A general analysis of approximate nonlinear lumping in chemical kinetics. I. Unconstrained lumping

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A general analysis of approximate nonlinear lumping for a chemical kinetic system described by an n-dimensional first order ordinary differential equation system $d\mathbf{y}/dt=\mathbf{f}(\mathbf{y})$ is presented. There is a one-to-one relation between the differential equation system and the linear partial differential operator $A=\sum_{i=1}^{n} f_i(\mathbf{y})(\partial/\partial y_i)$. The algebraic method in nonlinear perturbation theory is utilized to approximately transform A into some canonical forms in which the new dependent variables are partly separated. These canonical forms of A will give the generalized eigenfunctions or other higher dimensional unconstrained nonlinear lumping schemes of the original system approximately. Unconstrained nonlinear lumping gives a reduced differential equation system describing new variables which are nonlinear functions of the original ones. This approach may supply some purely fast variables. The solutions of original dependent variables can be obtained by the inverse transformation from the lumped variables and the approximate analytical solutions of the purely fast variables. The theoretical basis of this approach is presented. A simple example is used for illustration.

I. INTRODUCTION

Dimension reduction for the dynamic or kinetic equations of a large system is a very important problem in many areas. This reduction from a high dimensional differential equation system to a lower dimensional one is often achieved by *lumping*, in which the new dependent variables are some functions of the original ones. The lumping is called *exact* or *approximate* according to whether the solution of the lumped differential equation system does or does not have error compared to that given by the original system. When the lumping transformation is linear, we call it linear lumping, otherwise we call it nonlinear lumping. The authors have developed several approaches for exact and approximate linear lumping.[1-6] We also presented a general analysis of exact nonlinear lumping, where linear lumping was included as a special case.[7] In this analysis, three necessary and sufficient conditions for the existence of exact nonlinear lumping schemes were established.

Suppose the kinetics of the original n-dimensional system can be described by an n-dimensional first order ordinary differential equation system

$$\frac{d\mathbf{y}}{dt}=\mathbf{f}(\mathbf{y}), \quad \mathbf{y}\in\mathscr{R}^n, \tag{1}$$

where $\mathbf{y}$ is an n-dimensional vector, $\mathbf{f}(\mathbf{y})$ is an n-dimensional and C^2 (second order differentiable) function vector with $\mathbf{f}(\mathbf{0})=\mathbf{0}$. We have demonstrated that for an $\hat{n}(\hat{n}\leqslant n)$-dimensional nondegenerate exact lumping transformation

$$\hat{\mathbf{y}}=\mathbf{h}(\mathbf{y}), \tag{2}$$

the lumped system can be represented as

$$\frac{d\hat{\mathbf{y}}}{dt}=\mathbf{h}_{\mathbf{y}}[\bar{\mathbf{h}}(\hat{\mathbf{y}})]\mathbf{f}[\bar{\mathbf{h}}(\hat{\mathbf{y}})], \tag{3}$$

where $\mathbf{h}_{\mathbf{y}}(\mathbf{y})$ is the Jacobian matrix of $\mathbf{h}(\mathbf{y})$ and $\bar{\mathbf{h}}$ is the generalized inverse transformation of $\mathbf{h}$ satisfying the relation

$$\mathbf{h}(\bar{\mathbf{h}})=I_{\hat{n}}. \tag{4}$$

When the lumping transformation $\mathbf{h}$ consists of linear functions of y_i, $\bar{\mathbf{h}}$ can be readily determined.[1] When $\mathbf{h}$ is not linear, in some cases $\bar{\mathbf{h}}$ may not be represented by elementary or other simple functions. Under these circumstances, one cannot directly use Eq. (3) to describe the lumped systems as we have done before in the case of linear lumping.

To avoid this difficulty, we have tried to analyze the lumping problem using algebraic considerations. Equation (1) is equivalent to a linear partial differential operator

$$A=\sum_{i=1}^{n} f_i(\mathbf{y})\frac{\partial}{\partial y_i}. \tag{5}$$

This comes from the fact that

$$\frac{dy_i}{dt}=f_i(\mathbf{y})=Ay_i \quad (i=1,2,\ldots,n). \tag{6}$$

For the operator A, we have defined the generalized eigenfunction $\psi(\mathbf{y})$, the normal generalized eigenfunction $\Psi(\mathbf{y})$, and the eigenfunction $\varphi(\mathbf{y})$ as follows, respectively:[7]

$$A\psi=\Omega(\psi), \tag{7}$$

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$$A\Psi = 1, \tag{8}$$

$$A\varphi = \lambda(\mathbf{y})\varphi, \tag{9}$$

where Ω is an arbitrary function, $\lambda(\mathbf{y})$ is referred to as the eigenvalue corresponding to $\varphi(\mathbf{y})$ and is an invariant of A satisfying

$$A\lambda(\mathbf{y}) = 0. \tag{10}$$

It has been shown that exact lumping schemes are related to the eigenfunctions or generalized eigenfunctions of the operator A. An $\hat{n}$-dimensional exact lumping transformation $\mathbf{h}(\mathbf{y})$ consists of $\hat{n}$ functionally independent functions of $\hat{n}$ functionally independent generalized eigenfunctions. The determination of lumping transformations becomes the determination of eigenfunctions or generalized eigenfunctions of A. Actually, using the eigenfunctions or generalized eigenfunctions as a new basis, A can be transformed to some canonical form under which the new dependent variables in the corresponding transformed differential equation system have been partly or completely separated. Transforming A into canonical forms presents some exactly lumped systems, and therefore lumped differential equation systems can be directly obtained from canonical forms of A. Hence, the lumping analysis is equivalent to transforming A into some canonical forms. The advantage of this approach is that one does not need the generalized inverse transformation $\bar{\mathbf{h}}$.

