Economic Model Predictive Control of Parabolic PDE Systems Using Empirical Eigenfunctions

Liangfeng Lao, Matthew Ellis, Antonios Armaou, and Panagiotis D. Christofides

Abstract—This work focuses on the development of reduced-order models (ROMs) of transport-reaction processes described by nonlinear parabolic partial differential equations (PDEs) and their application in the formulation of economic model predictive control (EMPC) systems. Specifically, the reduced-order models of the PDEs are constructed on the basis of historical data-based empirical eigenfunctions by applying Karhunen-Loève expansion. Several EMPC systems each using a different ROM (i.e., different number of modes and derived from either using analytical sinusoidal/cosinusoidal eigenfunctions or empirical eigenfunctions as basis functions) are applied to a tubular reactor example where a second-order reaction occurs. The model accuracy, computational time and closed-loop economic performance of the closed-loop tubular reactor under the different EMPC systems are compared.

I. INTRODUCTION

The control problem for parabolic PDE systems arising in the modeling of transport-reaction processes primarily focuses on two aspects: 1) computationally efficient model reduction methodologies for the construction of finite-dimensional approximations, and 2) finite-dimensional controller design and analysis of the closed-loop PDE system. With respect to model reduction, the application of modal (eigenfunction) expansion techniques in the context of Galerkin’s method (using empirical or analytical basis functions), is usually adopted. Even though Galerkin’s method based on analytical basis functions of the spatial differential operator reduces the dimension of the control problem (e.g., [3], [5], [7], [8], [9], [14]), it may not be very computationally efficient and may not be highly accurate for the problems that involve nonlinear reaction rates or spatially varying coefficients because the basis functions may only contain information about the spatial differential operators and not the other terms in the PDE system.

In terms of the optimal control of PDE systems, model predictive control (MPC) has become a popular control method owing to its ability to handle constraints (both on manipulated inputs and state variables) within an optimal control setting using quadratic cost functions (e.g., [7], [8]).

Recently, significant work on economic model predictive control (EMPC) has been developed in the context of finite dimensional systems (e.g., [6], [12], [10], [15], [1]). Within the context of distributed parameter systems (DPS), however, only limited work has been completed using EMPC. In our previous work [14], two EMPC systems for transport-reaction processes described by nonlinear parabolic PDEs were developed on the basis of low-order and high-order nonlinear ordinary differential equation (ODE) models derived through Galerkin’s method using analytical basis functions. Considering the possible limitation for using analytical basis functions and to improve the reduced-order model (ROM) accuracy, empirical eigenfunctions may be considered as the basis functions for Galerkin’s method. The empirical eigenfunctions may be constructed by applying Karhunen-Loève (K-L) expansion to PDE system solution data (e.g., [18], [11]). By collecting an ensemble of the system solution data from process historical data or simulation data, the K-L expansion method considers the presence of the dominant spatial patterns in the solution of the parabolic PDEs and results in a more comprehensive and accurate ROM than a ROM based on analytical basis functions. This data-based construction of the basis functions for order reduction of PDE systems has been widely adopted in the recent years in the context of model-based control problems for parabolic PDE systems (e.g., [4], [19], [3], [2], [20], [16]).

In this work, reduced-order models of transport-reaction processes described by nonlinear parabolic PDEs are developed and used in the formulation of EMPC systems. Specifically, the reduced-order models of the PDEs are constructed on the basis of historical data-based empirical eigenfunctions by applying Karhunen-Loève expansion. Several EMPC systems each using a different ROM (i.e., different number of modes and derived from either using analytical sinusoidal/cosinusoidal eigenfunctions or empirical eigenfunctions) are applied to a non-isothermal tubular reactor where a second-order chemical reaction takes place. The model accuracy, computational time and closed-loop economic performance of the closed-loop tubular reactor under the different EMPC systems are compared.

