (5a)$$

$$z = 1 \quad \frac{\partial y_1(t,1)}{\partial z} = 0 \quad \frac{\partial y_2(t,1)}{\partial z} = 0 \quad (5b)$$

$$t = 0 \quad y_{10} = y_{20} = u_C = 0 \quad (5c)$$

The sensitivity coefficients can be calculated based on the local sensitivity analysis (Morbidelli and Varma, 1988, Vajda and Rabitz, 1992, Tildem et al., 1981, Juncu and Floarea, 1995). Indicating any of the reactor parameters [Pe_C, Pe_T, B_C, γ, B_T and β_T] as ϕ, the first-order sensitivity coefficient of Y, with Y being y_1 and y_2, is defined as,

$$s(Y,\varphi) = s_{Y,\varphi} = \frac{\partial Y}{\partial \varphi} \quad (6)$$

In this work, to take into account the pseudoadiabatic behaviour of the system, the sensitivity coefficients are computed using the direct method (Bauman et al., 1990, Coste and Aris, 2004). According to this method, the sensitivity coefficients can be expressed by the following equations,

$$\frac{\partial s_{y_1,\varphi}}{\partial t} = -\frac{\partial s_{y_1,\varphi}}{\partial z}\frac{\partial}{\partial \varphi}\left(\frac{1}{Pe_C}\frac{\partial^2 y_1(t,z)}{\partial z^2}\right) + \frac{\partial R_{i3}}{\partial y_2} s_{y_2,\varphi} + \frac{\partial R_{i3}}{\partial y_1} s_{y_1,\varphi} \quad (7)$$

$$\frac{\partial s_{y_2,\varphi}}{\partial t} = -\frac{\partial s_{y_2,\varphi}}{\partial z}\frac{\partial}{\partial \varphi}\left(\frac{1}{Pe_T}\frac{\partial^2 y_2(t,z)}{\partial z^2}\right) + \frac{\partial R_{i1}}{\partial y_2} s_{y_2,\varphi} + \frac{\partial R_{i1}}{\partial y_1} s_{y_1,\varphi} + \frac{\partial R_{i2}}{\partial y_2} s_{y_2,\varphi} \quad (8)$$

The boundary and initial conditions for each case study are,

a. Stable case,

$$z = 0 \quad \frac{\partial s_{y_1,\varphi}}{\partial z} = \frac{\partial}{\partial \varphi}\left(Pe_C y_1(t,0)\right)$$

$$z = 0 \quad \frac{\partial s_{y_2,\varphi}}{\partial z} = \frac{\partial}{\partial \varphi}\left(Pe_T y_2(t,0)\right) \tag{9a}$$

$$z = 1 \quad \frac{\partial s_{y_1,\varphi}}{\partial z} = 0 \quad \frac{\partial s_{y_2,\varphi}}{\partial z} = 0 \tag{9b}$$

$$t = 0 \qquad s_{y_1,\varphi} = s_{y_2,\varphi} = 0 \tag{9c}$$

b. Unstable case,

$$z = 0 \quad \frac{\partial s_{y_1,\varphi}}{\partial z} = \frac{\partial}{\partial \varphi}\left(Pe_C\left[y_1(t,0) - (1-r)y_{10} - r y_1(t,1)\right]\right)$$

$$\frac{\partial s_{y_2,\varphi}}{\partial z} = \frac{\partial}{\partial \varphi}\left(Pe_T\left[y_2(t,0) - (1-r)y_{20} - r y_2(t,1)\right]\right) \tag{10a}$$

$$z = 1 \quad \frac{\partial s_{y_1,\varphi}}{\partial z} = 0 \quad \frac{\partial s_{y_2,\varphi}}{\partial z} = 0 \tag{10b}$$

$$t = 0 \qquad s_{y_1,\varphi} = s_{y_2,\varphi} = 0 \tag{10c}$$

Equations (7) – (10) are obtained by differentiating the model equations (1) – (2), and (4) or (5) (depending of the case study), with respect to ϕ. The direct approach to obtain the sensitivity coefficients consists of solving (1) – (2) and (4), together with (7) – (9) for the stable case, and solving (1) – (2) and (5), together with (7) – (8) and (10) for the unstable example. For each case study, a system of fourteen coupled nonlinear partial differential equations is formed, with their respective initial and boundary conditions. This system can be solved using the Matlab® partial differential equation solver "pdepe", which solves initial-boundary value problems for systems of parabolic and elliptical partial differential equations in one space variable and time. The solver converts the partial differential equations to ordinary differential equations using a second-order accurate spatial discretization based on a set of nodes specified by the user. Time integration is then performed with a multistep variable-order method based on the numerical differentiation formulae. The spatial domain was divided into 21 equidistant intervals, and n time reporting intervals were considered. The nominal values of the parameter for the systems studied in this work are shown in Table 1.

Table 1: Nominal values of the parameters

Stable case			Unstable case		
$Pe_C = 1.0$	$B_C = 1.0$	$\gamma = 20.0$	$Pe_C = 7.0$	$B_C = 0.1$	$\gamma = 10.0$
$Pe_T = 1.0$	$B_T = 2.0$	$\beta_T = 1.0$	$Pe_T = 7.0$	$B_T = 2.5$	$\beta_T = 2.0$

In many cases, it can be assumed that some, albeit rough, a priori value of the parameters vector ϕ is on hand, e.g., determined from preliminary experiments. The aim in this work is to select a state sampling schedule to maximise the expected accuracy of the parameter estimates to be obtained from data generated in new experiments. This parameter should be determined with the lower uncertainties.

SENSITIVITY OF THE OPTIMUM PARAMETER $\hat{\varphi}$ WITH RESPECT TO THE EXPERIMENTAL DATA

A knowledge of how the solution of a system can vary with respect to small changes in the data or the parameters can yield insights into the model behaviour and can assists the modelling process.

Christopher and Fathalla (1999) proposed a new method to estimate the sensitivity of the state variables to the parameter estimates and the sensitivity of the parameter estimates to the observation. Using a set of analytical and numerical approaches, they concluded that the sensitivity of the parameter estimates to the observations is low if the sensitivity of the state variable to the parameter estimates is high. Similar results have been reported by Binder (2007). Next, the demonstration of the observation mentioned before can be found.

In order to compute $\frac{\partial \hat{\varphi}}{\partial u_{ij}}$, the sensitivity of the parameter $\hat{\varphi}$ to the experimental data u_{ij}, the objective function in the parameter estimation process has the form,

$$\Im(\varphi) \equiv \Im(\varphi, u) = \sum_i \sum_j \left(y\left(t_j, z_i, \varphi\right) - u_{ij}\right)^2 \tag{11}$$

This function can be considered to be a smooth function of φ in the vicinity of the optimal parameter $\hat{\varphi}$. Then the first and second derivatives are,

$$\frac{\partial \Im(\varphi,u)}{\partial \varphi_k} = 2\sum_i \sum_j \left(y\left(t_j,z_i,\varphi\right) - u_{ij}\right)\frac{\partial y\left(t_j,z_i,\varphi\right)}{\partial \varphi_k} \tag{12}$$

$$\frac{\partial^2 \Im(\varphi,u)}{\partial \varphi_l \partial \varphi_k} = 2\sum_i \sum_j \frac{\partial y\left(t_j,z_i,\varphi\right)}{\partial \varphi_l}\frac{\partial y\left(t_j,z_i,\varphi\right)}{\partial \varphi_k} + 2\sum_i \sum_j \left(y\left(t_j,z_i,\varphi\right) - u_{ij}\right)\frac{\partial^2 y\left(t_j,z_i,\varphi\right)}{\partial \varphi_l \partial \varphi_k} \tag{13}$$