Unfortunately, there is no general approach to transform an arbitrary operator to a canonical form. However, the idea of approximately transforming A to some canonical form may serve as a basis for developing an approach to approximate nonlinear lumping. Bogaevski and Povzner[8] have given a general analysis of approximately transforming an operator A containing a small positive parameter ϵ to some canonical forms by the algebraic method in nonlinear perturbation theory. We will employ this method to develop a general approach to approximate nonlinear lumping for chemical kinetic systems.

In a previous paper, the authors presented a singular perturbation method for the determination of an approximately lumped differential equation system with independent variable t.[9] The *purely fast variables* played the key role in this approach. However, the original differential equations must be linear in the deleted dependent variables and therefore this approach cannot be used to treat an arbitrary reaction system. In the present paper, the algebraic method in nonlinear perturbation theory will give some purely fast variables without such a restriction on the original system. As the explicit solutions of the purely fast variables can be approximately obtained by a singular perturbation method, one can obtain the original dependent variables by the inverse transformation from the lumped variables and the purely fast variables.

The paper is organized as follows: In Sec. II, we introduce the definitions of some canonical forms for a linear partial differential operator, such as diagonal, Jordan, and blockwise diagonal forms. In Sec. III, the theoretical basis of the algebraic method in nonlinear perturbation theory as developed by Bogaevski and Povzner is presented. We then show how the algebraic method in nonlinear perturbation theory can be used to approximately transform such an operator A of the form

$$A = A_0 + \epsilon A_1 + \epsilon^2 A_2 + \cdots$$

to a canonical form by defining a transformation of the basis variables. We include details of some of the proofs given by Bogaevski and Povzner since they illustrate the techniques used to select such transformations. The canonical form of A will be shown to lead to a lower dimensional lumped system. In Sec. IV, we present a brief summary of the method followed by a simple example which illustrates its application to unconstrained lumping. Finally, in Sec. V we present conclusions and a discussion.

II. CANONICAL FORMS

In the next two sections we will briefly introduce the theoretical basis of the algebraic method in nonlinear perturbation theory. We direct the reader to the example in Sec. IV, which serves to illustrate many of the theoretical points raised in the following sections. The proofs of some important conclusions or theorems can be found in the book written by Bogaevski and Povzner.[8]

A. Representations of *A* in different bases

Equation (5) is the representation of A upon the basis $\mathbf{y}=\{y_1, y_2, \ldots, y_n\}$. A new basis $\mathbf{x}=\{x_1(\mathbf{y}), x_2(\mathbf{y}), \ldots, x_n(\mathbf{y})\}$ of A consists of n functionally independent functions of $\mathbf{y}$. One can transform $\mathbf{y}$ to the new basis $\mathbf{x}$ by a nonsingular transformation. Upon the new basis, A is of the form

$$A = \sum_{i=1}^{n} g_i(\mathbf{x}) \frac{\partial}{\partial x_i}, \tag{11}$$

where the coefficients $g_i(\mathbf{x})$ are equal to Ax_i.

B. Canonical forms of operator *A*

Next, we will give the definitions of some canonical forms for a linear partial differential operator A defined by Eq. (5). Even though A cannot be represented as a matrix, the same terminology of matrix canonical forms such as *diagonal, Jordan, blockwise diagonal*, etc. may be utilized for A, after giving appropriate definitions.

1. Diagonal form

Suppose there exists a basis consisting of eigenfunctions $\varphi_i(\mathbf{y})$ and invariants $\omega_j(\mathbf{y})$ of A, i.e.,

$$\varphi_1(\mathbf{y}), \varphi_2(\mathbf{y}), \ldots, \varphi_k(\mathbf{y}), \quad \omega_1(\mathbf{y}), \omega_2(\mathbf{y}), \ldots, \omega_m(\mathbf{y}),$$

$$\text{for } k+m=n,$$

where the eigenvalues $\lambda_i[\omega(\mathbf{y})]$ corresponding to $\varphi_i(\mathbf{y})$ are not identically equal to zero, and are required to be functions of the invariant vector $\omega=(\omega_1, \omega_2, \ldots, \omega_m)^T$ only. This can always be assumed without the restriction of generality, because if λ_i does not satisfy this requirement, we can define a new eigenfunction $\tilde{\varphi}_i$ as follows:

$$\tilde{\varphi}_i = \varphi_i^{[\tilde{\omega}_i(\omega)]/\lambda_i}. \tag{12}$$

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For this new eigenfunction, the corresponding eigenvalue is only a function of ω,

$$A\tilde{\varphi}_i=\frac{\tilde{\omega}_i}{\lambda_i}\varphi_i^{[(\tilde{\omega}_i/\lambda_i)-1]}A\varphi_i=\frac{\tilde{\omega}_i}{\lambda_i}\varphi_i^{[(\tilde{\omega}_i/\lambda_i)-1]}\lambda_i\varphi_i=\tilde{\omega}_i\tilde{\varphi}_i. \quad (13)$$

Upon this basis, the operator A possesses the form

$$A=\sum_{i=1}^{k}\lambda_i(\omega)\varphi_i(\mathbf{y})\frac{\partial}{\partial\varphi_i(\mathbf{y})}=(\Lambda\varphi,\nabla_\varphi), \quad (14)$$

where Λ is a $k\times k$ diagonal matrix with $\lambda_i(\omega)$ as its ith diagonal element, and

$$\varphi=(\varphi_1\varphi_2\cdots\varphi_k)^T, \quad (15)$$

$$\nabla_\varphi=\left(\frac{\partial}{\partial\varphi_1}\frac{\partial}{\partial\varphi_2}\cdots\frac{\partial}{\partial\varphi_k}\right)^T. \quad (16)$$

In this representation, A is referred to as having a *diagonal* form. When $m=0$, i.e., $k=n$, λ_i are constants.