II. PRELIMINARIES

A. Class of Parabolic PDE Systems

We consider parabolic PDEs of the form:

$$\frac{\partial \bar{x}}{\partial t} = A \frac{\partial \bar{x}}{\partial z} + B \frac{\partial^2 \bar{x}}{\partial z^2} + W u(t) + f(\bar{x}(z, t))$$  \hspace{1cm} (1)

$$\frac{\partial^2 \bar{x}}{\partial z^2}$$ \hspace{1cm} (2)
with the boundary conditions:
\[
\frac{\partial \bar{x}}{\partial z}
\bigg|_{z=0} = g_0 \bar{x}(0, t), \quad \frac{\partial \bar{x}}{\partial z}
\bigg|_{z=1} = g_1 \bar{x}(1, t)
\]
for \( t \in [0, \infty) \) and the initial condition:
\[
\bar{x}(z, 0) = \bar{x}_0(z)
\]
where \( z \in [0, 1] \) is the spatial coordinate, \( t \in [0, \infty) \) is the time, \( \bar{x}'(z, t) = [\bar{x}_1(z, t); \cdots; \bar{x}_n(z, t)] \) is the vector of the state variables (\( \bar{x}' \) denotes the transpose of \( \bar{x} \)), and \( f(\bar{x}(z, t)) \) denotes a nonlinear vector function. The notation \( A, B, W, \)
\( g_0 \) and \( g_1 \) is used to denote (constant) matrices of appropriate dimensions. The control input vector is denoted as \( u(t) \in \mathbb{R}^n_u \) and is subject to the following constraints:
\[
u_{\text{min}} \leq u(t) \leq u_{\text{max}}
\]
where \( u_{\text{min}} \) and \( u_{\text{max}} \) are the lower and upper bound vectors of the manipulated input vector, \( u(t) \). Moreover, the system states are also subject to the following state constraints:
\[
x_{i,\text{min}} \leq \int_0^1 r_x(z) x_i(z) dz \leq x_{i,\text{max}}, \; i = 1, \ldots, n_x
\]
where \( x_{i,\text{min}} \) and \( x_{i,\text{max}} \) are the lower and upper state constraint for the \( i \)-th state, respectively. The function \( r_x(z) \in L_2(0, 1) \) where \( L_2(0, 1) \) is the space of measurable, square-integrable functions on the interval \([0, 1]\) is the state constraint distribution function.

III. METHODOLOGICAL FRAMEWORK FOR LOW-ORDER EMPC USING EMPIRICAL EIGENFUNCTIONS

The methodology used to carry out the order reduction and EMPC design is summarized below.

1) Initially, we form an ensemble of solutions of the PDE system of Eq. 1 for different values of manipulated input variables \( u(t) \).
2) Then, we apply Karhunen-Loève (K-L) expansion to this ensemble to derive a set of empirical eigenfunctions (dominant spatial patterns that minimize the mean square error over all the ensemble elements) [2].
3) The empirical eigenfunctions are used as basis functions within a Galerkin’s model reduction framework to transform the infinite dimensional nonlinear PDE system into a ROM in the form of a low-dimensional nonlinear ODE system.
4) Finally, an EMPC formulation is developed with the ROM and applied to the tubular reactor example.

IV. APPLICATION TO A TUBULAR REACTOR

A. Reactor Description

We consider a non-isothermal tubular reactor where an irreversible second-order reaction of the form \( A \rightarrow B \) takes place. The process model in dimensionless variable form consists of two parabolic PDEs (process details and model notation can be found in [14] and [17]):
\[
\frac{\partial \bar{x}_1}{\partial t} = -\frac{\partial \bar{x}_1}{\partial z} + \frac{1}{Pe_1} \frac{\partial^2 \bar{x}_1}{\partial z^2} + \delta(z-0)T_t + B_T B_C \exp\left(\frac{\gamma \bar{x}_1}{1 + \bar{x}_1}\right)(1 + \bar{x}_2)^2 + \beta_T (T_s - \bar{x}_1)
\]
\[
\frac{\partial \bar{x}_2}{\partial t} = -\frac{\partial \bar{x}_2}{\partial z} + \frac{1}{Pe_2} \frac{\partial^2 \bar{x}_2}{\partial z^2} + \delta(z-0)u - B_C \exp\left(\frac{\gamma \bar{x}_1}{1 + \bar{x}_1}\right)(1 + \bar{x}_2)^2
\]
where the states \( \bar{x}_1 \) and \( \bar{x}_2 \) are the temperature and concentration of \( A \) in the reactor, respectively, the input \( u \) is the inlet concentration of \( A \), and \( \delta \) is the standard Dirac function, subject to the following transformed boundary conditions:
\[
z = 0 : \frac{\partial \bar{x}_1}{\partial z} = Pe_1 \bar{x}_1, \quad \frac{\partial \bar{x}_2}{\partial z} = Pe_2 \bar{x}_2;
\]
\[
z = 1 : \frac{\partial \bar{x}_1}{\partial z} = 0, \quad \frac{\partial \bar{x}_2}{\partial z} = 0;
\]