In order to minimise the objective function (11), the right hand side of Equation (12) vanishes at $\varphi = \hat{\varphi}$ (where $\hat{\varphi} = \hat{\varphi}(u)$),

$$\sum_i \sum_j \left(y\left(t_j,z_i,\hat{\varphi}(u)\right) - u_{ij}\right) s_k\left(t_j,z_i,\hat{\varphi}(u)\right) = 0 \tag{14}$$

with, $s_k\left(t_j,z_i,\hat{\varphi}(u)\right) = \dfrac{\partial y\left(t_j,z_i,\varphi\right)}{\partial \varphi_k}$

At this moment, the left hand side of Equation (14) is a function of $\hat{\varphi}(u)$ and u_{ij}; differentiating both sides with respect to u_{ij} yields, for $k = 1,...,L_p$,

$$\sum_{i=1}^{N}\sum_{j=1}^{M}\sum_{l=1}^{L_p}\left(s_k\left(t_j,z_i,\hat{\varphi}\right)s_l\left(t_j,z_i,\hat{\varphi}\right) + \left(y\left(t_j,z_i,\hat{\varphi}\right) - u_{ij}\right)\frac{\partial^2 y\left(t_j,z_i,\hat{\varphi}\right)}{\partial \varphi_l \partial \varphi_k}\right)\frac{\partial \hat{\varphi}}{\partial u_{ij}} = s_k\left(t_j,z_i,\hat{\varphi}\right) \tag{15}$$

If we assume that $y\left(t_j,z_i,\hat{\varphi}\right)$ is close to the observed measured values u_{ij}, then the term $\left(y\left(t_j,z_i,\hat{\varphi}(u)\right) - u_{ij}\right)$ on the left hand side of Equation (15) can be neglected. Finally, the sensitivity of the best fit parameter estimate $\hat{\varphi}$ to the experimental measurements u_{ij} can be approximated using the following compact form,

$$\frac{\partial \hat{\varphi}}{\partial u_{ij}} \approx \left[\Theta(\hat{\varphi})\right]^{-1} s\left(t_j,z_i,\hat{\varphi}\right) \tag{16}$$

Here $s\left(t,z,\hat{\varphi}\right)$ is a L_px1 vector, given by the derivatives of the governing equations of the system with respect to the parameters, and $\Theta(\hat{\varphi}) = \sum_{i=1}^{N}\sum_{j=1}^{M} s\left(t_j,z_i,\hat{\varphi}\right)s^T\left(t_j,z_i,\hat{\varphi}\right)$ is a L_pxL_p non-singular matrix.

A desirable property of the model is that the sensitivity of the parameter estimate to the experimental measurement, $\dfrac{\partial \hat{\varphi}}{\partial u_{ij}}$, should be small in order to minimise the effect of the noise present in the experimental observation on the parameter estimation process. Equation (16) suggests that increasing $s\left(t_j,z_i,\hat{\varphi}\right)$ (the sensitivity of the state variable with respect to the unknown parameter) decreases the sensitivity of the parameter estimate to the experimental measurement. Then it is reasonable to expect that the best estimation of the parameters should be obtained when the experimental data are taken at the locations where the sensitivity coefficients reach their extrema values (the largest absolute values). It is our intention to verify here how useful these observations are to define a set of measurement locations for parameter estimation purposes using numerical experimentation.

PARAMETER ESTIMATION

Model calibration consists of finding a set of parameter values that produces the best model output which fit the observed data. This calibration is usually done by the minimisation of the objective function (17).

Once the sensor locations have been determined, the parameter estimation problem can be viewed as matching the model to the real system through the

minimisation of an error criterion over a set of admissible parameters. This can be defined as,

$$J(\varphi)=\frac{1}{m}\left[\frac{1}{t_f}\int_0^{t_f}\sum_{i=1}^{m}\left(y_e(z_i,t)-y_p(z_i,t)\right)^2 dt\right] \quad (17)$$

where, $y_p(z_i,t)$ is defined as the predicted response of the model at location z_i, and $y_e(z_i,t)$ as the experimental response at the same location, m is the number of optimal measurement locations determined by the different methods studied in this work. Unfortunately, elements in the vector $y_p(z_i,t)$ are not linear functions of the parameters ϕ, and multiple solutions of (17) are possible.

It is well known that problem (17) is challenging for numerous reasons. The existence of a solution is not certain, particularly if the observed data contain errors or if the model is grossly incorrect. It is unusual that any parameter set can accurately match the experimental data used, especially when these data are contaminated with noise. The presence of noise can promote difficulties during the optimisation process, causing spurious local minima and discontinuities. The gradient-based methods are the most affected of all. In this work, several different optimisation techniques (already existing in the Matlab® library) were used. The method of Nelder–Mead produced the best results for the scenarios studied. This can be explained by the fact that, using this technique, poor gradient approximations are not a problem, and continuity and differentiability of the objective function are not required.

Covariance Matrix of Parameter Estimates

When assessing the quality of an identified dynamic model, the covariance matrix of the estimated parameters gives an important measure (Ljung, 1999, Söderström and Stoica, 1989). In a maximum likelihood context, the inverse of the expected value of the negative of the Hessian provides the Cramer-Rao lower bound on the variance-covariance matrix of the parameter estimates. Large variances imply imprecise parameter estimates. The arrival of new data, or data measurement, can lead to substantial change in parameter estimates if the variance-covariance matrix is ill-conditioned. So, the goal of the estimation procedure is to determine unknown parameters in such a way that the difference between the sample covariance matrix and the implied covariance matrix is minimised in a certain sense (Davidson and MacKinnon, 1980, Sorenson, 1980, Zhun and Stein, 2005).

Based on the system studied here, the approximation of the parameter covariance matrix (Yen and Yoon, 1981) can be approximated by,

$$\mathrm{Cov}\left(\hat{\varphi}_{nv}\right)\approx\left(\frac{1}{\sigma_{y_1}^2}J_{y_1}^T J_{y_1}+\frac{1}{\sigma_{y_2}^2}J_{y_2}^T J_{y_2}\right)^{-1} \quad (18)$$

where J_{y_1} and J_{y_2} represent the Jacobian matrix of estimated variables; y_1 and y_2, respectively, with respect to changes in the parameters. nv is the parameter dimension, and σ_k^2 is the variance of the variable k. In this equation it is easy to view the influence of field data quality and quantity in parameter uncertainty. Since these Jacobian matrices are evaluated at those locations for which observations are available, any experimental design should aim at sampling at those locations where the variables are most sensitive to the estimated parameters. Such a design is said to provide the maximum amount of information about the unknown parameters (Knopman and Voss, 1987).

It is intuitively obvious that the experimental design objective should be intended to minimise the norm of the covariance matrix (18), i.e., to make matrices $\left(J_{y_1}^T J_{y_1}\right)^{-1}$ and $\left(J_{y_2}^T J_{y_2}\right)^{-1}$ as small as possible. The variance terms $\sigma_{y_1}^2$ and $\sigma_{y_2}^2$ are constants, and can be dropped from the formulation. To measure the accuracy of the estimates, we prefer to summarise the information about the variability in the covariance matrix into a single number. Here we used the determinant of (18) as the function that transforms a matrix into a scalar. This is quite informative since in fact it is related to the volume of the multidimensional simplex defined by the column/row vectors of the matrix (Kumar and Seinfeld, 1978, Rutzler, 1987).