2. Jordan form

If there exist l eigenvalues $\lambda_i(\omega)$ $(i=1,2,\ldots,l)$ and for each λ_i there are k_i functions $\varphi_j^i(\mathbf{y})$ $(j=1,2,\ldots,k_i)$ such that

$$\begin{aligned}&A\varphi_1^i=\lambda_i\varphi_1^i,\\&A\varphi_2^i=\lambda_i\varphi_2^i+\varphi_1^i,\\&\quad\ldots,\\&A\varphi_{k_i}^i=\lambda_i\varphi_{k_i}^i+\varphi_{k_i-1}^i,\end{aligned} \quad (17)$$

then $\varphi_j^i(\mathbf{y})$ $(j=1,2,\ldots,k_i)$ are referred to as Jordan basis functions of A corresponding to eigenvalue λ_i. According to this definition, if $\varphi(\mathbf{y})$ is a Jordan basis function of A corresponding to eigenvalue λ, then

$$(A-\lambda)^q\varphi(\mathbf{y})=0 \quad (18)$$

for a sufficiently large positive integer q.

Suppose there exists a basis consisting of Jordan basis functions φ_j^i $(i=1,2,\ldots l;\ j=1,2,\ldots,k_i)$ and invariants $\omega_i(\mathbf{y})$ $(i=1,2,\ldots,m)$, where the eigenvalues $\lambda_i\neq 0$ and $\Sigma_{i=1}^{l}k_i+m=n$ (m can be zero). Upon this basis, the operator A possesses the form

$$A=(\mathscr{J}\varphi,\nabla_\varphi), \quad (19)$$

where $\mathscr{J}$ is the Jordan matrix with $k_i\times k_i$ $(i=1,2,\ldots,l)$ diagonal blocks $\mathscr{J}_i$, and

$$\mathscr{J}_i=\begin{pmatrix}\lambda_i & & & \\ 1 & \lambda_i & & \\ & \ddots & \ddots & \\ & & 1 & \lambda_i\end{pmatrix}, \quad (20)$$

$$\varphi=(\varphi_1^1\varphi_2^1\cdots\varphi_{k_1}^1\varphi_1^2\cdots\varphi_{k_l}^l)^T, \quad (21)$$

$$\nabla_\varphi=\left(\frac{\partial}{\partial\varphi_1^1}\frac{\partial}{\partial\varphi_2^1}\cdots\frac{\partial}{\partial\varphi_{k_1}^1}\frac{\partial}{\partial\varphi_1^2}\cdots\frac{\partial}{\partial\varphi_{k_l}^l}\right)^T \quad (22)$$

and we say that A possesses a *Jordan* form. Obviously, the diagonal form is a special case of the Jordan form.

3. Blockwise diagonal form

Suppose there exists a basis consisting of $x_1^1(\mathbf{y}),x_2^1(\mathbf{y}),\ldots,x_{k_1}^1(\mathbf{y}),x_1^2(\mathbf{y}),\ldots,x_{k_l}^l(\mathbf{y})$ and invariants $\omega_1(\mathbf{y}),\omega_2(\mathbf{y}),\ldots,\omega_m(\mathbf{y})$ ($\Sigma_{i=1}^{l}k_i+m=n$ and m can be zero). Upon this basis, the operator A possesses the form

$$A=\sum_{i=1}^{l}\sum_{j=1}^{k_i}f_j^i(x^i)\frac{\partial}{\partial x_j^i}, \quad (23)$$

where

$$\mathbf{x}^i=(x_1^ix_2^i\cdots x_{k_i}^i)^T \quad (24)$$

and we say that A possesses a *blockwise diagonal* form. This property trivially holds for all operators with $l=1$, and we shall only use it for $l>1$.

4. Quasilinear form

Finally, if there exists a basis consisting of $z_1(\mathbf{y}),z_2(\mathbf{y}),\ldots,z_k(\mathbf{y})$ and invariants $\omega_1(\mathbf{y}),\omega_2(\mathbf{y}),\ldots,\omega_m(\mathbf{y})$ ($k+m=n$ and m can be zero) such that

$$A=(D\mathbf{z},\nabla_z), \quad (25)$$

where D is a $k\times k$ matrix whose (i,j) entry is an invariant $\omega_{ij}(\mathbf{y})$ of A, we say that A possesses a *quasilinear* form. Obviously, the diagonal and Jordan forms are quasilinear.

III. THE ALGEBRAIC METHOD IN NONLINEAR PERTURBATION THEORY

A. Main formulas

Bogaevski and Povzner[8] developed an approach to approximately transform a special linear partial differential operator A to a canonical form. The operator A should be of the form

$$A=A_0+\epsilon A_1+\epsilon^2A_2+\cdots, \quad (26)$$

where ϵ is a small positive parameter and all A_i $(i=0,1,\ldots)$ are defined in a common basis and the magnitudes of the coefficients for all A_i are comparable to one another. In addition, the *leading operator* A_0 should be of a diagonal, Jordan, or quasilinear canonical form. An important special case emerges for chemical kinetic systems with *time scale separation* between variables or between reaction fluxes, where the corresponding operator A can be expressed in a form

$$A=A_0+\epsilon A_1.$$

We shall see from the example in Sec. IV that the reaction system need not have time scale separation since the technique can sometimes be applied even when $\epsilon=1$. This point will be discussed further in the Conclusions section. The algebraic method in nonlinear perturbation theory is therefore directly applicable to chemical reaction systems.

Using the algebraic method in nonlinear perturbation theory, we wish to find a transformation operator S such that the resultant operator

$$M=e^{-S}Ae^{S}, \quad (27)$$

where

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$$S=\epsilon S_1+\epsilon^2 S_2+\cdots, \tag{28}$$

is blockwise diagonal and its diagonal size and location are the same as the Jordan blocks of A_0. In the following, we will simply say that M is of a canonical form similar to A_0. From Eq. (23), one can see that the dependent variables in the corresponding differential equation system for a blockwise diagonal operator are partly separated. The differential equations for x_j^i $(j=1,2,\ldots,k_i)$ only contain these variables. Since there is a one-to-one relation between an operator and its corresponding differential equation system, we can simply write down the corresponding differential equation system after we obtain the canonical form M.

