Provided for non-commercial research and educational use only.
Not for reproduction or distribution or commercial use.

Volume 376 15 March 2007 ISSN 0378-4371

PHYSICA A

STATISTICAL MECHANICS AND ITS APPLICATIONS

Recognized by the European Physical Society

Editors:
K.A. DAWSON
J.O. INDEKEU
H.E. STANLEY
C. TSALLIS

Available online at
ScienceDirect
www.sciencedirect.com

http://www.elsevier.com/locate/physa

This article was originally published in a journal published by Elsevier, and the attached copy is provided by Elsevier for the author's benefit and for the benefit of the author's institution, for non-commercial research and educational use including without limitation use in instruction at your institution, sending it to specific colleagues that you know, and providing a copy to your institution's administrator.

All other uses, reproduction and distribution, including without limitation commercial reprints, selling or licensing copies or access, or posting on open internet sites, your personal or institution's website or repository, are prohibited. For exceptions, permission may be sought for such use through Elsevier's permissions site at:

http://www.elsevier.com/locate/permissionusematerial

Available online at www.sciencedirect.com
ScienceDirect
Physica A 376 (2007) 215–222
PHYSICA A
www.elsevier.com/locate/physa

Greatly enhancing the modeling accuracy for distributed parameter systems by nonlinear time/space separation

Hai-Tao Zhang[a], Chen-Kun Qi[b], Tao Zhou[c,*], Han-Xiong Li[b]

[a]*Department of Control Science and Engineering, and the Key Laboratory of Image Processing and Intelligent Control, Huazhong University of Science and Technology, Wuhan 430074, PR China*
[b]*Department of Manufactory Engineering and Engineering Management, City University of Hong Kong, Hong Kong SAR, PR China*
[c]*Department of Modern Physics and Nonlinear Science Center, University of Science and Technology of China, Hefei 230026, PR China*

Received 15 June 2006; received in revised form 26 September 2006
Available online 20 November 2006

Abstract

An effective modeling method for nonlinear distributed parameter systems (DPSs) is critical for both physical system analysis and industrial engineering. In this paper, we propose a novel DPS modeling approach, in which a high-order nonlinear Volterra series is used to separate the time/space variables. With almost no additional computational complexity, the modeling accuracy is improved more than 20 times in average comparing with the traditional method.
© 2006 Elsevier B.V. All rights reserved.

Keywords: Nonlinear-DPS; Nonlinear time/space separation; Modeling accuracy

1. Introduction

Most of the physical processes (e.g. thermal diffusion process [1–7], thermal radiation process [8], distributed quantum systems [9,10], concentration distribution process [11–13], crystal growth process [1,6], etc.) are nonlinear distributed parameter systems (DPSs) with boundary conditions determined by the system structure. Thus, it is an urgent task to design an effective modeling method for nonlinear DPSs. The key problem in the design of nonlinear-DPS modeling method is how to separate the time/space variables. Some modeling approaches are previously proposed: these include the Karhunen–Loève (KL) approach [1,4,14,15], the spectrum analysis [16], the singular value decomposition (SVD) combined with the Galerkin's method [1,17], and so on. Among them, the KL approach is the most extensively studied and the most widely applied one. In this approach, the output $T(z,t)$ is expanded as

$$T(z,t)=\sum_{i=1}^{N} c_i(z)l_i(t) \triangleq C(z)L(t), \tag{1}$$

where z and t are the space and time variables, respectively. This operation can be implemented by spatial basis $\{c_i(z)\}$ combined with time-domain coefficients $\{l_i(t)\}$, or time-domain basis $\{l_i(t)\}$ combined with spatial

*Corresponding author.
E-mail address: zhutou@ustc.edu (T. Zhou).