Experimental design for parameter estimation deals with the problem of defining experimental conditions that increase the reliability of a simulation model. This can be formulated by using a measure of the covariance matrix of the parameter estimates. Among these, the most widely used design criteria are,

- A-optimality: A design is said to be A-optimal if it minimises the trace of matrix (18).
- D-optimality: A design is said to be D-optimal if it minimises the determinant of (18).
- E-optimality: A design is said to be E-optimal if it minimises the maximal eigenvalue of (18).

Using different norms leads to slightly different conclusions regarding the optimal design. The D-optimality criterion minimises the volume of the hyper-ellipsoid in the parameter space, which makes no consideration of the relationship between the ellipsoid's axes lengths, which are in turn proportional to the square root of the covariance matrix eigenvalues.

In general, it can be shown that, under some assumptions of regularity and for a sufficiently large sample size N, the vector $\left(\hat{\varphi}_{(N)} - \overset{*}{\varphi}\right)$ (with $\overset{*}{\varphi}$ denoting the 'true' but unknown value of the parameters and $\hat{\varphi}_{(N)}$ the least square parameter estimates) has approximately a normal distribution with zero mean and covariance matrix,

$$\frac{\sigma^2}{N} M^{-1}\left(\xi, \overset{*}{\varphi}\right) \tag{19}$$

where σ^2 denotes the standard deviation of the errors in the model, ξ represent a design experiment (including the measurement locations) and $M\left(\xi, \overset{*}{\varphi}\right)$ is the FIM, defined by,

$$M\left(\xi, \overset{*}{\varphi}\right) = \left(\sum_{k=1}^{n} \frac{\partial y\left(z_k, t, \varphi\right)}{\partial \varphi_i} \frac{\partial y\left(z_k, t, \varphi\right)}{\partial \varphi_j}\right)_{i,j=0}^{N} \tag{20}$$

In principle, the covariance matrix is a measure for the precision of the least square estimator for the unknown parameter $\overset{*}{\varphi}$ and a 'smaller' matrix yields more precise estimates. For example, the i^{th} diagonal element of (19) will be denoted by $\frac{\sigma^2}{N} M^{-1}\left(\xi, \overset{*}{\varphi}\right)_{ii}$ and is an approximation of the variance or mean squared error for the i^{th} component $\hat{\varphi}_{i,(N)}$ of the least squared estimator $\hat{\varphi}_{(N)}$. An approximate confidence interval for the i^{th} component φ_i of the vector φ is given by,

$$\left[\hat{\varphi}_{i,(N)} - \frac{\hat{\sigma} u_{1-\alpha/2}}{\sqrt{N}} \sqrt{M^{-1}\left(\xi, \overset{*}{\varphi}\right)_{ii}}, \hat{\varphi}_{i,(N)} + \frac{\hat{\sigma} u_{1-\alpha/2}}{\sqrt{N}} \sqrt{M^{-1}\left(\xi, \overset{*}{\varphi}\right)_{ii}}\right] \tag{21}$$

where $u_{1-\alpha/2}$ denotes the $1-\alpha/2$ quantile of the standard normal distribution and $\hat{\sigma}^2$ is an estimate of the unknown variance of the error. For most cases, it was shown that, for moderate sample sizes N, the sampling variances of the parameter estimates are well approximated.

The precision of the estimates can always be decreased by increasing the sample size N, which yields a 'smaller' covariance matrix and smaller variances of the least square estimates. However, in practice the sample size is usually fixed, due to cost considerations of each additional experiment. To improve the quality of the estimates or, from a different point of view, to reduce the number of experimental measurements needed to obtain the estimates with a given accuracy, we note that the variances of the estimates $\hat{\varphi}_{i,(N)}$ and the covariance matrix of the vector $\hat{\varphi}_{(N)}$ also depend on the given design, ξ, which determines the relative proportion of total observations to be taken at the experimental locations.

It is advisable to check that the confidence interval magnitude agrees with the sensitivity analysis, where the parameter that has the largest sensitivity coefficient should have the smallest confidence interval. Because of the consideration of the measurement error only, if the FIM is well-defined, the confidence intervals may result in very small values. Grimstadt and Mannseth (1998) indicate that the use of such an approximation of the confidence intervals was almost always justified, even for the highly nonlinear model they analysed.

NUMERICAL RESULTS

The spatial variability of sensitivities has a significant impact on parameter estimation and sampling design for studies of distributed parameter systems. Information about a physical parameter will be most accurately gained at points in space with a high sensitivity to the parameter.

The set of partial differential equations described above was solved using nominal values for the parameters and random noise with zero mean, $N(0,\sigma^2)$, was added to the outputs, the variance, σ^2, was manipulated in order to produce up to ±15% of stochastic deviation from the outputs. For each case 10 replications of the digital experiment were collected.

Data set averaging is used to reduce the effect of random noise in the measurements, which typically

arises from the data acquisition system. In practice, this implies that several data sets of the same signal, in response to identical perturbations, have been taken. Data set averaging may be obtained as,

$$\hat{y}(t_i) = \frac{1}{nt}\sum_{j=1}^{nt} y_j(t_i) \qquad i = 1,...,N_S \qquad (22)$$

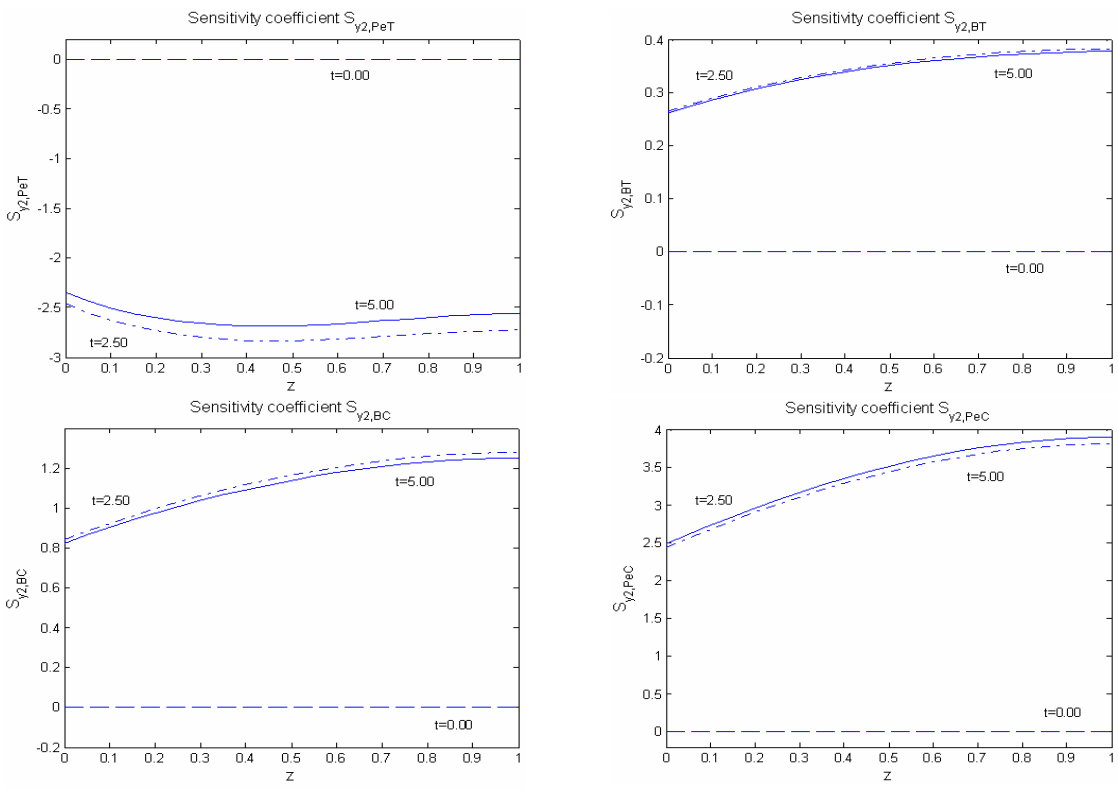
where nt is the number of data sets and N_S is the number of observations per set. The effects of the random noise tend to cancel when several sets of data are averaged. However, the noise can only be reduced to a certain degree and not totally eliminated. In this work, only minimal improvements were achieved by averaging together more than ten sets of data. In addition to averaging, the output can be low pass filtered to remove the residual random noise and the systematic noise.