The following typical values are given to the process parameters: \( Pe_1 = 7, Pe_2 = 7, B_T = 2.5, B_C = 0.1, \beta_T = 2, T_s = 0, T_t = 0 \) and \( \gamma = 10 \). The second-order finite-difference method was used to discretize, in space, the two parabolic PDEs and obtain a 101th-order set of ODEs in time. The following simulations were carried out using Java programming language in a Intel Core i7-2600, 3.40GHz computer with a 64-bit Windows 7 operating system.

B. Implementation of K-L Expansion to Open-loop System

In order to compute the empirical eigenfunctions, we first derive and solve a high-order and convergent discretization of the PDE of Eq. 7. In detail, 20 different initial conditions and arbitrary (constant) input values, \( u(t) \) were applied to the process model to get the spatiotemporal solution profiles. Consequently, from each simulation solution profile, 125 uniformly sampled solutions (which are typically called “snapshots”) were taken and combined to generate an ensemble of 2500 solutions. The K-L expansion was applied to the developed ensemble of solutions to compute empirical eigenfunctions that describe the dominant spatial solution patterns embedded in the ensemble where the Jacobian in the K-L expansion is calculated through a finite-difference method. After truncating the eigenfunctions with relatively small eigenvalues (smaller than \( 1 \times 10^{-5} \)), we were left with the first 4 eigenvalues which occupy more than 99.99% of the total energy included in the entire ensemble. In contrast to the sinusoidal/cosinusoidal eigenfunctions, these empirical eigenfunctions are not symmetric with respect to the center of the spatial domain owing to the nonlinear term \( f \) and the input \( u(t) \).

Remark 1: As a practical implementation note, we point out that even though the increase of the eigenfunctions applied to the series expansion of the states of Eq. 7 could improve the accuracy of the computed approximate
model, eigenfunctions that have high frequency spatial profiles with small eigenvalues are discarded because of the probable round off errors. For this case, the descending first 5 empirical eigenvalues are listed as follows: for $\bar{x}_1(z,t), \lambda_{1,1} = 2.365, \lambda_{1,2} = 1.157 \times 10^{-1}, \lambda_{1,3} = 4.926 \times 10^{-2}, \lambda_{1,4} = 9.315 \times 10^{-4}, \lambda_{1,5} = 7.255 \times 10^{-6}$ and for $\bar{x}_2(z,t), \lambda_{2,1} = 9.719 \times 10^{-1}, \lambda_{2,2} = 1.371 \times 10^{-1}, \lambda_{2,3} = 5.138 \times 10^{-2}, \lambda_{2,4} = 9.405 \times 10^{-4}, \lambda_{2,5} = 8.930 \times 10^{-6}$.

C. Galerkin’s Method

To reduce the PDE model of Eq. 7 into an ODE model, we take advantage of the orthogonality of the empirical eigenfunctions obtained from the K-L expansion. Specifically, using Galerkin’s method, we first derive a low-order ODE system for each of the PDEs describing the temporal evolution of the amplitudes corresponding to the first $m_i$ eigenfunctions. The low-order finite-dimensional model for the first $j = 1, \ldots, m_i$ eigenfunctions of the $i$-th PDE has the following form:

$$a_i(t) = A_i a_i(t) + F_i(a_1(t), a_2(t)) + B_i u(t) \quad (9)$$

for $i = 1, 2$ where $a_i'(t) = [a_{i1}(t), \ldots, a_{im_i}(t)]$ is a vector of the amplitudes of the first $m_i$ eigenfunctions, the vector consisting of all amplitudes for both PDEs is denoted as $a(t) = [a_1'(t) \quad a_2'(t)]'$, and $\phi_{ij}(z)$ denotes the $j$-th empirical eigenfunction of the $i$-th PDE.