Notice that even though A and M use the same symbols for the dependent variables, they are not identical. If we use y_i and $\hat{y}_i$ to represent the dependent variables for A and M, respectively, it can be verified that

$$\hat{y}_i=e^S y_i \quad (i=1,2,\ldots,n) \tag{29}$$

and the operator e^S is naturally referred to as the *change of variable operator*.[8] Since

$$A=e^S M e^{-S}, \tag{30}$$

similarly we have

$$y_i=e^{-S}\hat{y}_i \quad (i=1,2,\ldots,n). \tag{31}$$

If we express e^S and e^{-S} by

$$e^S=I+S+\tfrac{1}{2}S^2+\cdots=I+\epsilon S_1+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)+\cdots \tag{32}$$

and

$$e^{-S}=I-S+\tfrac{1}{2}S^2-\cdots=I-\epsilon S_1-\epsilon^2(S_2-\tfrac{1}{2}S_1^2)-\cdots, \tag{33}$$

then

$$\hat{y}_i=y_i+\epsilon S_1 y_i+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)y_i+\cdots \tag{34}$$

and

$$y_i=\hat{y}_i-\epsilon S_1\hat{y}_i-\epsilon^2(S_2-\tfrac{1}{2}S_1^2)\hat{y}_i-\cdots. \tag{35}$$

In Eqs. (34) and (35), the operators S_i are defined in the bases $\mathbf{y}$ and $\hat{\mathbf{y}}$, respectively. Therefore, if we solve the differential equation system corresponding to M, the initial values should be taken as

$$\hat{y}_i(0)=y_i(0)+\epsilon S_1 y_i(0)+\epsilon^2(S_2+\tfrac{1}{2}S_1)y_i(0)+\cdots, \tag{36}$$

and the solutions $y_i(t)$ of the original differential equation system can be obtained by Eq. (35) from the solutions $\hat{y}_i(t)$. In the following, except for some special cases, we do not distinguish between the dependent variables in A and M; the reader should bear it in mind that y_i in A and M are different and they have the relations given by Eqs. (34) and (35). It becomes clear from Eq. (34) that finding the approximate canonical forms for A requires the application of a nonlinear transformation which is close to the identity transformation for small ϵ.

According to Eqs. (27) and (28), it can be readily verified that

$$M=M_0+\epsilon M_1+\epsilon^2 M_2+\cdots \tag{37}$$

and

$$M_0=A_0, \quad M_1=[A_0,S_1]+A_1,$$
$$M_2=[A_0,S_2]+A_2+[A_1,S_1]+\tfrac{1}{2}[[A_0,S_1],S_1],\ldots, \tag{38}$$

where $[X,Y]$ is the *commutator* of operators X and Y defined as

$$[X,Y]=XY-YX. \tag{39}$$

The formulas in Eq. (38) are recursive

$$M_i=[A_0,S_i]+Y_i \quad (i=1,2,\ldots), \tag{40}$$

where $Y_1=A_1$ and Y_i for $i>1$ are known if $S_1,\ldots,S_{i-1}$ are known. By appropriate choices of S_i's, M_i and consequently M will possess a canonical form similar to A_0.[8]

B. Derivative, integral, and canonical forms of an operator

The operator Y' will be referred to as the *derivative* of the operator Y with respect to A_0 if

$$Y'=[A_0,Y]. \tag{41}$$

The name of this operation reflects the fact that with appropriate definitions, it has similar properties common in elementary calculus, e.g., the derivative of a sum of operators is the sum of the derivatives of the summands; the derivative of a product of two operators is the sum of two products composed of one operator and the derivative of the other. Moreover, we say that the *height* of Y equals μ if the μth derivative of Y vanishes while the $(\mu-1)$th one does not. If no derivative of Y is zero, then Y will be referred to as *unbounded in height*. Obviously, the operator with height 1 commutes with A_0. Furthermore, the operator Y is integrable if there exists an operator Z such that

$$Y=Z'. \tag{42}$$

It has been verified that **operator Y possesses a canonical form similar to A_0 if and only if its height is bounded**, i.e., there exists $\mu\geqslant 1$ such that

$$Y^{(\mu)}=0. \tag{43}$$

The necessary and sufficient condition for Y having a bounded height has been obtained as follows:[8] if A_0 is of a Jordan form, then Y is bounded in height if and only if there exist a positive integer p, $\lambda(\mathbf{y})$ and $\varphi(\mathbf{y})$ such that

$$[A_0(\mathbf{y})-\lambda(\mathbf{y})]^p\varphi(\mathbf{y})=0 \quad \text{implies}$$
$$[A_0(\mathbf{y})-\lambda(\mathbf{y})]^q Y\varphi(\mathbf{y})=0 \tag{44}$$

for a sufficiently large positive integer q. This condition implies that Y transforms a Jordan basis function $\varphi(\mathbf{y})$ corresponding to the eigenvalue $\lambda(\mathbf{y})$ of A_0 to a Jordan basis function $\phi(\mathbf{y})$ corresponding to the same eigenvalue of A_0 or $Y\varphi(\mathbf{y})=0$. As $\phi(\mathbf{y})$ is only a function of the Jordan basis functions $\varphi_\lambda^j(\mathbf{y})$ $(j=1,2,\ldots,k_\lambda)$ corresponding to eigenvalue λ, Y must possess a blockwise diagonal form similar to A_0. Each diagonal block of Y has the same basis variables as those of the corresponding Jordan block of A_0. Thus our purpose is finding appropriate S_i such that M_i and consequently M have bounded heights.

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Using the definition of the derivative of an operator, Eq. (40) can be expressed as

$$M_i=[A_0,S_i]+Y_i=S_i'+Y_i. \tag{45}$$

The basic idea to obtain a canonical M_i is the following: if we can separate Y_i into two terms

$$Y_i=Y_{i1}+Y_{i2}, \tag{46}$$

where Y_{i1} has a bounded height and Y_{i2} is integrable, i.e.,

$$Y_{i2}=Z', \tag{47}$$

then we have

$$M_i=S_i'+Y_{i1}+Z'. \tag{48}$$

Choosing $S_i=-Z$ allows M_i to be equal to Y_{i1}.