The average of the resulting ten responses was then treated as experimental data and was used in the minimisation of the objective function (17). The calculated parameters were compared with their corresponding nominal values.

The analysis of the sensitivity coefficients and of the determinant of the FIM reveals the most appropriate sensor locations for the estimation of the unknown parameters (Storch et al, 2007). It is well known that sensitivity analysis quantifies the dependence of the system behaviour on the parameters that affect the process dynamics. Prasad and Vlachos (2010) presented results that show that high values of the FIM are correlated with large normalised sensitivity coefficients. These results can be very helpful to reinforce the analysis carried out here.

Figures 1 and 2 show the results of the sensitivity coefficients obtained for the stable tubular reactor case, i=1. From these figures the positions where the extrema values are reached can be extracted easily.

The extrema values of the sensitivity coefficients for temperature are located at 0.00, 0.45, and 1.00 and at 0.00, 0.30, and 1.00 for concentration. The parameter showing the lowest absolute sensitivity coefficient is γ, which implies that more sampling effort would be required to estimate this parameter. These measurement locations were considered and their effects on the parameter estimation procedure were verified. The minimum of the determinant of the covariance matrix, Equation (18) was used to measure the quality of the parameter estimates considering the spatial positions established by the extrema analysis of the sensitivity coefficients. Table 2 shows the scenarios considered for the parameter estimation of the stable example.



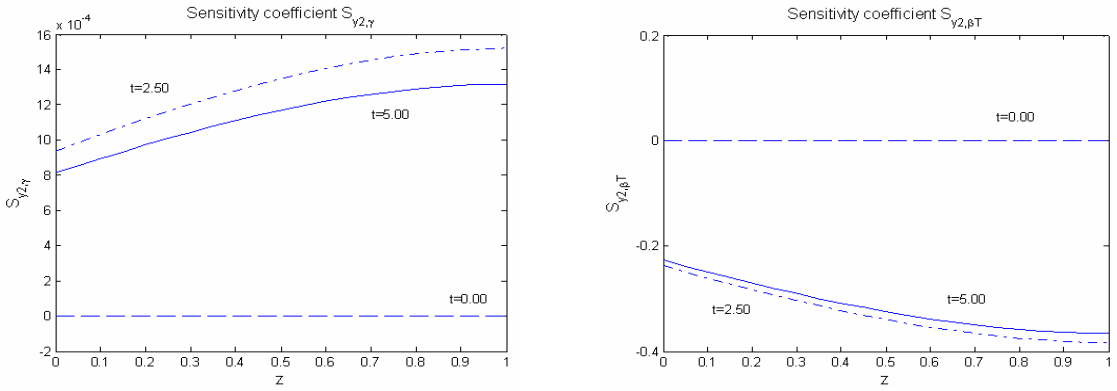


Figure 1: Sensitivity coefficients behaviour in the spatial domain, stable case.

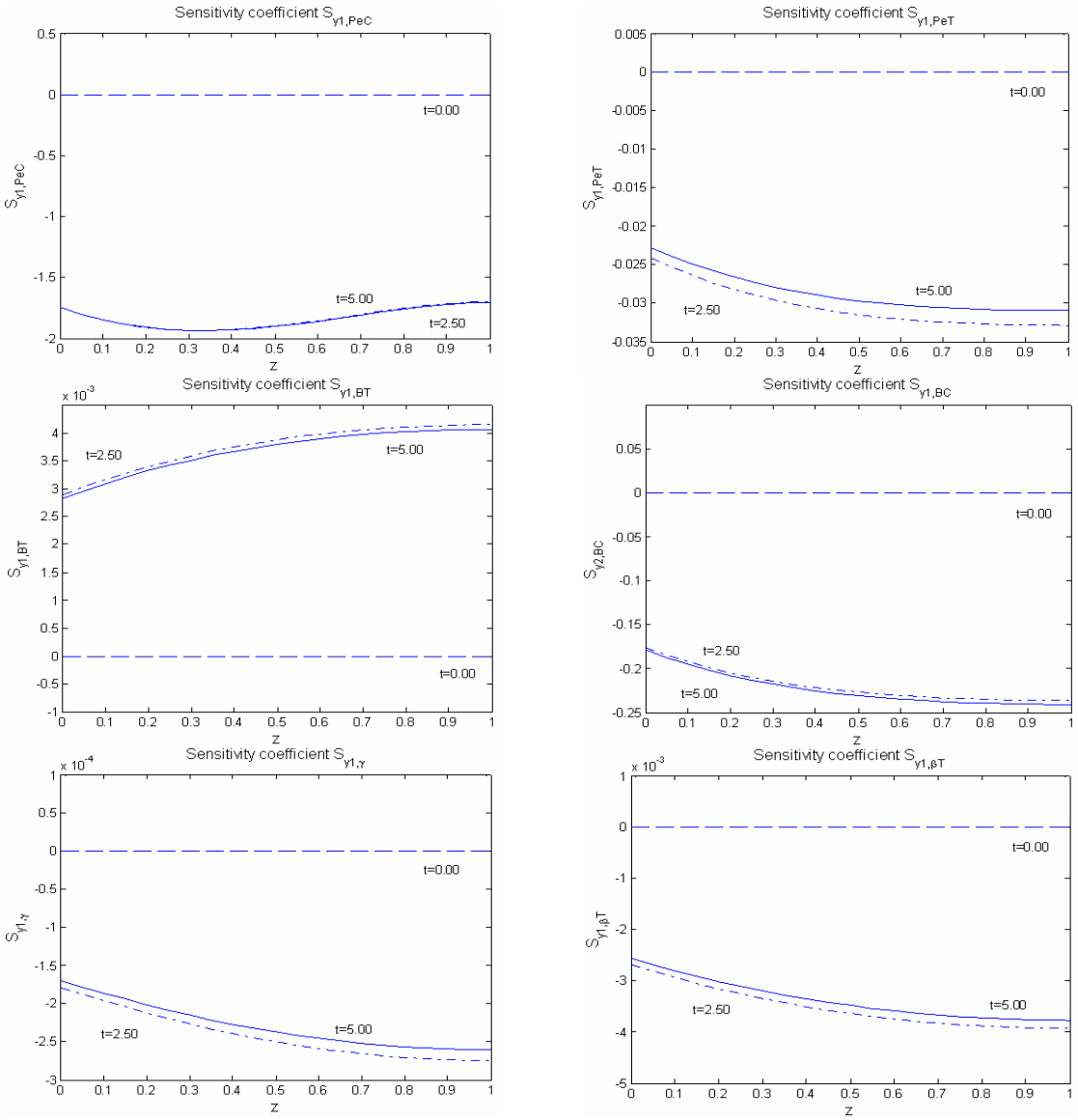


Figure 2: Sensitivity coefficients behaviour in the spatial domain, stable case.

It is our intention to consider the spatial locations where the sensitivity coefficients show extrema values to verify the accuracy of the parameter estimates using experimental data contaminated with noise. At these positions it would be logical to expect that the confidence intervals for each parameter should be small, according to Equation (21).