0378-4371/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physa.2006.10.014

Author's personal copy

coefficients $\{c_i(z)\}$. The basis could be Jacobi series [18], orthonormal functional series (OFS, such as Laguerre series [18,19], Kautz series [18], etc.), spline functional series [20], trigonometric functional series, or some others. However, no matter how elaborately the basis is designed, the infinite-dimensional nature of DPSs does not allow being accurately modeled with small number of truncation length N of the basis series. Moreover, the nonlinear nature of the DPSs will even increase this modeling difficulty. Thus for nonlinear DPSs' modeling, the extending of N to a sufficiently large number is generally required, which would definitely increase the computational burden. Consequently, in order to improve the efficiency of the modeling algorithms, many former efforts focused on designing suitable time-domain basis $\{l_i(t)\}$ or spatial basis $\{c_i(z)\}$ according to the prior knowledge of the DPSs [1,14]. In addition, some scholars also presented neural networks to model the nonlinearities of transitional flows and distributed reacting systems based on proper orthogonal decomposition and Galerkin's method [21,22]. However, if the prior knowledge is unavailable or inadequate, the general design methods of the bases are very limited so far. On the other hand, the conventional finite difference and finite element method often lead to very high-order ODEs which are inappropriate for dynamical analysis and real-time implementation [22]. Another conventional approach, spectral method [16], is popularly used for modeling DPSs because it may result in very low-dimensional ODE systems. However, it requires a regular boundary condition [1,23].

Thus, in this paper, we argue that the linear separation is a bottleneck to better modeling performance, and to introduce some kinds of nonlinear terms may sharply enhance the performance, since they have the capability to compensate the residuals of the linear separation.

2. The implement of nonlinear space/time separation

For nonlinear lumping systems, if their dependencies on past inputs decrease rapidly enough with time, their input/output relationship can be precisely described by *Volterra series* [24–28], which is a generalization of the convolution description of linear time-invariant to time-invariant nonlinear operators. This kind of system is called fading memory nonlinear system (FMNS) [25], which is well-behaved in the sense that it will not exhibit multiple steady states or other related phenomena like chaotic responses. Fortunately, most industrial processes are FMNSs. Accordingly, one can naturally extend the concept of Volterra series from lumping systems to DPSs by allowing each kernel to contain both time variable t and space variable z, and then design the time/space separation method via the so-called *distributed Volterra series* (see Fig. 1 for the mechanism of this modeling method). Firstly, the system output can be represented by

$$T(z,t) = h_0(z) + \int_0^\infty h_1(z,\tau_1)u(t-\tau_1)\,\mathrm{d}\tau_1 + \int_0^\infty\int_0^\infty h_2(z,\tau_1,\tau_2)u(t-\tau_1)u(t-\tau_2)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2 + \cdots, \tag{2}$$

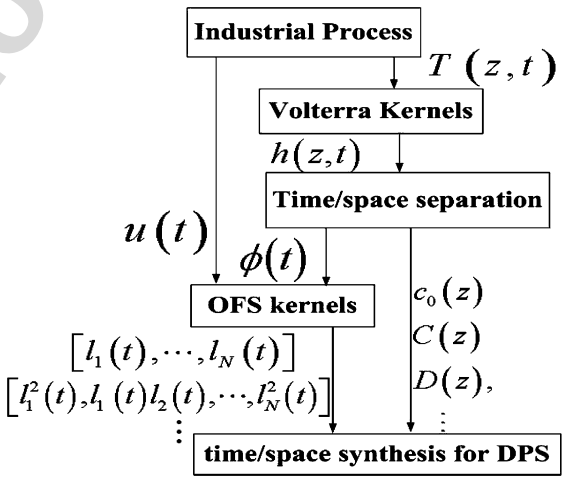

Fig. 1. The sketch map of OFS-Volterra modeling for nonlinear DPS.

