Model reduction as a tool for robust predictive control: application to OPR

Estefanía López-Quiroga, Luís T. Antelo, Antonio A. Alonso*

Process Engineering Group IIM-CSIC, Eduardo Cabello 6, Vigo 36208, Galiza, Spain,

** Corresponding Author: antonio@iim.csic.es*

Abstract

The production of some chemicals or pharmaceuticals has been improved over the years by the development of a new concept of reactors, the reactor-heat exchangers, that overcome the classical constraints affecting many reaction units related to dissipation of heat and dilution/separation of products. The aim of this work is to propose a methodology for robust predictive control which aims at capturing the slow and most relevant, dynamics of the system. This model reduction constitutes the preliminary step to apply a real time optimization (RTO) framework for the robust control of reaction systems. The Open Plate Reactor (OPR) developed by the Swedish company Alfa Laval is used as a benchmark to validate the proposed methodology.

Keywords: OPR, Process Dynamics, Time Scales, Reduced Order Models, Robust Control.

1. Introduction

The synthesis of some chemicals or pharmaceuticals products constitutes a highly constrained process due to restrictions related to the dissipation of heat generated by the reactions [1]. One of the most common ways of solving these dissipation problems is to dilute the reactants, so that the reaction rate and therefore the heat released are reduced, which facilitates the process. Once the reaction ends, a separation of the solvent is carried out in order to increase the product concentrations. This separation process implies energy and time expenses which should be avoided. In order to overcome these problems, a new concept of heat-exchange reactors which combine both the advantages of plate exchangers for heat transferring as well as the mixing efficiency and reaction control of micro-reactors was developed [2,3]. As a consequence, full process performance is improved and time and energy costs are reduced. In this new framework, the Open Plate Reactor (OPR) developed by Alfa Laval presents such features. The dynamic behavior of the OPR is described by a large nonlinear system of partial differential equations involving temperature and reactant concentrations [4]. Due to the high dimensionality of the full model, reduced order representations of partial differential equations are developed. These follow the strategies proposed in [5], based on Laplacian Spectral Decomposition (LSD) and Proper Orthogonal Decomposition (POD). The aim is to capture the most relevant (slow) dynamics of the system without significant loss of accuracy in the representation with respect to those corresponding to the full model. These reduced models constitute the core of a real time optimization (RTO) methodology for controlling the OPR. The objective will be the minimization of process, so time to attain a desired yield while keeping the maximum temperature inside the unit within the established security margins defined for the process.

In this paper, the full dynamic model for OPR is presented in Section 2. Model reduction is described in Section 3. Finally, in Section 4, the formal statement of the RTO control problem for the Open Plate Reactor is proposed.

2. The Open Plate Reactor dynamic model.

The OPR unit is based on plate heat exchangers, which separate the hot and cold fluids in alternate plates with a large surface area, so to attain a higher heat transfer. The mixing of the reactants is performed in reactor plates, being each of them located between two cooling plates. This configuration allows flexible operation conditions such as several reactant injection points all along the reactor, changes in residence time, etc.

Since the cross section of the horizontal channels in the OPR is too small when compared with its length [4], an equivalent design consisting in a continuous plug reactor with cooling jacket can be used. In this work, the following exothermic reaction is considered:

The system of nonlinear partial differential equations (PDE) describing the dynamic behavior of the resulting plug flow reactor [6] is obtained from the energy balance inside the OPR and the reactants mass balances when a unique reactant injection point is considered. The equations are as follows:

$$\rho c_p \frac{\partial T_r}{\partial t} = k \frac{\partial^2 T_r}{\partial z^2} - \rho c_p v_r \frac{\partial T_r}{\partial z} + \frac{4h}{D_r} (T_c - T_r) + \Delta H r(C_A, C_B, T_r) \quad \text{Eq.(2)}$$