Matrix $\Theta(\hat{\varphi})$ in Equation (16) resembles the FIM, and Equation (20), the inverse of (16) can be considered as an approximation of the inverse of the FIM, which is a lower bound on the parameter covariance matrix. Even though Christopher and Fathalla (1999) derived their conclusions for purposes other than sensor location for parameter estimation, it is our intent to use their results to reinforce our hypothesis that a tentative set of optimal measurement positions could be defined considering the spatial locations of the extrema values of the sensitivity coefficients, which should result in small confidence intervals for the parameter estimates.

The procedure followed in this work resembles the conventional D-optimal experimental design. In the D-optimal design, the sensors are allocated by the minimisation of the determinant of the parameter covariance matrix. In our approach, the measurement positions are defined by a mere extrema analysis of the sensitivity coefficients, which can be defined as a locally optimal design, with a further evaluation of the determinant of the parameter covariance matrix to verify the quality of the parameter estimates. Both approaches need a previous estimate of the parameters.

Table 3 shows the values of the parameters estimated taking the experimental data at the locations mentioned in Table 2. The data estimated from the model at these same positions are used to minimise the objective function (17). The initial guess used corresponds to 50% of the nominal values. During each iteration the sensitivity coefficients were calculated using (7) and (8) together with (9) and/or (10). The values obtained for each case studied are shown in Tables 3 and 5. Finally, the parameters calculated were compared with their nominal values.

It can be seen in Table 3 that the parameter with the highest deviation was γ in most cases. The best estimation is obtained when the experimental measurements are taken at the locations where the sensitivity coefficients reached the extrema values for each variable of the system. The sampling scheme experienced a significant reduction from the original process, consisting of 21xn measurement locations for each state variable, to 3xn (based on the positions where the sensitivity coefficients reached extrema values). This reduction represents 86% of the original spatial domain.

For the tubular reactor with recycle operating under unstable conditions, Figures 3 and 4 show the behaviour of the sensitivity coefficients in the spatial domain for temperature and concentration, respectively.

Table 2: Locations considered for each variable, stable case

Case	Concentration locations	Temperature locations
A	Whole domain	Whole domain
B	0.00, 0.15, 1.00	0.00, 0.15, 1.00
C	0.00, 0.15, 0.95, 1.00	0.00, 0.15, 0.95, 1.00
D[a]	0.00, 0.30, 1.00	0.00, 0.45, 1.00

[a]Based on the extrema values of the sensitivity coefficients and considering the largest absolute value

Table 3: Parameters estimated, stable case

Case	Pe_C	Pe_T	B_C	B_T	γ	β_T	SSE	det[Cov]
A	1.0030 0.30%	1.0035 0.35%	0.9954 0.46%	2.0039 0.20%	20.0085 0.04%	0.9992 0.08%	1.33e-8	6.32×10^{-8}
B	0.9841 1.59%	0.9964 0.36%	1.0301 3.01%	1.9905 0.48%	6.8791 65.61%	0.9780 2.20%	0.0034	81.27×10^{-2}
C	0.9910 0.90%	1.0073 0.73%	1.0317 3.17%	1.9849 0.76%	7.2747 63.63%	0.9740 2.60%	0.0042	73.33×10^{-2}
D	1.0099 0.99%	0.9984 0.16%	1.0107 1.07%	1.9688 1.56%	19.0229 4.89%	0.9982 0.18%	2.15e-4	4.06×10^{-5}

Numbers in bold represent the deviation of the parameter from the nominal value.

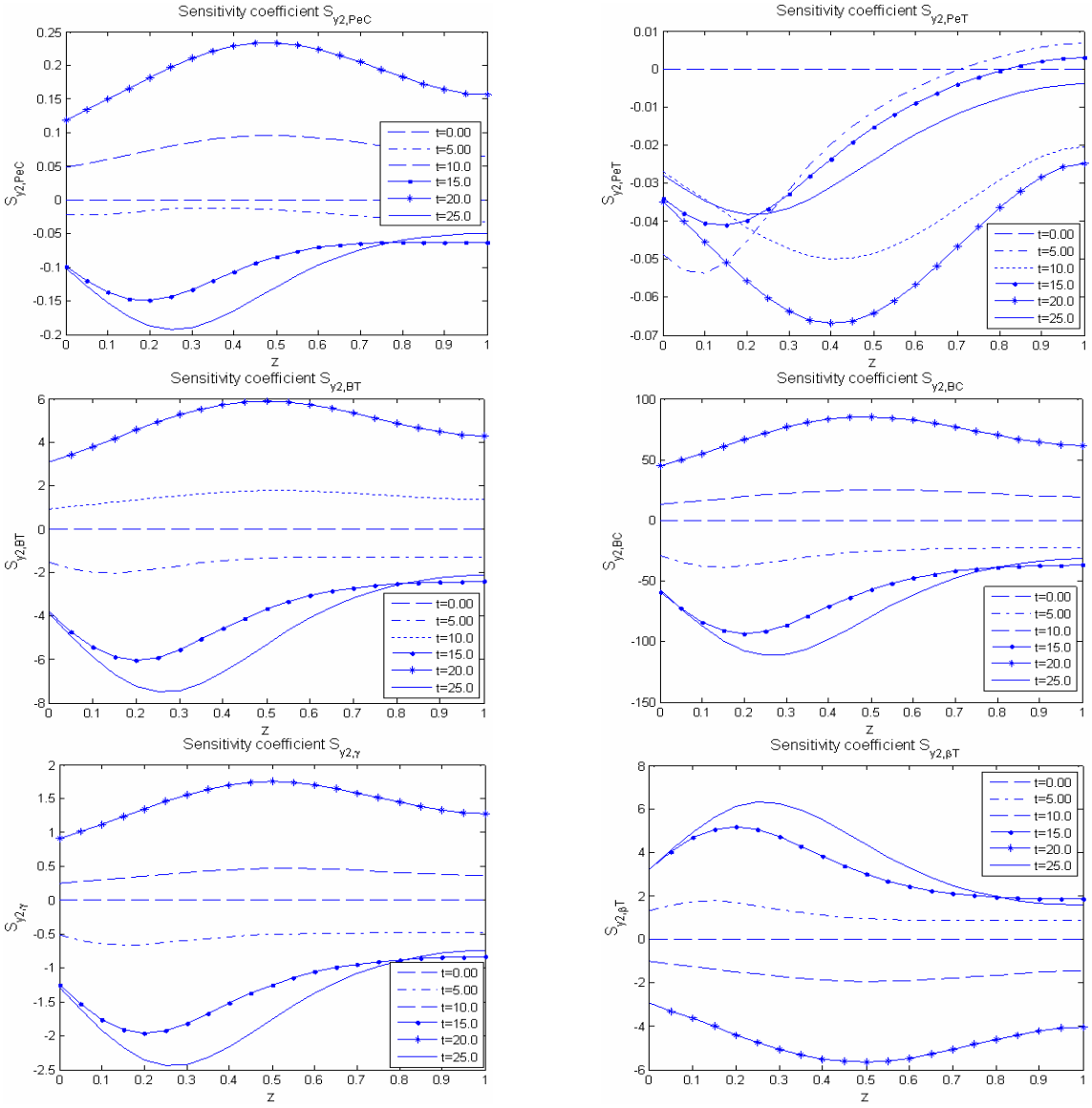
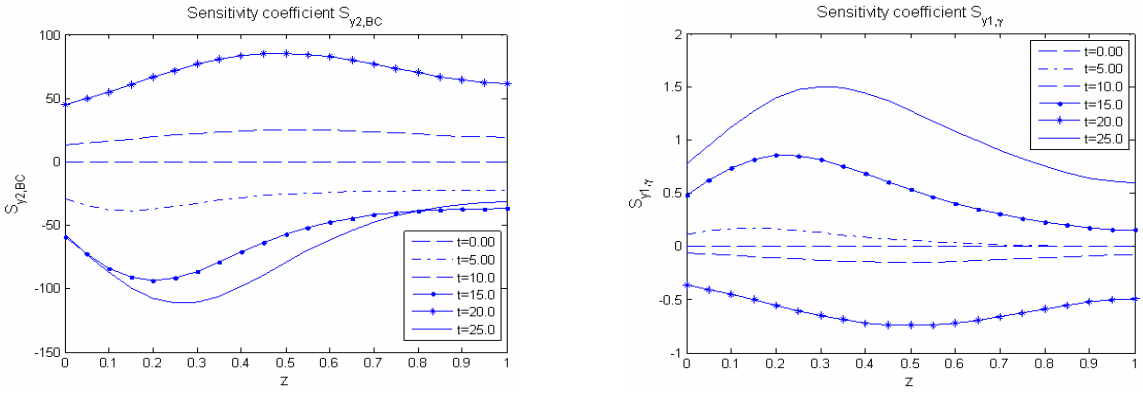