Author's personal copy

where $h_i(z,\tau_1,\ldots,\tau_i)$ is the ith order distributed Volterra kernel. Then denote $\phi_i(t)$ as the ith order OFS and $l_i(t)=\int_0^\infty \phi_i(t)u(t-\tau)\,d\tau$ as the ith order OFS filter output. Since $\{\phi_i(t)\}$ forms a complete orthonormal set in functional space l_2, each kernel can be approximately represented as

$$h_1(z,\tau_1)=\sum_{k=1}^{N} c_k(z)\phi_k(\tau_1),$$
$$h_2(z,\tau_1,\tau_2)=\sum_{n=1}^{N}\sum_{m=1}^{N} c_{nm}(z)\phi_n(\tau_1)\phi_m(\tau_2),$$
$$\cdots \tag{3}$$

where $c_k(z)$ and $c_{nm}(z)$ are spatial coefficients. Then, the input/output relationship can be written as (see Eq. (1) for comparison)

$$T(z,t)=c_0(z)+C(z)L(t)+L^{\mathrm{T}}(t)D(z)L(t)+\cdots, \tag{4}$$

where $L(t)=[l_1(t)\cdots l_N(t)]^{\mathrm{T}}$, $C(z)=[c_1(z)\cdots c_N(z)]$, and $D(z)=[c_{ij}(z)]_{N\times N}$.

To obtain the spatial coefficients, firstly we pre-compute all the OFS kernels according to the polynomial iterations [18] or the following state equation:

$$L(t+1)=AL(t)+Bu(t), \tag{5}$$

where $u(t)$ is the system input, and A and B are pre-optimized matrices (see Ref. [29] for details). Then the input/output relationship Eq. (4) is represented by a linear regressive form, and these spatial coefficients $c_0(z), C(z), D(z),\ldots$ can be obtained by using the least-square estimation combined with spline interpolation [20]. Finally, the model is obtained by synthesizing the OFS kernels and the spatial coefficients according to Eq. (4).

Fig. 2 shows the operation details of this modeling method. The first order OFS filter is the Laguerre series, in which

$$G_0(q^{-1})=\frac{q^{-1}\sqrt{1-a^2}}{1-q^{-1}a}, \quad G_1(q^{-1})=\frac{q^{-1}-a}{1-q^{-1}a}, \tag{6}$$

where a is the time-scaling constant and q^{-1} is the one-step backward shifting operator (i.e., $q^{-1}u(t)=u(t-1)$). The second order OFS filter is the Kautz Series, in which $G_0(q^{-1})$ and $G_1(q^{-1})$ are second order transfer functions. Analogically, Heuberger et al. [30] introduced the higher-order OFS model. As the order increases, OFS model can handle more complex dynamics.

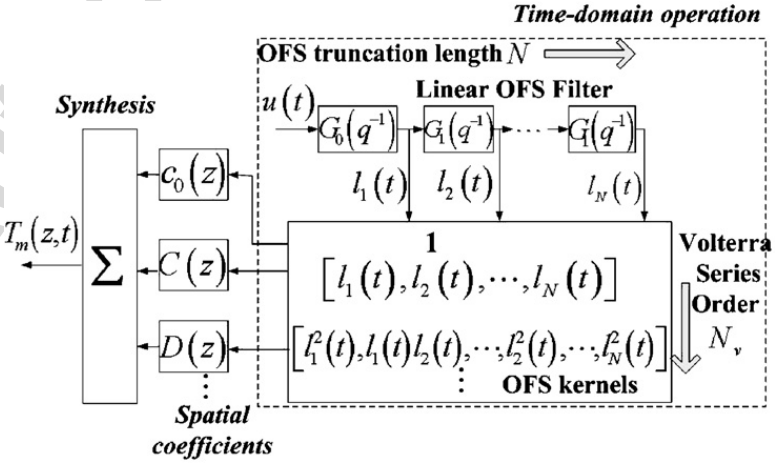

Fig. 2. Operation details of OFS-Volterra modeling.