$$\frac{\partial C_A}{\partial t} = D \frac{\partial^2 C_A}{\partial z^2} - v_r \frac{\partial C_A}{\partial z} - r(C_A, C_B, T_r) \quad \text{Eq.(3)}$$

$$\frac{\partial C_B}{\partial t} = D \frac{\partial^2 C_B}{\partial z^2} - v_r \frac{\partial C_B}{\partial z} - 2r(C_A, C_B, T_r) \quad \text{Eq.(4)}$$

where: z is the position in the reactor, t is the time variable, D_r is the diameter of the tube and h is the heat transfer coefficient. The reaction heat is represented by ΔH ; T_r and T_c are the temperatures in the reactor and of the cooling medium, respectively. The reacting mixture defined by its density ρ , thermal conductivity k , and heat capacity c_p flows through the reactor with velocity v_r . Finally, D is the mass diffusion coefficient, and C_A, C_B are the concentrations of reactants A and B, respectively. It must be noted that the reaction rate is given by the Arrhenius law: $r(C_A, C_B, T_r) = k_0 C_A C_B \exp(-E_a / RT_r)$; and that the initial conditions are: $C_A(z, 0) = 0$, $C_B(z, 0) = 0$, $T_r(z, 0) = 273 \text{ K}$, $\forall 0 \leq z \leq L$, being L the reactor length.

In order to both facilitate the analysis and control of the OPR dynamic model, and to reduce the amount of parameters while achieving a well-conditioned system for numerical simulation, the model described by Eqs.(2-4) is transformed into a dimensionless one, by taking as independent spatial variable $\xi = z / L$, and as independent temporary variable $\tau = t v_r / L$. This leads to:

$$\frac{\partial y}{\partial \tau} = \frac{1}{Pe_1} \frac{\partial^2 y}{\partial \xi^2} - \frac{\partial y}{\partial \xi} + W(u - y) + Da_3 \cdot f(x_A, x_B, y) \quad \text{Eq.(5)}$$

$$\frac{\partial x_A}{\partial \tau} = \frac{1}{Pe_2} \frac{\partial^2 x_A}{\partial \xi^2} - \frac{\partial x_A}{\partial \xi} - Da_{1a} \cdot f(x_A, x_B, y) \quad \text{Eq.(6)}$$

$$\frac{\partial x_B}{\partial \tau} = \frac{1}{Pe_2} \frac{\partial^2 x_B}{\partial \xi^2} - \frac{\partial x_B}{\partial \xi} - 2Da_{1b} \cdot f(x_A, x_B, y) \quad \text{Eq.(7)}$$

where $f(x_A, x_B, y) = (1 + x_A)(1 + x_B) \exp\left(\frac{E_a}{RT_{ref}} \left(\frac{y}{1 + y}\right)\right)$; x_A, x_B, y are the dimensionless variables for reactants A, B, and reactor temperature, respectively, with:

$Pe_1 = \rho L v_r c_p / k$; $Pe_2 = L v_r / D$; $Da_{1a} = L r_{ref} / v_r C_{Ae}$; $Da_{1b} = L r_{ref} / v_r C_{Be}$; $Da_3 = r_{ref} L \Delta H / \rho v_r c_p T_{ref}$; $W = 4hL / c_p \rho D_r v_r$ and $r_{ref} = k_0 C_{Ae} C_{Be} \exp(-E_a / RT)$.