To present the effectiveness of empirical eigenfunctions in capturing the dominant trends that appear during closed-loop process evolution, we let the process evolve starting from a certain initial condition and under a constant input value, $u(t) = 1$. Four different ROMs are presented and compared to show the ROM accuracy in the context of EMPC handling manipulated input and state constraints. Specifically, the following ROMs are considered:

1) ROM using 8 analytical sinusoidal/cosinusoidal eigenfunctions (e.g., 8 eigenfunctions for each PDE state; 16 eigenfunctions total).
2) ROM using 7 analytical sinusoidal/cosinusoidal eigenfunctions.
3) ROM using 4 empirical eigenfunctions.
4) ROM using 3 empirical eigenfunctions.

We compared the square of the $L_2$ norm, denoted as $||dX||_2$, to quantify the error of each of the reduced-order models. Specifically, we define $||dX||_2$ as

$$||dX||_2 = \sum_{i=1}^{2} \sum_{j=1}^{101} (x_{i,j} - \hat{x}_{i,j})^2, \quad i = 1, 2 \quad (10)$$

where $x_{i,j}$ and $\hat{x}_{i,j}$ are the state values of the $i$-th PDE at the $j$-th discrete points equally distributed along the spatial domain obtained from reduced order model and the finite difference method, respectively. The four different reduced-order models are compared with respect to the evolution profile from the higher-order discretization finite difference method (i.e., the two 101th-order set of ODEs obtained by discretizing, in space, the two parabolic PDEs of Eq. 7) under the same initial condition and input value in Fig. 1. From

![Fig. 1](image1.png)

**Fig. 1.** $L_2$ norm of the closed-loop evolution profiles of Eq. 7 using 4 different ROMs with respect to the evolution profile from the higher-order discretization finite difference method.

![Fig. 2](image2.png)

**Fig. 2.** Computational time profiles of Eq. 7 using 4 different ROMs.

Fig. 1, comparing the $L_2$ norm between the ROM using 4 empirical eigenfunctions and the ROM using 8 analytical eigenfunctions, the ROM constructed from the empirical eigenfunctions is more accurate than the accuracy of the ROM constructed from analytical eigenfunctions with more modes. The average approximation error of each reduced-order model is at maximum of the order of $10^{-1}$.

Furthermore, we compared the computational efficiency under the above two different model reduction methods. The comparison of the computational time corresponding to these 4 different ROMs is given in Fig. 2. The ROM based on empirical eigenfunctions shows its advantage on the computational efficiency compared with the ROM based on the analytical sinusoidal/cosinusoidal eigenfunctions.

D. Implementation of EMPC

We formulate an EMPC system as in [14] for the tubular reactor with the ROM derived from the procedure described above. Ipopt [21] was used to solve the EMPC optimization problem. The EMPC is designed via Lyapunov-based techniques and a quadratic Lyapunov function of the following form was adopted:

$$V(a) = a'(t)Pa(t) \quad (11)$$
where $P$ is an identity matrix of approximate dimension, respectively and $\bar{\rho} = 3$ (see [10] for more details on Lyapunov-based EMPC).

The cost function considered for the EMPC involves maximizing the overall reaction rate along the length of the reactor:

$$J = \frac{1}{N\Delta} \int_{t_k}^{t_{k+N}} \left( \int_0^1 r(z, \tau) dz \right) d\tau$$

where

$$r(z, t) = B_C \exp \left( \frac{\gamma \bar{x}_1}{1 + \bar{x}_2} \right) (1 + \bar{x}_2)^2$$

is the reaction rate.

The control input is subject to constraints as follows: $-1 \leq u \leq 1$. Owing to practical considerations, the amount of reactant material which can be fed to the tubular reactor over the period $t_f$ is fixed. Specifically, $u$ should satisfy the following constraint over the period $t_f$:

$$\frac{1}{t_f} \int_0^{t_f} u(\tau) d\tau = 0.5$$

which will be referred to as the reactant material constraint and will be denoted as $u \in g(t_k)$ to simplify the notation.