Figure 3: Sensitivity coefficients behaviour in the spatial domain, unstable case.



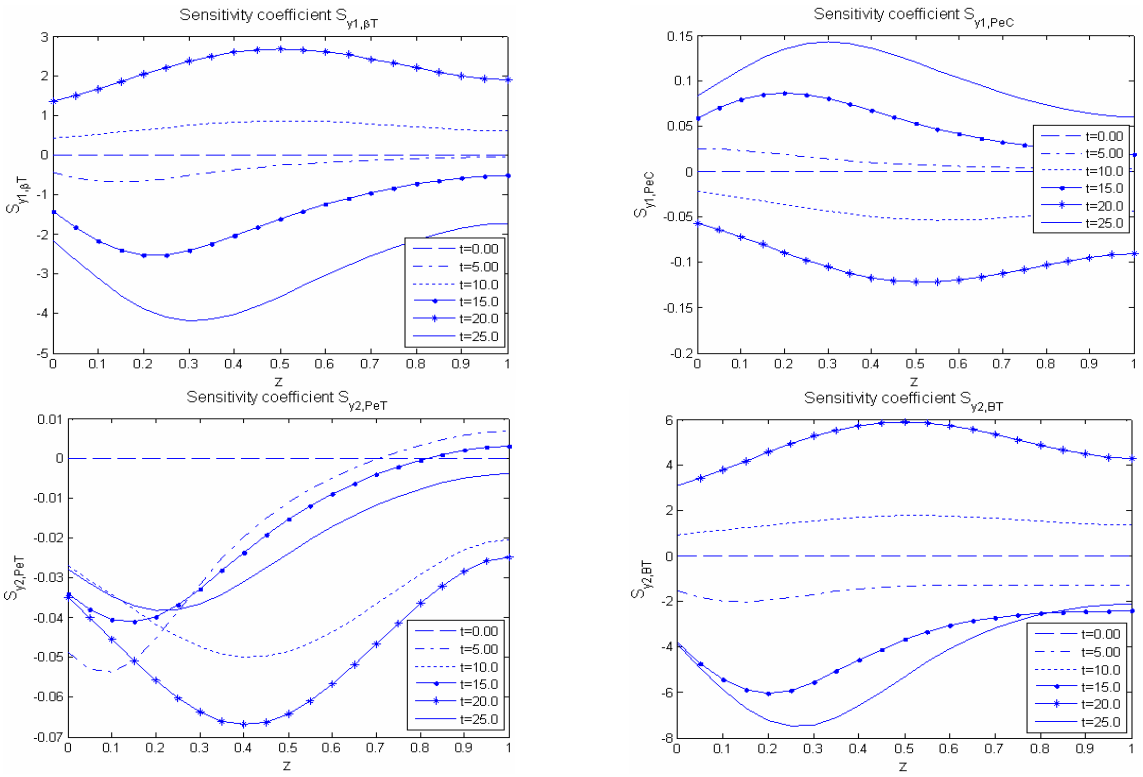


Figure 4: Sensitivity coefficients behaviour in the spatial domain, unstable case.

Examining these figures, the variety of extrema for different values of time can be seen. The largest absolute values for temperature are located at 0.15, 0.20, and 0.30 and at 0.15, 030, and 0.35 for concentration. The parameter showing the lowest absolute sensitivity coefficient is Pe_T. This system is very unstable, showing numerous extrema values in the whole spectrum of constant time lines, as can be seen in Figures 3 and 4. Even though that is not shown here, a quantification of the most recurrent extrema was carried out, which are resumed as Case D in Table 4. This table shows the cases considered to analyse the parameter estimation procedure for the unstable case.

The parameters estimated, taking the experimental measurements at the locations mentioned in Table 4 and following the procedure explained above, are shown in Table 5.

Table 4: Locations considered for each variable, unstable case

Case	Concentration locations	Temperature locations
A	Whole domain	Whole domain
B	0.05 0.10 … 0.65 0.70	0.05 0.10 … 0.65 0.70
C	0.15 0.30 0.35 0.45	0.15 0.20 030 0.40
D[a]	0.15 0.30 0.35	0.15 0.20 0.30

[a] Based on the extrema values of the sensitivity coefficients and considering the largest absolute value

Table 5: Parameter estimated, unstable case

Case	Pe_C	Pe_T	B_C	B_T	γ	β_T	10^{-3}*SSE	det[Cov]
A	7.2560 3.66%	6.3010 9.997%	0.1005 0.50%	2.4799 0.80%	9.9243 0.76%	2.0068 0.34%	3.049	$2.10\text{x}10^{-7}$
B	7.5560 7.93%	6.0010 14.27%	0.0974 2.60%	2.4480 2.08%	10.2121 2.12%	2.0799 3.40%	15.008	$7.95\text{x}10^{-4}$
C	7.7381 10.54%	4.6780 33.17%	0.1026 2.60%	2.3040 7.84%	10.2191 2.19%	1.9354 3.23%	19.482	$45.38\text{x}10^{-1}$
D	7.2279 3.26%	6.1370 12.33%	0.0998 0.20%	2.5233 0.93%	10.0330 0.33%	2.0231 1.16%	3.098	$3.89\text{x}10^{-7}$

Bold numbers represent the deviation of the parameter from the nominal value.

Due to the complex nature of this example, not even considering the whole experimental data in the spatial domain, the nominal values of the parameters are reproduced. Pe_T is the parameter showing the highest deviation from its nominal value. This gives another motivation for using sensor placement strategies based on the extrema evaluation of the predominant sensitivity functions showing the largest absolute value. Thus, not only the uncertainty in parameter estimation was reduced (see the deviation from the nominal values, number in parentheses, shown in Tables 3 and 5), but also the cost associated with such measures was reduced as well, which can be significant, especially in situations where experimental measurements are very expensive. Information about a physical parameter may be most accurately gained at points in space with a high sensitivity to the parameter. Taking observations at locations showing high sensitivity to the parameter tends to yield relatively low variance, as can be seen in Tables 3 and 5. Level of noise, above the ones considered here, affect considerably the parameter estimates.