C. Determination of S_i and M_i

1. The commutation relation

There are several ways to choose S_i. One way is using the *commutation relation*. Let us compute $Y',Y'',\ldots,Y^{(r)}$. If there exist invariants ω_0, $\omega_1,\ldots,\omega_r$ of A_0 not all equal to zero and such that

$$\omega_0 Y+\omega_1 Y'+\cdots+\omega_r Y^{(r)}=0, \tag{49}$$

the equation is referred to as a commutation relation. If $\omega_0\neq 0$, then Y is integrable because

$$Y=\left[-\frac{1}{\omega_0}(\omega_1 Y+\omega_2 Y'+\cdots+\omega_r Y^{(r-1)})\right]'. \tag{50}$$

Here we have used the property that the derivative of a sum of operators is the sum of the derivatives of the operators, and the ratio of two invariants is again an invariant. If $\omega_i=0$ $(i=0,1,\ldots,\mu-1)$, but $\omega_\mu\neq 0$, then one can define

$$\tilde{Y}=Y+\frac{1}{\omega_\mu}(\omega_{\mu+1}Y'+\cdots+\omega_r Y^{(r-\mu)}) \tag{51}$$

and then

$$Y-\tilde{Y}=\left[-\frac{1}{\omega_\mu}(\omega_{\mu+1}Y+\cdots+\omega_r Y^{(r-\mu-1)})\right]'. \tag{52}$$

It is easy to see that $\tilde{Y}^{(\mu)}=0$ and $Y-\tilde{Y}$ is integrable. Now returning to the formula for M_1 [Eq. (38)], we find that $M_1=S_1'+A_1$. If a commutation relation holds for A_1, then A_1 can be represented as the sum of an integrable operator $A_1-\tilde{A}_1$ and an operator $\tilde{A}_1$ with a bounded height. The integrable part can be eliminated by setting $S_1'=\tilde{A}_1-A_1$, which also defines S_1. Thus M_1 equals the rest part $\tilde{A}_1$ whose height is bounded. For $\mu=0$, $\tilde{A}_1=0$ and $S_1'=-A_1$. Hence, operator M_1 with a bounded height is of a canonical form similar to A_0. After the determination of S_1,

$$Y_2=A_2+[A_1,S_1]+\tfrac{1}{2}[[A_0,S_1],S_1] \tag{53}$$

is known and we have

$$M_2=S_2'+Y_2. \tag{54}$$

If a commutation relation also holds for Y_2 we can choose S_2 such that M_2 has a canonical form similar to A_0. Following the same procedure, one can determine the other S_i's $(i=3,4,\ldots)$ to obtain canonical M_i's.

The necessary and sufficient conditions for the existence of a commutation relation for some special operators have been obtained. For example, when A_0 is quasilinear and Y defined in the basis $z_1,z_2,\ldots,z_k,\omega_1,\omega_2,\ldots,\omega_m$ is of the form

$$Y=\sum_{i=1}^{k} P_i\frac{\partial}{\partial z_i}+\sum_{i=1}^{m} Q_i\frac{\partial}{\partial \omega_i}, \tag{55}$$

where P_i and Q_i are polynomials in z_i whose coefficients are invariants of A_0, then there exists a commutation relation for Y. This condition is usually satisfied for a mass action kinetic system with $Y=A_1$.

2. Using the mapping property of Jordan basis functions

Determination of S_i such that $M_i^{(\mu)}=0$ by a commutation relation is sometimes quite complicated. This is because the calculation of different derivatives is time consuming and there is no easy way to determine the combination coefficients ω_i in Eq. (49). There is another way to determine S_i and consequently M_i if Y_i satisfies the following conditions:

(1) For any Jordan basis function $\varphi_\lambda(\mathbf{y})$ corresponding to the eigenvalue $\lambda(\mathbf{y})$ of A_0 which is used in the basis, the image of $\varphi_\lambda(\mathbf{y})$ under Y_i is only the sum of some Jordan basis functions $\phi_k(\mathbf{y})$ corresponding to eigenvalue $\mu_k(\mathbf{y})$ of A_0 that will be denoted as

$$Y_i\varphi_\lambda(\mathbf{y})=\phi_0(\mathbf{y})+\sum_{k\in I}\phi_k(\mathbf{y}), \tag{56}$$

where $\phi_0(\mathbf{y})$ is an invariant (it can be 0) and I is a set of integers.

(2) Either $\mu_k(\mathbf{y})\equiv\lambda(\mathbf{y})$ or $\mu_k(\mathbf{y})\neq\lambda(\mathbf{y})$ for all $\mathbf{y}$ in the considered domain of $\mathbf{y}$.

If these two conditions hold, then Eq. (40) $M_i=[A_0,S_i]+Y_i$ is solvable and the resultant M_i is of a bounded height.

Here we reproduce the proof given by Bogaevski and Povzner for diagonal A_0, where any eigenvalue is only a function of invariants ω_j of A_0 since it illustrates a method for the determination of S_i and M_i, which we shall also use in the example below. In this case, the basis is composed of the eigenfunctions $\varphi_i(\mathbf{y})$ $(i=1,2,\ldots,k)$ and the invariants $\omega_j(\mathbf{y})$ $(j=1,2,\ldots m)$ of A_0. For A_0 being Jordan, the proof can be found in Ref. 8. We refer the reader to the example in Sec. IV for an illustration of this method.