Author's personal copy

3. Numerical results

Consider a long, thin rod in a reactor as shown in Fig. 3. The reactor is fed with pure species A and a zeroth order exothermic catalytic reaction of the form $A \to B$ takes place in the rod. Since the reaction is exothermic, a cooling medium that is in contact with the rod is used for cooling. Assume the density, heat capacity, conductivity and temperature are all constant, and species A is superfluous in the furnace, then the mathematical model which describes the spatiotemporal evolution of the rod temperature consists of the following parabolic partial differential equation:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial z^2} + \beta_T e^{-\gamma/(1+z)} - \beta_T e^{-\gamma} + \beta_u(b(z)u(t) - T), \tag{7}$$

which subjects to the Dirichlet boundary conditions

$$T(0,t) = 0, \quad T(\pi,t) = 0, \quad T(z,0) = 0, \tag{8}$$

where $T(z,t)$, $b(z)$, β_T, β_u, γ, and u denote the temperature in the reactor (output), the actuator distribution function, the heat of reaction, the heat transfer coefficient, the activation energy, and the temperature of the cooling medium (input), respectively. Here we set $\beta_T = 50.0$, $\beta_u = 2.0$, and $\gamma = 4.0$. In the numerical calculation, without loss of generality, we set $b(z) = 1$, and $u(t) = [1.4, 1.4, 1.4, 1.4]$. The order of Volterra series is two, the OFS is chosen as one-order Laguerre series [18] with $a = 0.6$, and the truncation length is given $N = 4$.

The system output is shown in Fig. 4. Denote by $e(z,t)$ the modeling error, that is, the difference between system output and modeling result at the point (z,t). Figs. 5 and 6 exhibit the modeling errors of the traditional and the present methods, respectively. Clearly, the method proposed here has remarkably smaller

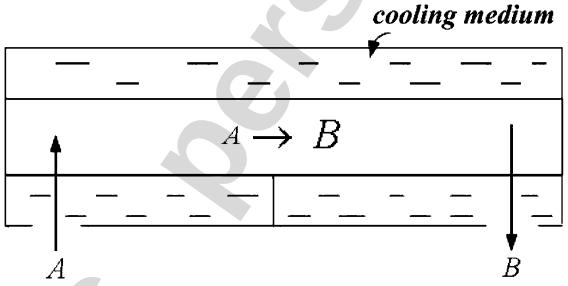

Fig. 3. The sketch map of catalytic rod.

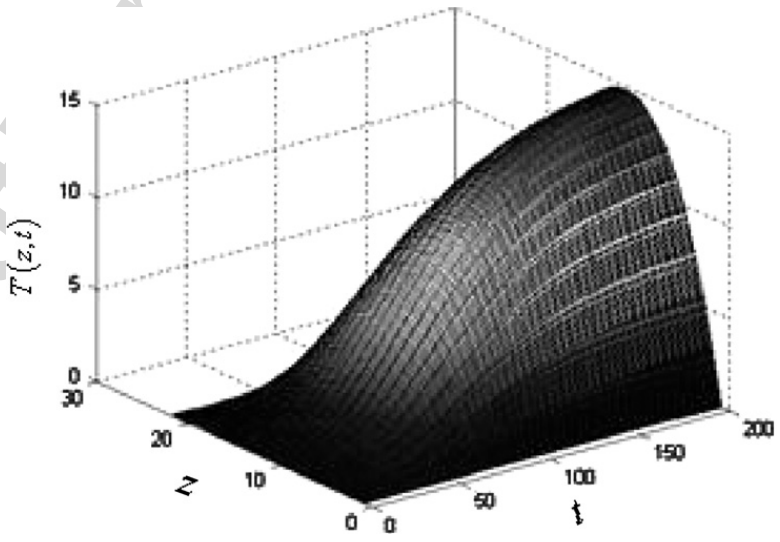

Fig. 4. *Color online*: System output.