The parameters with the lowest absolute sensitivity coefficients are the most difficult to estimate, especially if the experimental measurements are taken far from the optimal locations. When at least one parameter shows a very low absolute sensitivity, an optimisation algorithm based on the gradient and/or Hessian matrix generally gets stuck in a local minimum, distant from the optimal solution. Considering the measurement locations where the sensitivity coefficients show extrema values provided very good parameter estimates.

Taking into account the largest absolute sensitivity coefficients of the parameter of interest through a careful choice of observation points in a sampling design will lower the variance of the parameter estimate. This is the motivation for examining the behaviour of sensitivities in the system when refinement of parameter estimates is an objective of field sampling.

CONCLUSIONS

A sensor placement strategy to estimate parameters is presented. The spatial location selection is essential in the parameter estimation procedure. To optimally estimate the parameters of the system, the measurements can be taken where the extrema values of the sensitivity coefficients are reached in the spatial domain. The parameters determined with the highest deviation from the nominal values are usually the ones showing the lowest absolute sensitivity coefficients. To improve this estimation, it is advisable to measure at the locations where the sensitivity functions reach their extrema. The results are strongly affected by the presence of noise in the system, but this can be partly solved by using common filtering techniques. Not only the uncertainty in parameter estimation can be reduced by using these sensor locations, but cost is decreased also, which is significant, especially in situations where experimental observations are expensive.

NOMENCLATURE

$C_A(t,z)$	Concentration
$T(t,z)$	Temperature
$y_1(t,z)$	Dimensionless concentration
$y_2(t,z)$	Dimensionless temperature
r	Recycle to reactor
z	Spatial variable
Pe_T	Temperature Peclet number
Pe_C	Concentration Peclet number
B_C	Damkohler number
γ	Activation energy
B_T	Heat of reaction
β_T	Heat transfer
t	Time variable
t_0	Initial time
t_f	Final time
ϕ	A vector parameter of the system
Y	Output of the system
$s(Y,\varphi)$ or $s_{Y,\varphi}$	Local sensitivity of Y with respect parameter ϕ
$\frac{\partial\hat{\varphi}}{\partial u_{ij}}$	Sensitivity of the parameter $\hat{\varphi}$ to the experimental data u_{ij}
u_{ij}	Experimental data
$\Im(\varphi)$ or $\Im(\varphi,u)$	Objective function
$s(t,z,\hat{\varphi})$	Vector of local sensitivities
$\Theta(\hat{\varphi})$	Non-singular matrix
$\overset{*}{\varphi}$	the 'true' but unknown value of the parameters
$\hat{\varphi}_{(N)}$	the least square parameter estimates
ξ	the design experiment (including the measurement locations)
$M\left(\overset{*}{\xi,\varphi}\right)$	Fisher Index Matrix
$Cov(\hat{\varphi}_{nv})$	Parameter covariance matrix

$N(0,\sigma^2)$	random noise with zero mean and variance σ^2
$u_{1-\alpha/2}$	the 1-α/2 quantile of the standard normal distribution
J_y	Jacobian of the variable y
J_{y_k}	Variance of the variable k
SSE	Sum of square errors
$y_p(z_i,t)$	Predicted response at location z_i
$y_e(z_i,t)$	Experimental response at location z_i
$\hat{y}(t_i)$	Averaged data
m	Optimal number of spatial locations
nt	Number of data sets
N_S	Number of observations per data set

Acronyms

FIM	Fisher Index Matrix

REFERENCES

Alaña, J. E., Estimation of the Temporal Coefficients for an Empirical Approximator. New Approach based on the Proper Orthogonal Decomposition Modes. Computer and Chemical Engineering, doi:10.1016/j.compchemeng.2010.02.001 (2010).

Balsa-Canto, E., Alonso, A. A., Banga, J. R., Computing optimal dynamic experiments for model process calibration in predictive microbiology. Journal of Food Process Engineering, 31 (2), 186 (2008).

Bauman, E., Varma, A., Lorusso, J., Dente, M., Morbidelli, M., Parametric sensitivity in tubular reactors with co-current external cooling. Chemical Engineering Science, 45, 1301 (1990).

Bendersky, E., Christofides, P. D., Optimisation of transport-reaction processes using nonlinear model reduction. Chemical Engineering Science, 55, 4349 (2000).

Binder, T., Parameter estimation for dynamic process described with DDEs. Theses, Fakultät für Mathematik und Informatik, Ruprecht-Karls-Universität Heidelberg, Germany (2007).

Carotenuto, L., Raiconi, G., Identifiability and identification of a Galerkin approximation for a class of distributed parameter systems. Int. Journal Syst. Sci., 11, 1035 (1980).

Carotenuto, L., Raiconi, G., On the identification of a random parameter function in the one-dimensional diffusion equation and related location. Proc. 8th IFAC Triennial World Congress, Kyoto, Vol. II, 76 (1981).

Chistopher, T. H., Fathalla, A. R., Sensitivity analysis of parameters in modelling with delay-differential equations. Numerical Analysis Report No. 349, Manchester Centre for Computational Mathematics, Departments of Mathematics, The University of Manchester, England (1999).

Christofides, P. D., Antoniades, C., Computation of optimal actuator locations for nonlinear controllers in transport-reaction processes. Computer and Chemical Engineering, 24, 577 (2000).

Christofides, P. D., Antoniades, C., Integrated optimal actuator/sensor placement and robust control of uncertain transport-reaction processes. Computer and Chemical Engineering, 26, 187 (2002).

Christofides, P. D., Antoniades, C., Integrating nonlinear output feedback control and optimal actuator/sensor placement for transport-reaction processes. Chemical Engineering Science, 56, 4517 (2001).

Coste, J., Aris, R., Amundson, N. R., Tubular reactor sensitivity. AIChE Journal, 7, (1), 124 (2004).

Cotae, P., Yalamnchili, S., Chen, C. L., Ayon, A., Optimization of sensor locations and sensitivity analysis for engine health monitoring using minimum interference algorithms. EURASIP Journal on Advances in Signal Processing, 9 (2008).

Courdesses, M., Amouroux, M., Identifiabilité et identification des systémes á paramétres repartis. Proc. 3rd IFAC Symp. On Control of D. P. S., Toulouse, XXI. 1 (1982).

Courdesses, M., Polis, M. P., Amouroux, M., On identifiability of parameters in a class of parabolic distributed systems. IEEE Trans. Aut. Control, AC-26, 474 (1981).

Davidson, R., MacKinnon, J. G., Estimating the covariance matrix for regression models with ar(1) errors and lagged dependent variables. Economics Letters, 6, (2), 119 (1980).

Grimstaadt, A. A., Mannseth, T., Nonlinearity, Scale, and Sensitivity for a class of parameter estimation problem. Proc. 9th Conf. Inverse Problems in Eng., Muncie, IN (1998).

Harris, T. J., Macgregor, J. F., Wright, J. D., Optimal sensor location with an application to a packed bed tubular reactor. AIChE Journal, 26, (6), 910 (2004).

Hernandez, M. L., Kirubarajan, T., Bar-Shalom, Y., Multisensor resource deployment using posterior Cramer-Rao bounds. IEEE Transactions on Aerospace and Electronic Systems, 40, 399 (2004).

Juncu, G., Floarea, O., Sensitivity analysis of tubular packed-bed reactor by pseudohomogeneous 2D model. AIChE Journal, 41, (12), 2625 (1995).

Kitamura, S., Taniguchi, Y., Parameter estimation of one- and two–dimensional heat conduction processes using a minicomputer. Int. Journal Control, 34, 955 (1981).

Knopman, D. S., Voss, C. I., Behavior of sensitivities in the one-dimensional advection-dispersion equation: implications for parameter estimation and sampling design. Water Resour. Res., 23, (2), 253 (1987).