We start by defining the coefficients of operators M_i and S_i for the terms of the partial derivative with respect to invariant $\omega_j(\mathbf{y})$ of A_0. An invariant can be considered as an eigenfunction corresponding to eigenvalue zero. According to the assumption

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$$Y_i\omega_j(\mathbf{y})=\phi_0(\mathbf{y})+\sum_{k\in I_{i,j}}\phi_k(\mathbf{y}), \tag{57}$$

where $\phi_0(\mathbf{y})$ is an invariant (it can be 0) of A_0, $I_{i,j}$ is a set of integers, and

$$A_0\phi_k(\mathbf{y})=\mu_k(\mathbf{y})\phi_k(\mathbf{y}) \quad (k=1,2,\ldots) \tag{58}$$

with

$$\mu_k(\mathbf{y})\neq 0. \tag{59}$$

From Eq. (40), we have

$$M_i\omega_j(\mathbf{y})=A_0S_i\omega_j(\mathbf{y})-S_iA_0\omega_j(\mathbf{y})+Y_i\omega_j(\mathbf{y})$$

$$=A_0S_i\omega_j(\mathbf{y})+\phi_0(\mathbf{y})+\sum_{k\in I_{i,j}}\phi_k(\mathbf{y}). \tag{60}$$

By choosing

$$S_i\omega_j(\mathbf{y})=-\sum_{k\in I_{i,j}}\phi_k(\mathbf{y})/\mu_k(\mathbf{y}), \tag{61}$$

we have a solution of Eq. (60) and

$$M_i\omega_j(\mathbf{y})=\phi_0(\mathbf{y}). \tag{62}$$

Equation (62) shows that M_i transforms an invariant of A_0 to an invariant of A_0.

Now we determine the coefficients $S_i\varphi_\lambda(\mathbf{y})$ and $M_i\varphi_\lambda(\mathbf{y})$ for the term of the partial derivative with respect to eigenfunction $\varphi_\lambda(\mathbf{y})$ of A_0 corresponding to eigenvalue λ. We have

$$M_i\varphi_\lambda(\mathbf{y})=A_0S_i\varphi_\lambda(\mathbf{y})-S_iA_0\varphi_\lambda(\mathbf{y})+Y_i\varphi_\lambda(\mathbf{y})=A_0S_i\varphi_\lambda(\mathbf{y})$$

$$-(S_i\lambda)\varphi_\lambda(\mathbf{y})-\lambda S_i\varphi_\lambda(\mathbf{y})+Y_i\varphi_\lambda(\mathbf{y}). \tag{63}$$

Since under our assumption any eigenvalue is only a function of the invariants ω_j of A_0, one has

$$S_i\lambda=\sum_{j=1}^{m}\frac{\partial\lambda}{\partial\omega_j(\mathbf{y})}S_i\omega_j(\mathbf{y}). \tag{64}$$

From Eq. (61), we know that $(S_i\lambda)\varphi_\lambda$ is a sum of eigenfunctions corresponding to the eigenvalues $\gamma_k=\mu_k+\lambda$ such that $\lambda-\gamma_k\neq 0$. Here we used the property that the product of two eigenfunctions ϕ_k and φ_λ is still an eigenfunction corresponding to the sum of the original two eigenvalues μ_k and λ. From Eq. (56), we also know that $Y_i\varphi_\lambda(\mathbf{y})$ is a sum of some eigenfunctions of A_0. Then $M_i\varphi_\lambda(\mathbf{y})$ can be represented as follows:

$$M_i\varphi_\lambda(\mathbf{y})=A_0S_i\varphi_\lambda(\mathbf{y})-\lambda S_i\varphi_\lambda(\mathbf{y})+\phi_\lambda(\mathbf{y})+\sum_{k\in I_{i,\lambda}}\phi_k(\mathbf{y}), \tag{65}$$

where $\phi_\lambda(\mathbf{y})$ and $\phi_k(\mathbf{y})$ are eigenfunctions of A_0 corresponding to eigenvalues λ and μ_k with $\lambda-\mu_k\neq 0$, and $\phi_\lambda(\mathbf{y})$ may be absent. Setting

$$S_i\varphi_\lambda(\mathbf{y})=\sum_{k\in I_{i,\lambda}}\frac{\phi_k(\mathbf{y})}{\lambda-\mu_k}, \tag{66}$$

we obtain

$$M_i\varphi_\lambda(\mathbf{y})=\phi_\lambda(\mathbf{y}). \tag{67}$$

It may also be the case that $M_i\varphi_\lambda(\mathbf{y})=0$ when $\phi_\lambda(\mathbf{y})$ is absent in Eq. (65). This shows that M_i transforms an eigenfunction $\varphi_\lambda(\mathbf{y})$ of A_0 corresponding to eigenvalue λ to an eigenfunction of A_0 with the same eigenvalue or to 0. Hence, Eqs. (62) and (67) show that M_i satisfies the condition defined by Eq. (44). Therefore, the height of M_i is bounded, i.e., M_i is of a canonical form similar to A_0. Moreover, Eqs. (61) and (66) present a method for the selection of S_i. When conditions (1) and (2) are not satisfied, in some cases we can still transform Y_i to a canonical form M_i by the determination of an appropriate S_i. The interested reader should consult Appendix A for the techniques used.

IV. DETERMINATION OF UNCONSTRAINED APPROXIMATE LUMPING SCHEMES BY THE ALGEBRAIC METHOD IN NONLINEAR PERTURBATION THEORY

The algebraic method in nonlinear perturbation theory can be used to determine unconstrained approximate lumping schemes of a chemical reaction system described by the following ordinary differential equation system:

$$\frac{d\mathbf{y}}{d\tau}=\mathbf{f}^1(\mathbf{y},\mathbf{z})+\epsilon\mathbf{f}^2(\mathbf{y},\mathbf{z}), \tag{68}$$

$$\frac{d\mathbf{z}}{d\tau}=\mathbf{g}^1(\mathbf{y},\mathbf{z})+\epsilon\mathbf{g}^2(\mathbf{y},\mathbf{z}), \tag{69}$$

where $\mathbf{y}$ and $\mathbf{f}^i$, $\mathbf{z}$ and $\mathbf{g}^i$ are m- and k-dimensional vectors and function vectors, respectively, and $k+m=n$; ϵ is a small positive parameter which arises due to the separation between the magnitudes of reaction rates in chemical systems.