Author's personal copy

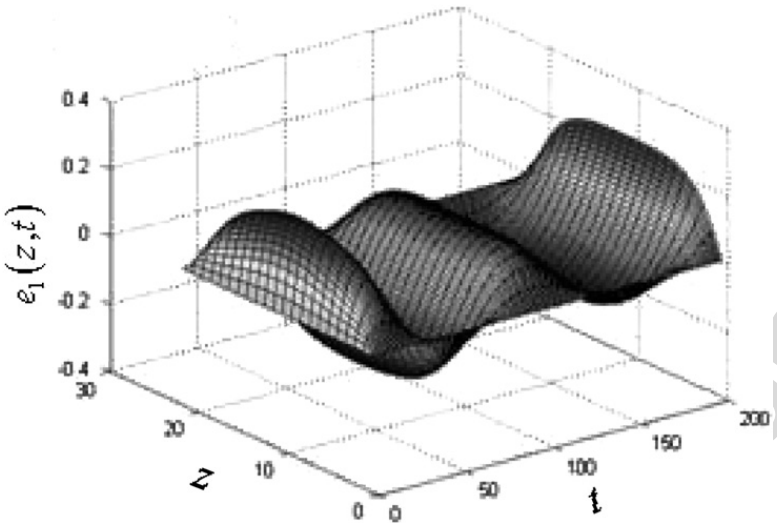

Fig. 5. *Color online*: Modeling error of the traditional method.

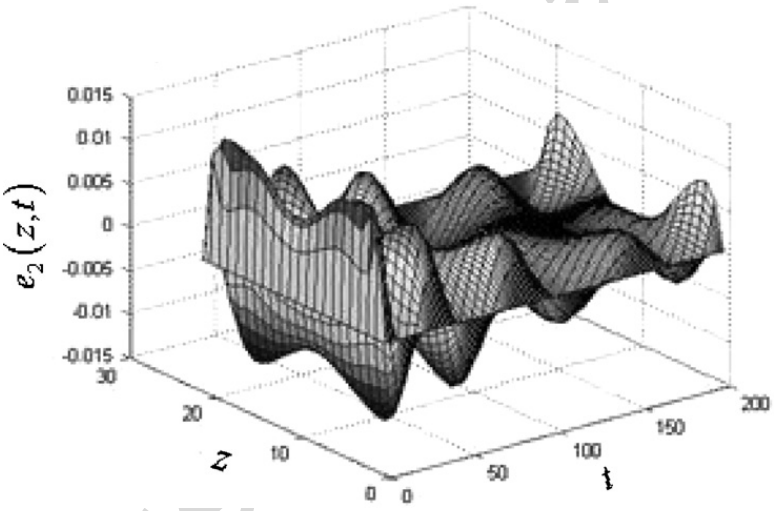

Fig. 6. *Color online*: Modeling error of the present method.

error than that of the traditional one. To provide a vivid contrast between these two methods, we calculate the integral of absolute error (IAE, $\int |e(z,t)|\,\mathrm{d}z$) and time-weighted absolute errors (ITAE, $\int t|e(z,t)|\,\mathrm{d}t$), which are two standard error indexes to evaluate modeling performances of DPS and can be considered as the modeling errors along the temporal dimension t and the spatial dimension z. As are shown in Figs. 7 and 8, both the IAE and ITAE of the present method is reduced by >20 times comparing with those of the traditional one, which strongly demonstrates the advantage of the present method. Actually, to obtain the shapes of IAE and ITAE, one can cut the error surfaces of Figs. 5 and 6 along the temporal coordinate t and the spatial dimension z. In addition, we calculate the average of absolute modeling error $1/\iint \mathrm{d}z\,\mathrm{d}t \iint |e(z,t)|\,\mathrm{d}z\,\mathrm{d}t$. From Fig. 9, it is found that, in comparison with the traditional method, the modeling accuracy of the present one is enhanced by 14–32 times with less than 15% increase of the consumed time. It should be noted that the modeling accuracy would increase along with the increase of the Volterra series order N_v, however, the computational complexity will increase too. For lumping systems, this fact has been proved, and for DPSs, this fact is also validated by experimental results [24]. So a tradeoff between the modeling accuracy and the computational complexity must be made. That is why here we set the order $N_v = 2$.