Furthermore, the temperature along the length of the reactor is subject to the following constraint:

$$x_{1, \text{min}} \leq x_1(z, t) \leq x_{1, \text{max}}$$

where $x_{1, \text{min}} = -1$ and $x_{1, \text{max}} = 3$ are the lower and upper limits, respectively. Since the models used in the formulations of the EMPC optimization problems have the order of $m_i$, we reformulate the state constraint using the amplitudes of the eigenmodes to simplify the optimization problem calculations:

$$-1 \leq \sum_{j=1}^{m_i} a_{ij}(t) \phi_{ij}(z) \leq 3$$

Explicit Euler’s method was used with an sufficiently small integration step of $1 \times 10^{-4}$ to numerically integrate the finite-dimensional ODE model of the transport-reaction process.

**E. Case 1: Low-Order EMPC: Input Constraint**

In this set of simulations, we consider an EMPC formulation using the model of Eq. 9 and considering only input constraints which is of the form:

$$\max_{u \in S(\Delta)} \frac{1}{N\Delta} \int_{t_k}^{t_{k+N}} \left( \int_0^1 r(z, \tau) dz \right) d\tau$$

s.t. $\dot{a}_i(t) = A_i \tilde{a}_i(t) + F_i(\tilde{a}_1(t), \tilde{a}_2(t)) + B_i u(t)$

$$\tilde{a}_{ij}(t_k) = (\tilde{\phi}_{ij}(\cdot), \tilde{x}_i(\cdot, t_k))$$

$$-1 \leq u(t) \leq 1, \forall t \in [t_k, t_{k+N}]$$

$$u \in g(t_k)$$

$$\tilde{a}'(t) P \tilde{a}(t) \leq \bar{\rho}$$

where $j = 1, \ldots, m_i$ and $i = 1, 2$, $S(\Delta)$ is the family of piecewise constant functions with sampling period $\Delta$, the notation $\tilde{a}_i(t)$ denotes the predicted temporal evolution of the amplitudes of the eigenmodes of the $i$-th PDE using the ROM of Eq. 17b, the prediction horizon is $N = 3$ and the sampling time is $\Delta = 0.01$ (dimensionless).

In the optimization problem of Eq. 17, the constraint of Eq. 17c is the inner product of the adjoint eigenfunction $\tilde{\phi}$ and the current state profile obtained through a state measurement and is used to initialize the dynamic model. The bound on the input is the constraint of Eq. 17d. The constraint of Eq. 17e is the integral input constraint of Eq. 14 formulated for the sampling time $t_k$ on the basis of the material usage from $t = 0$ to $t = t_k$ to ensure that the integral input constraint is satisfied over the window $t_f = 1.0$ (the beginning of the operating window is denoted as $t = 0$). The constraint of Eq. 17f is used to maintain the predicted temporal evolution in an invariant set.

The tubular reactor is initialized at an off-steady-state state profile. The closed-loop behavior of the tubular reactor under an EMPC formulated with four different ROMs were considered: ROMs based on 3 and 4 empirical eigenfunctions and ROMs based on 7 and 8 analytical sinusoidal/cosinusoidal eigenfunctions. For $x(z, 0) = 0$, all of these 4 ROMs achieve the same manipulated input under the EMPC of Eq. 17 which is shown in Fig. 3. We emphasize here on the computational efficiency under the above two different methods. The comparison of the computational time corresponding to these 4 different situations is given in Fig. 4. The ROM based on empirical eigenfunctions shows its advantage on the computational efficiency compared with the ROM based on the analytical sinusoidal/cosinusoidal eigenfunctions.

**F. Case 2: Low-Order EMPC Formulation With State and Input Constraints**

In this case, the EMPC formulation considering the above input, state and Lyapunov function constraints takes the form:

$$\max_{u \in S(\Delta)} \frac{1}{N\Delta} \int_{t_k}^{t_{k+N}} \left( \int_0^1 r(z, \tau) dz \right) d\tau$$

s.t. $\dot{\tilde{a}}_i(t) = A_i \tilde{a}_i(t) + F_i(\tilde{a}_1(t), \tilde{a}_2(t)) + B_i u(t)$

$$\tilde{a}_{ij}(t_k) = (\tilde{\phi}_{ij}(\cdot), \tilde{x}_i(\cdot, t_k))$$

$$\tilde{a}'(t) P \tilde{a}(t) \leq \bar{\rho}$$
Fig. 4. Computational time profiles of the EMPC formulation of Eq. 17 using 4 different ROMs over one operation period.