Kubrously, C. S., Malebranche, H., Sensors and controllers location in distributed systems–A survey. Automatica, 21, (2), 117 (1985).

Kubrusly, C. S., Linear DPS identification in a stochastic environment. R. A. I. R. O. System Anal. and Control, 14, 343 (1980).

Kumar, S., Seinfeld, S. H., Optimal location of measurements in tubular reactors. Chemical Engineering Science, 33, 1507 (1978).

Le Pourhiet, A. M., Le Letty, L., Optimization of sensors location in distributed parameter system identification. Proc. 4th IFAC Symp. On Identification & System Parameter Estimation, Tibilisi, 1581 (1976).

Li, M., Chistofides, P. D., Optimal control of diffusion–convection–reaction processes using reduced–order models. Computers and Chemical Engineering, doi: 10.1016/j.compchemeng. 2007.10.018 (2007).

Ljung, L., System Identification–Theory for the user. 2nd Edition, Prentice Hall, Upper Saddle River, NJ, USA (1999).

Löhner, R., Camelli, F., Optimal Placement of Sensors for Contaminant Detection Based on Detailed 3D CFD. Simulations Engineering Computations. International Journal for Computer-Aided Engineering, 22, (3), 260 (2005).

Morbidelli, M., Varma, A., A generalized criterion for parametric sensitivity application to thermal explosion theory. Chem. Eng. Sci., 43, 91 (1988).

Nahor, H. B., Scheerlinck, N., Van Impe, J. F., Nicolaï, B. M., Optimization of temperature sensor position in a hot wire probe set up for estimation of the thermal properties of foods using optimal experimental design. J. Food. Eng., 57, 103 (2003).

Nakagiri, S., Identifiability of linear systems in Hilbert spaces. SIAM J. Control & Optimization, 21, 501 (1983).

Olanrewaju, M. J., Al-Arfaj, M. A., Estimator-based control of reactive distillation system: Application of an extended Kalman filtering. Chemical Engineering Science 61, 3386 (2006).

Papadimitriou, C., Optimal sensor placement methodology for parametric identification of structural systems. J. Sound Vibration 278, 923 (2004).

Peng, T., Fault Detection Methods Based on Optimal Sensor Location. Hunan: Central South University (2005).

Prasad, V., Vlachos, D. G., Combined multiscale model and informatics based design of experiments: Application to the catalytic decomposition of Ammonia on Ruthenium. Ind. Eng. Chem. Res., (accepted).

Punithakumar, K., Kirubarajan, T., Hernandez, M., Multisensor deployment using PCRLBs, incorporating sensor deployment and motion uncertainties. IEEE Transactions on Aerospace and Electronic Systems 42, 1474 (2006).

Qureshi, Z. H., Ng, T. S., Goodwin, G. C., Optimum experimental design for identification of distributed parameter systems. International Journal of Control, 31, (1), 21 (1980).

Rafajlowics, E., Optimal experiment design for identification of linear distributed-parameter systems: Frequency domain approach. IEEE Transactions on Automatic Control, 28, (7), 806 (1983).

Rafajlowicz, E., Design of experiments for eigenvalues identification in DPS, International. Journal of Control, 34, (6), 1079 (1981).

Rutzler, W., Nonlinear and adaptive parameter estimation methods for tubular reactors. Ind. Eng. Chem. Res., 26, (2), 325 (1987).

Rutzler, W., Nonlinear and adaptive parameter estimation methods for tubular reactors. Ind. Eng. Chem. Res., 26, (2), 325 (1987).

Singh, A. K., Hahn, J., Determining optimal sensor locations for state and parameter estimation for stable nonlinear systems. Industrial and Eng. Chem. Res., 44, (15), 5645 (2005).

Singh, A. K., Hahn, J., Sensor Location for Stable Nonlinear Systems: Placing Multiple Sensors. Proceedings Chemical Process Control 7, Lake Louise, Canada (2006).

Söderström, T., Stoica, P., System Identification. Prentice Hall International, Hemel Hempstead, UK (1989).

Sokollik, F., Zur Parameterschätzung von Systemen mit verteilten Parametern mittels on–line. Verfahren. Messen. Steuern. Regeln., 19, 84 (1976).

Sorenson, H. W., Parameter estimation: principles and problems. New York, M. Dekker, 183 (1980).

Storch, R. B., Pimentel, L. C. G., Orlande, H. R. B., Identification of atmospheric boundary layer parameters by inverse problem. Atmospheric Environment, 41, (7), 1417 (2007).

Tilden, J. W., Constanza, V., McRae, G. J., Seinfeld, J. H., Sensitivity analysis of chemically reacting systems. In: K. H. Ebert, P. Deuflhard and W. Jager, Editors, Modeling of Chemical Reaction Systems, Springer, New York, 69 (1981).

Uciński, D., Bogacka, B., Construction of T-optimum designs for multiresponse dynamic models. In COMPSTAT 2002 (Berlin), Heidelberg: Physica, pp. 267 (2002).

Uciński, D., Demetriou, M., An approach to the optimal scanning measurement problem using optimum experimental design. Proceeding of the 2004 American Control Conference, June 30-July 2, Boston, Massachusetts (2004).

Uciński, D., Measurement Optimization for Parameter Estimation of Distributed Systems. Technical University Press, Zielona Gora (1999).

Uciński, D., On the determination of moving sensor policies for parameter estimation of distributed systems. 11th Mediterranean IEEE Conference on Control and Automation MED'03, June 18-20, Rhodes, Greece (2003).

Uciński, D., Optimal measurement method for distributed parameter system identification. CRC Press. USA (2005).

Uciński, D., Optimal sensor location for parameter estimation of distributed processes. International Journal of Control, Vol. 73, No. 13, 1235 (2000a).

Uciński, D., Optimal sensor location for parameter identification of distributed systems. Applied Mathematics and Computer Science, 2, (1), 119 (1992).

Uciński, D., Optimization of sensors' allocation strategies for parameter estimation in distributed systems. System Analysis Modell. Simul., Vol. 37, 243 (2000b).

Vajda, S., Rabitz, H., Parametric sensitivity and self-similarity in thermal explosion theory. Chem. Engng. Sci., 47, 1063 (1992).

Van den Berg, F. W. J., Hoefsloot, H. C. J., Boelens, H. F. M., Smilde, A. K., Selection of optimal sensor position in a tubular reactor using robust degree of observability criteria. Chemical Engineering Science, 55, (4), 827 (2000).

Vande Wouwer, A., Point, N., Porteman, S., Remy, M., An approach to the selection of optimal sensor locations in distributed parameter systems. Journal of Process Control, 10, (4), 291 (2000).

Venkateswarlu, C. B. J., Kumar, B. J., Composition estimation of multi component reactive batch distillation with optimal sensor configuration. Chemical Engineering Science, 61, 5560 (2006).

Waterhouse, T. H., Eccleston, J. A., Duffull, S. B., Optimal design criteria for discrimination and estimation in nonlinear models. J. Biopharmaceutical Statistics, 19, (2) 386 (2009).

Yen, W. W-G., Yoon, Y. S., Aquifer parameter identification with optimum dimension in parameterization. Water Resour. Res., 17, (3), 664 (1981).

Zamprohna, E., Barolo, M., Seborg, D. E., Optimal Selection of Sensors Inputs for Batch Distillation Columns Using Principal Component Analysis. Journal of Process Control, 15, 39 (2005).

Zhu, Z., Stein, M. L., Spatial sampling design for parameter estimation of the covariance function. Journal of Statistical Planning and Inference, 134, (2), 583 (2005).