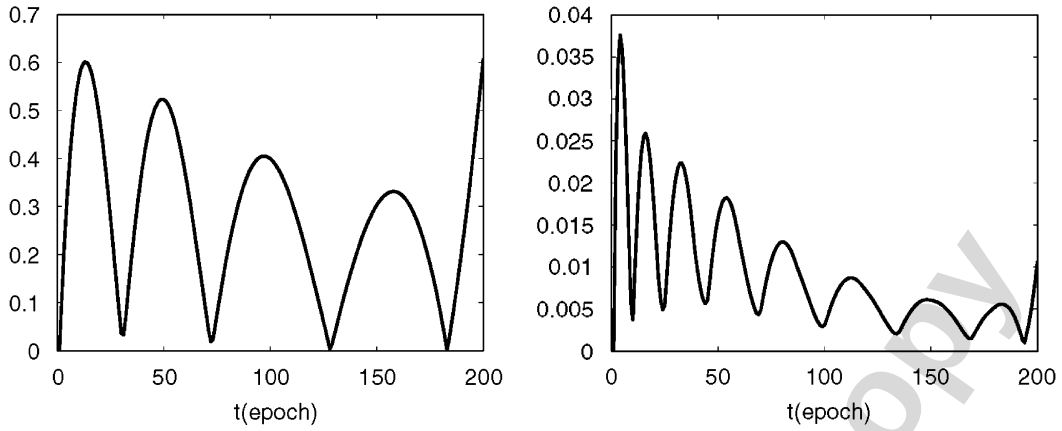

Fig. 7. IAEs of the traditional method (left) and the present method (right).

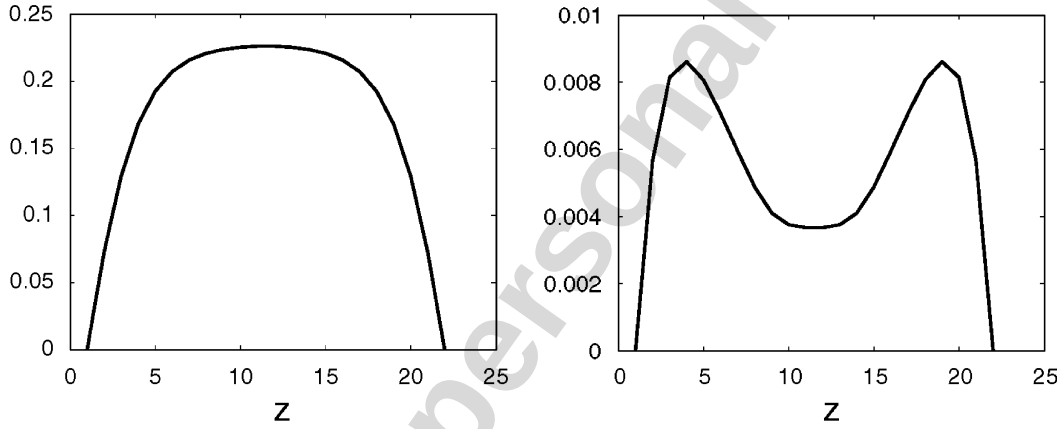

Fig. 8. ITAEs of the traditional method (left) and the present method (right).