Fig. 5. Closed-loop profile of $x_1$ of EMPC formulation of Eq. 18 using the ROM based on 4 empirical eigenfunctions over one operation period.

\begin{align*}
-1 & \leq \sum_{j=1}^{m_1} \alpha_{1j}(t) \phi_{1j}(z) \leq 3 \quad (18d) \\
-1 & \leq u(t) \leq 1, \forall t \in [t_k, t_{k+N}) \\
u & \in g(t_k) \\
\alpha'(t) & \bar{P} \alpha(t) \leq \bar{\rho} \\
(18f) & \quad (18g)
\end{align*}

where $j = 1, \ldots, m_1$ and $i = 1, 2$ and the notation is similar to that used in the EMPC of Eq. 17. The constraint of Eq. 18d is the state constraint.

The tubular reactor is initialized at an off-steady-state state profile and we apply the EMPC of Eq. 18 to the tubular reactor. We compared the simulation results from the ROM based on 4 empirical eigenfunctions (i.e., $m_1 = m_2 = 4$) and ROMs based on 8 and 12 sinusoidal/cosinusoidal eigenfunctions, respectively, for $x(z, 0)$ equal to the steady-state of the system under constant input value, $u(t) = 0.8$. Figs. 5-6 show the closed-loop evolution of the states under the EMPC formulation of Eq. 18 from the ROM based on 4 empirical eigenfunctions. The manipulated input profiles for the above 3 different ROMs are given in Fig. 7, which have the same behavior as the ones in Case 1. For the input profile of ROM based on 4 empirical eigenfunctions in Fig. 7 (solid line), the chattering is caused by the over-estimated maximum temperature by the ROM in EMPC, which is also seen in Fig. 8 (solid line).

Fig. 6. Closed-loop profile of $x_2$ of EMPC formulation of Eq. 18 using the ROM based on 4 empirical eigenfunctions over one operation period.

Fig. 7. Manipulated input profiles of the EMPC formulation of Eq. 18 using 3 different ROMs and uniform in time distribution of the reactant material profile over one operation period.

Fig. 8. Maximum temperature of $x_1$ profiles of the EMPC formulation of Eq. 18 using 3 different ROMs over one operation period.
For this case study, we compared the integral of the reaction rate along the length of the reactor among the above 3 different ROMs and the case of the system under uniform in time distribution of the reactant material, i.e., \( u(t) = 0.5 \) Over \( t_f = 1.0 \), the reaction rate from the system under the EMPC formulation from the ROM on the basis of 4 empirical eigenfunctions is 11.25% greater than that from the system under uniform in time distribution of the reactant material. The total economic cost of the ROM on the basis of 4 empirical eigenfunctions is 0.79% and 1.85% greater than that of the ROM on the basis of 8 and 12 analytical eigenfunctions, respectively. This is because the empirical eigenfunctions capture more information of the influence of the nonlinear terms and the input effect in the original PDE model which is not considered by the analytical eigenfunctions.

The comparison of the computational time corresponding to the EMPC systems based on the above 3 different ROMs is given in Fig. 9. The ROM based on 4 empirical eigenfunctions shows its advantage on the computational efficiency compared with the ROM based on both 8 and 12 analytical eigenfunctions.

**Remark 2:** Additional simulation results with other EMPC systems using empirical eigenfunctions applied to the tubular reactor (e.g., output feedback EMPC systems using empirical eigenfunctions) can be found in [13].

**V. Conclusion**

In this work, reduced-order models of transport-reaction processes described by nonlinear parabolic partial differential equations were first constructed on the basis of data-based empirical eigenfunctions by applying Karhunen-Loève expansion and used in the formulation of economic model predictive control systems. Several EMPC systems each using a different ROM (i.e., different number of modes and derived from either using analytical sinusoidal/cosinusoidal eigenfunctions or empirical eigenfunctions) were applied to a tubular reactor example where a second-order reaction occurs. The model accuracy, computational time and closed-loop economic performance of the closed-loop tubular reactor under the different EMPC systems were evaluated and discussed.

**References**