A subset of the above class of equations arises when there is time scale separation between the species concentrations. In this case, Eqs. (68) and (69) take the form

$$\frac{d\mathbf{y}}{d\tau}=\epsilon\mathbf{f}(\mathbf{y},\mathbf{z}), \tag{70}$$

$$\frac{d\mathbf{z}}{d\tau}=\mathbf{g}(\mathbf{y},\mathbf{z}), \tag{71}$$

or

$$\frac{d\mathbf{y}}{dt}=\mathbf{f}(\mathbf{y},\mathbf{z}), \tag{72}$$

$$\epsilon\frac{d\mathbf{z}}{dt}=\mathbf{g}(\mathbf{y},\mathbf{z}), \tag{73}$$

where

$$t=\epsilon\tau. \tag{74}$$

For Eqs. (70) and (71), the corresponding linear partial differential operator has the form

$$A=A_0+\epsilon A_1, \tag{75}$$

where

$$A_0=\sum_{i=1}^{k}g_i(\mathbf{y},\mathbf{z})\frac{\partial}{\partial z_i}, \tag{76}$$

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$$A_1=\sum_{i=1}^{m} f_i(\mathbf{y},\mathbf{z})\frac{\partial}{\partial y_i}. \tag{77}$$

Notice that all y_i are invariants of A_0. If we can transform A_0 into a Jordan canonical form by determining its Jordan basis functions $\varphi_i(\mathbf{y},\mathbf{z})(i=1,2,\ldots,k)$, we can construct a new basis for A as follows:

$$\varphi_1,\varphi_2,\ldots,\varphi_k,y_1,y_2,\ldots,y_m.$$

For this basis, the operators possess the forms

$$A_0=\sum_{i=1}^{k} G_i(\mathbf{y},\varphi)\frac{\partial}{\partial\varphi_i}=(\mathscr{J}\varphi,\nabla_\varphi), \tag{78}$$

$$A_1=\sum_{i=1}^{k} P_i(\mathbf{y},\varphi)\frac{\partial}{\partial\varphi_i}+\sum_{i=1}^{m} Q_i(\mathbf{y},\varphi)\frac{\partial}{\partial y_i}. \tag{79}$$

All y_i can be referred to as the eigenfunctions of A_0 with respect to the eigenvalue zero. Then for $\mathbf{y}$ and φ, A_0 is diagonal and Jordan, respectively. After the transformation of A to a canonical form, the resultant M is of a canonical form similar to A_0, i.e., the first part of the corresponding differential equation system for M only contains variables y_i $(i=1,2,\ldots,m)$ (actually they are lumped variables $\hat{y}_i$ denoted by the same symbols) and the second part contains all basis variables. Hence the first part composes an m-dimensional lumped differential equation system. As we can only take finite terms of M_i, the resultant system is an approximation of an exactly lumped system for the original differential equations. This is the basic idea in the application of the algebraic method in nonlinear perturbation theory for unconstrained approximate nonlinear lumping. We use the term unconstrained lumping since the choice of transformation S is determined purely by the method itself rather than with any previously imposed restrictions.

A. Summary of the method

(i) Choose an appropriate A_0 according to the separation in magnitudes of the terms of $\mathbf{f}$ and $\mathbf{g}$, which variables we choose to be invariants, or by other considerations;

(ii) if A_0 is not of a canonical form, transform it to some canonical form by using the Jordan basis functions of A_0 as a new basis for A;

(iii) find the representations of $A_i(i>0)$ upon the new basis;

(iv) find a canonical form for A_1 by choosing a suitable S_1 such that the equation

$$M_1=[A_0,S_1]+A_1$$

gives a canonical form for M_1 which is similar to A_0;

(v) repeat for higher order terms if necessary.

B. Unconstrained approximate nonlinear lumping

We will use an example to show the principle for the determination of an unconstrained approximate nonlinear lumping scheme. A simple biochemical reaction[10] will be used for illustration of this method

$$S+E\underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}}C\xrightarrow{k_2}P+E,$$

where S and P represent the substrate and product, respectively, E denotes the enzyme, and C the complex formed between S and E. k_1, k_{-1}, and k_2 are rate constants. If we use lower-case letters to represent their concentrations, the corresponding kinetic equation system is as follows:

$$\frac{ds}{dt}=-k_1se+k_{-1}c, \tag{80}$$

$$\frac{de}{dt}=-k_1se+(k_{-1}+k_2)c, \tag{81}$$

$$\frac{dc}{dt}=k_1se-(k_{-1}+k_2)c, \tag{82}$$

$$\frac{dp}{dt}=k_2c. \tag{83}$$

Notice that $e+c$ is a constant. If at time $t=0$, $s=s_0$, $e=e_0$, and $c=p=0$, then

$$e+c=e_0. \tag{84}$$

As there are only two independent equations, we choose Eqs. (80) and (82). Substituting Eq. (84) into them yields

$$\frac{ds}{dt}=-k_1e_0s+(k_1s+k_{-1})c, \tag{85}$$

$$\frac{dc}{dt}=k_1e_0s-(k_1s+k_{-1}+k_2)c. \tag{86}$$

For this system, c is small and we are usually only concerned with the evolution of s. We wish to obtain an approximation for ds/dt which does not contain c. In the following, we use the variable $y=s/s_0$ instead of s. Therefore, we want to construct an approximation of dy/dt which only contains y. We need to introduce a small positive parameter ϵ. In order to do so, let us make Eqs. (85) and (86) dimensionless by taking

$$y=\frac{s}{s_0},\quad z=\frac{c}{e_0},\quad \epsilon=\frac{e_0}{s_0}, \tag{87}$$

$$\tau=\frac{k_1e_0t}{\epsilon},\quad a=\frac{k_{-1}+k_2}{k_1s_0},\quad b=\frac{k_2}{k_1s_0}. \tag{88}$$