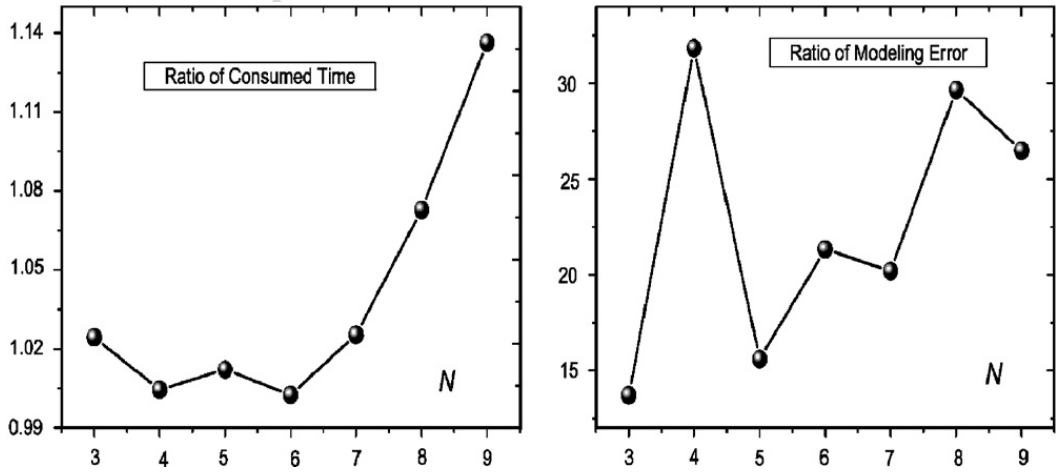

Fig. 9. Ratios of the consumed time t_2/t_1 (left) and the average of absolute modeling error $|e_1|/|e_2|$ (right) vs the truncation length N. The subscripts 1 and 2 denote the cases of the traditional and the present methods, respectively. The CPU time by using traditional method for $N \in [3, 9]$ is in the interval [100 s, 160 s]. All the numerical calculations are implemented by using a personal computer with CPU: 1.8G, RAM: 256M, OS: Windows XP, and software platform: MATLAB 6.5.

author's personal copy

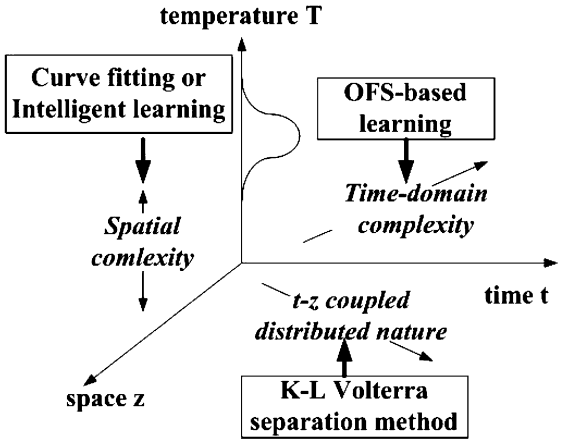

Fig. 10. Modeling methodology for DPSs.

4. Conclusion and discussion

Modeling method for nonlinear DPS plays an important role in physical system analysis and industrial engineering. Unfortunately, there exits two essential difficulties in this issue, (a) *distributed nature* due to time-space coupled, which causes different temperature responses at different locations; (b) *nonlinear complexity* from varying working point—different dynamics obtained even at the same location for a large change of working points. Owing to these difficulties, previous modeling methods via linear time/spatial separation techniques (e.g. KL approach, spectrum analysis, SVD-Galerkin technique, etc.) cannot yield satisfying modeling performance, especially for DPSs with severe nonlinearity. The modeling error is caused by the nonlinear residue of the linear time/space separation. Thus, it is natural to expect that a nonlinear time/space separation method may yield better modeling performance.

To validate this supposition, we design a novel modeling method by extending the concept of lumping Volterra series to the distributed scenario. As shown in Fig. 10, the nonlinear DPS is first decomposed into kernels, upon which the time-space separation is carried out. These two decompositions will gradually separate the complexity and provide a better modeling platform. The time/space separation will be handled by a novel KL Volterra method instead of the conventional KL method, the time-domain complexity by the OFS-based learning, and the spatial complexity by the curve fitting techniques (e.g. spline interpolation) or intelligent learning algorithms (e.g. neural network, fuzzy system, etc.). This novel method is applied on a benchmark nonlinear DPS of industrial process, a catalytic rod. It is found that the modeling accuracy has been remarkably improved comparing with the traditional method, with almost no additional computational complexity. The underlying reason may be that the high-order Volterra kernel can compensate the residuals of the linear separation. In addition, we have applied this method to another two benchmark nonlinear DPSs, a rapid thermal chemical vapor deposition process [1], and a Czochralski crystal growth process [1]. The corresponding results also strongly suggest that the nonlinear time/space separation can greatly enhance the modeling accuracy.