Finally, the dimensionless model is completed with the following boundary conditions:

$$\begin{aligned} \bullet \quad \text{At } \xi = 0 \quad & \bullet \quad \text{At } \xi = 1 \\ -\frac{\partial y}{\partial \xi} + Pe_1 y = 0 \quad & \frac{\partial y}{\partial \xi} = 0 \end{aligned} \quad \text{Eq.(8)} \quad \text{Eq.(11)}$$

$$-\frac{\partial x_A}{\partial \xi} + Pe_2 x_A = 0 \quad \frac{\partial x_A}{\partial \xi} = 0 \quad \text{Eq.(9)} \quad \text{Eq.(12)}$$

$$-\frac{\partial x_B}{\partial \xi} + Pe_2 x_B = 0 \quad \frac{\partial x_B}{\partial \xi} = 0 \quad \text{Eq.(10)} \quad \text{Eq.(13)}$$

and initial conditions:

$$x_A(\xi, 0) = -1 \quad x_B(\xi, 0) = -1 \quad y(\xi, 0) = -0,099, \quad 0 \leq \xi \leq 1 \quad \text{Eq.(14)}$$

For its characteristics, the Matlab toolbox MatMOL (www.matmol.org) has been selected to solve the EDP system by using Finite Element Method (FEM). In this case, a non homogeneous spatial discretization, with 121 Lagrange P1 elements (half in the first third of the OPR and half in the rest) has been chosen. The results obtained for this model will be presented in comparison with those corresponding to the reduced model in the next Section.

3. Construction of reduced order models.

Solving PDE systems by using classical methods, for instance FEM, Finite Difference or Finite Volumes, implies the handling of a high number of ODEs. This fact difficulties the application of these methods in many fields as real time optimization or predictive control, where the computing times are very important. In order to overcome this issue, new techniques capable of both simplifying the analysis and control of a given dynamic system as well as to reduce the computational effort have been developed. In this aim, Reduced Order Models will be employed to approximate the system by its slow and possibly unstable dynamics. Such approach will, in consequence, reduce the number of equations involved and thus the computation times [5,7]. In this work, the Laplacian Spectral Decomposition (LSD) and the Proper Orthogonal Decomposition (POD) are applied to the OPR model. Both methods consist of projecting the system of partial differential equations on a lower dimensional subspace characterized by a set of globally defined basis functions satisfying the boundary conditions [8]. These basis functions are also required to form an orthogonal set in L^2 on the spatial domain considered.

Laplacian Spectral Decomposition (LSD). The reduced model is obtained by using the `matlsd` function from the MatMOL toolbox. The procedure consists on solving the following eigenvalue problem:

$$-\frac{1}{Pe}\Delta\phi_i = \lambda_i\phi_i, \quad \text{en } (0,1), \quad i = 1, \dots, \text{neig};$$

$$-\frac{1}{Pe}\phi_i'(0) + \phi_i(0) = 0, \quad \phi_i'(1) = 0$$

where λ_i are the eigenvalues (increasing ordered), ϕ_i are the eigenfunctions and neig is the number of basis functions. Finally, the EDP system with boundary conditions is projected over the selected set of eigenfunctions ϕ_i .

One of the dimensionless parameters present in the dynamic model is the Péclet number, Pe . Each reactor has a characteristic Pe value which plays an important role on system reduction: the eigenvalues and eigenfunctions are determined by the diffusion coefficient ($1/Pe$), according to Eq.(15). In this section, two different OPR, with its own Pe values, are analyzed. For an OPR with a low Pe number ($Pe=7$), a spectral gap of characteristic time scales that separates slow and fast components of the system dynamics exists [9], as shown in Figure 1. For an OPR with a high Pe number ($Pe=59$), the identification of different time scales is not as clear since the gap is smaller (all eigenvalues are in the same order of magnitude), being the dynamics more homogeneous. According to this, the LSD method will be more efficient for obtaining a model reduction when dealing with low Péclet values (i.e. reaction systems in which diffusion is important).

Proper Orthogonal Decomposition (POD). In this method, the basis functions are calculated through sets of data, called *snapshots*, by solving the following eigenvalue problem:

$$\phi_i(\xi) = \lambda_i \int_{\Omega} K(\xi, \xi') \phi_i(\xi') d\xi', \quad \text{Eq.(16)}$$

where $K(\xi, \xi') = \frac{1}{l} \sum_{i=1}^l z_i(\xi) z_i(\xi')$ is the kernel defined by the *snapshots* $z_i(\xi)$.