Although its superiority has been demonstrated, the KL Volterra method is just a first attempt aiming at the motivation of nonlinear time/space separation. Thanks to its excellent modeling efficiency, this novel method is definitely a promising one for both physical system analysis and industrial engineering. We believe that our work can enlighten the readers on this interesting subject.

Author's personal copy

Acknowledgements

The author would like to thank Prof. Guanrong Chen for helpful discussion and suggestion. H.T. Zhang would like to acknowledge NSFC under Grant Nos. 60340420431 and 60274020, and the Youth Founding Project of HUST. T. Zhou would like to acknowledge NSFC under Grant No. 10635040. H.X. Li would like to acknowledge the grant from the RGC of Hong Kong SAR (CityU 116905).

References

[1] P.D. Christofides, Nonlinear and Robust Control of PDE Systems: Methods and Applications to Transport-Reaction Processes, Birkhauser, Boston, 2001.
[2] D.K. Hoffman, et al., Phys. Rev. E 57 (1998) 6152.
[3] A.V. Chechkin, et al., Phys. Rev. E 66 (2002) 046129.
[4] M. Sheintuch, Y. Smagina, Phys. Rev. E 70 (2004) 026221.
[5] P.V. Kuptsov, R.A. Satnoianu, Phys. Rev. E 71 (2005) 015204.
[6] W.J. Kossler, A.J. Greer, R.N. Dickes, D. Sicilia, Y. Dai, Physica B 374–375 (2006) 225.
[7] T. Yagi, N. Taketoshi, H. Kato, Physica C 412–414 (2004) 1337.
[8] V.A. Kazakov, R.S. Berry, Phys. Rev. E 49 (1994) 2928.
[9] M.I. Katsnelson, et al., Phys. Rev. A 62 (2000) 022118.
[10] J. Wakabayashi, A. Tamagawa, T. Nagashima, T. Mochiku, K. Hirata, Physica B 249–251 (1998) 102.
[11] M.O. Vlad, J. Ross, Phys. Rev. E 66 (2002) 061908.
[12] U. Hass, Physica A 215 (1995) 247.
[13] P.N. McGraw, M. Menzinger, Phys. Rev. E 68 (2003) 066122.
[14] W.H. Ray, Advanced Process Control, McGraw-Hill, New York, 1981.
[15] H.M. Park, D.H. Cho, Chem. Eng. Sci. 51 (1996) 81.
[16] D. Gottlieb, S.A. Orszag, Numerical Analysis of Spectral Methods: Theory and Applications, SIAM, Philadelphia, 1993.
[17] S. Chakravarti, et al., Phys. Rev. E 52 (1995) 2407.
[18] K.B. Datta, B.M. Mohan, Orthogonal Functions in System and Control, World Scientific, Singapore, 1995.
[19] X.G. Hu, Phys. Rev. E 59 (2004) 2471.
[20] C. de Boor, A Practical Guide to Splines, Springer, Berlin, 1978.
[21] R.A. Sahan, et al., in: Proceedings of the 1997 IEEE International Conference on Control and Applications, IEEE Press, New York, 1997, pp. 359–364.
[22] S.Y. Shvartsman, et al., J. Process Control 10 (2000) 177.
[23] C. Canuto, M.Y. Hussaini, A. Quarteroni, T.A. Zang, Spectral Methods in Fluid Dynamics, Springer, New York, 1988.
[24] M. Schetzen, The Volterra and Wiener Theory of Nonlinear System, Wiley, New York, 1980.
[25] S. Boyd, L.O. Chua, IEEE Trans. Circuits Syst. 32 (1985) 1150.
[26] V.A. Kuz, Phys. Rev. A 44 (1991) 8414.
[27] I.Y. Cherdantsev, R.I. Yamilov, Physica D 87 (1995) 140.
[28] L.J. Chen, et al., Phys. Rev. E 50 (1999) 551.
[29] L.P. Wang, J. Process Control 14 (2004) 131.
[30] P.S.C. Heuberger, et al., IEEE Trans. Autom. Control 40 (1995) 451.

Author's personal copy