The *snapshots* are chosen so to reproduce the leading dynamics of the system. In this work, the *snapshots* are obtained from the numerical simulation of the OPR model and the function `matpod` is employed to perform the reduction. As shown in Table 1, the POD method achieves a reduction in the degrees of freedom (DOF) of the model of around a 50% for each variable, while maintaining the accuracy with respect to the full model. The temperature evolution in the OPR for both full and reduced model is presented in Figure 2, confirming the good agreement between them.

Figure 1. Comparison between λ_i obtained from Eq.(15) for $Pe=7$ and $Pe=59$.

Figure 2. Temperature evolution in the OPR reactor: a) Full model; b) POD reduced model.

Table 1. POD results for the OPR model

Variable	DOF full model	DOF reduced model	Maximum absolute error
$x_A \in (-1, 0)$	121	56	0.0011
$x_B \in (-1, 0)$	121	49	0.0003
$y \in (-0.099, 2.15)$	121	54	0.0025

4. The OPR real time optimization problem.

The high dimension and nonlinearity inherent to the mass and energy balance equations of the OPR result into sets of control problems computational involved which justify a hierarchy two level approach:

1) The *upper layer* is responsible of obtaining different operation scenarios (i.e. different inlet configurations for reactants A and B or several reactant injection points distributed all along the reactor's length -Figure 3), which can be evaluated as a function of the reaction yield. Such assessment will be formally stated as a dynamic optimization problem to provide the required profile for the considered control variable u (cooling water temperature, T_c). The aim in this case is to minimize the process time t_f so to achieve a given yield γ in the OPR while satisfying both process dynamics f and operation constraints related to the reactor temperature T_r . Mathematically, the problem can be stated as follows:

Figure 3. OPR scheme for the case of multiple reactant injection points. Each block can be described by the reduce model defined for the OPR with a single injection point.

$$\min J = t_f$$

$$s.t. \quad f(\dot{x}, x, u, z, t) = 0; \quad \gamma(L, t_f) = 96\%; \quad T_r(z, t) \leq 155^\circ C; \quad 20^\circ C \leq T_c \leq 80^\circ C$$

Eq.(17)

As discussed above, the high dimensionality of the full model for the OPR could make the solution of problem in Eq.(17) computational involved. This calls for methodologies as the one proposed for model reduction to facilitate its analysis and solution [10].

2) The *lower layer* consists on the implementation of the pre-computed policies on a real time optimization framework designed to react to possible disturbances and to minimize the adverse effect of final product variability. It is at this level where once again model reduction techniques together with on-line observers and estimators could be employed to cope with parameter and structural uncertainty as well as to minimize the computational burden associated with on-line dynamic optimization. As mentioned in Section 3, such identification methods will be based on first principle models covering the relevant operation time scales of the process (slow dynamics).

5. Conclusions and future work

Reduced order models for the Open Plate Reactor were obtained by applying two different techniques, the Laplacian Spectral Decomposition (LSD) and the Proper Orthogonal Decomposition (POD). It was found that model reduction through LSD is efficient for low Péclet numbers. In addition, the POD has been revealed as an effective method to obtain the desired reduced model for the OPR, no matter the importance of the diffusive phenomenon (i.e. for all the Péclet values). The latter reduced model is the

core of the RTO problem proposed in this paper. As a future work, the resulting NLP control problems defined on the *upper layer* will be solved by employing the NDOT MATLAB toolbox [11] developed in the Process Engineering Group of the IIM-CSIC (<http://www.iim.csic.es/~gingproc>). Moreover, different strategies such as the distribution of reactant injection points all along the reactor's length together with some modifications on the OPR model design (to consider extensive variables –inventories– instead the current intensive ones) and on the operation conditions will be considered. These extensions are believed to provide a considerable improvement of the operation.

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