Then we obtain the desired form for the application of the algebraic method in nonlinear perturbation theory

$$\frac{dy}{d\tau}=\epsilon[-y+(y+a-b)z], \tag{89}$$

$$\frac{dz}{d\tau}=y-(y+a)z, \tag{90}$$

with the initial condition $y=1$, $z=0$ at $\tau=0$. For this differential equation system, the corresponding linear partial differential operator is

$$A=A_0+\epsilon A_1, \tag{91}$$

where

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$$A_0=[y-(y+a)z]\frac{\partial}{\partial z}, \tag{92}$$

$$A_1=[-y+(y+a-b)z]\frac{\partial}{\partial y}. \tag{93}$$

First we need to transform A_0 into a canonical form. Obviously, y is an invariant of A_0 and the other eigenfunction

$$\varphi=\frac{y}{y+a}-z \tag{94}$$

with eigenvalue $\lambda=-(y+a)$ can be readily obtained by solving the equation

$$A_0\varphi=\lambda\varphi. \tag{95}$$

Using the new basis y and φ, the operators are represented as

$$A_0=-(y+a)\varphi\frac{\partial}{\partial\varphi}, \tag{96}$$

$$A_1=-\left[\frac{by}{y+a}+(y+a-b)\varphi\right]\frac{\partial}{\partial y}-\left[\frac{aby}{(y+a)^3}+\frac{a(y+a-b)}{(y+a)^2}\varphi\right]\frac{\partial}{\partial\varphi}. \tag{97}$$

A_0 is of a diagonal form. Under the new basis, the corresponding ordinary differential equation system is

$$\frac{dy}{d\tau}=-\epsilon\left[\frac{by}{y+a}+(y+a-b)\varphi\right], \tag{98}$$

$$\frac{d\varphi}{d\tau}=-(y+a)\varphi-\epsilon\left[\frac{aby}{(y+a)^3}+\frac{a(y+a-b)}{(y+a)^2}\varphi\right], \tag{99}$$

with the initial condition $y(0)=1$, $\varphi(0)=1/(1+a)$.

Now we will employ Eq. (38) to transform A to M. From the equation, we know $M_0=A_0$ and M_1 can be determined by

$$M_1=[A_0,S_1]+A_1. \tag{100}$$

Notice that each term of the coefficients of A_1 is an eigenfunction of A_0 with respect to eigenvalue either zero or $-(y+a)$. Therefore, A_1 satisfies the requirement given by Eq. (56). Then for Eq. (100), the solution M_1 with a bounded height exists. Let us first determine the coefficient M_1y through Eq. (60)

$$M_1y=A_0S_1y+A_1y=A_0S_1y-\frac{by}{y+a}-(y+a-b)\varphi. \tag{101}$$

According to Eq. (61), setting

$$S_1y=-\frac{y+a-b}{y+a}\varphi \tag{102}$$

gives

$$M_1y=-\frac{by}{y+a}. \tag{103}$$

Similarly, using the result of M_1y and Eq. (63) as well as $\lambda=-(y+a)$ for φ, we have

$$\begin{aligned}M_1\varphi&=A_0S_1\varphi-(S_1\lambda)\varphi-\lambda S_1\varphi+A_1\varphi\\&=A_0S_1\varphi-\{S_1[-(y+a)]\}\varphi+(y+a)S_1\varphi+A_1\varphi\\&=A_0S_1\varphi+(y+a)S_1\varphi-\frac{y+a-b}{y+a}\varphi^2\\&\quad-\frac{aby}{(y+a)^3}-\frac{a(y+a-b)}{(y+a)^2}\varphi.\end{aligned} \tag{104}$$

Notice that the last three terms in Eq. (104) are all eigenfunctions of A_0 corresponding to eigenvalues $-2(y+a)$, 0, and $-(y+a)$, respectively. Thus setting

$$S_1\varphi=-\frac{y+a-b}{(y+a)^2}\varphi^2+\frac{aby}{(y+a)^4} \tag{105}$$

yields

$$M_1\varphi=-\frac{a(y+a-b)}{(y+a)^2}\varphi. \tag{106}$$

In summary, we obtain

$$M_1=-\frac{by}{y+a}\frac{\partial}{\partial y}-\frac{a(y+a-b)}{(y+a)^2}\varphi\frac{\partial}{\partial\varphi}, \tag{107}$$

$$S_1=-\frac{y+a-b}{y+a}\varphi\frac{\partial}{\partial y}+\left[\frac{aby}{(y+a)^4}-\frac{y+a-b}{(y+a)^2}\varphi^2\right]\frac{\partial}{\partial\varphi}. \tag{108}$$

The resultant M_1 is of a canonical form similar to A_0. The coefficient of $\partial/\partial y$ is only a function of the invariant y of A_0, and the coefficient of $\partial/\partial\varphi$ has the form $\omega(y)\varphi$.

It can be readily proved that $M_1'\neq 0$, but $M_1''=0$,

$$M_1'=[A_0,M_1]=A_0M_1-M_1A_0=-\frac{by}{y+a}\varphi\frac{\partial}{\partial\varphi}, \tag{109}$$

$$\begin{aligned}M_1''&=[A_0,M_1']=A_0M_1'-M_1'A_0\\&=\left\{-(y+a)\varphi\left(-\frac{by}{y+a}\right)+\frac{by}{y+a}\varphi[-(y+a)]\right\}\frac{\partial}{\partial\varphi}=0.\end{aligned} \tag{110}$$

There is a special problem in the transformation of A to M. The canonical form of M_1 is not unique. Actually for S_1, we can add a term

$$S_1^*=\omega_1(y)\frac{\partial}{\partial y}+\omega_2(y)\varphi\frac{\partial}{\partial\varphi} \tag{111}$$

without failing to give a canonical form for M_1. Here $\omega_i(y)$ are arbitrary functions of y. Let $\tilde{M}_1$ denote the new canonical form. Then

$$\begin{aligned}\tilde{M}_1&=[A_0,S_1+S_1^*]+A_1=[A_0,S_1]+A_1+[A_0,S_1^*]\\&=M_1+M_1^*,\end{aligned} \tag{112}$$

where

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$$M_1^* = A_0 S_1^* - S_1^* A_0 = [-(y+a)\omega_2(y) + \omega_1(y) + (y+a)\omega_2(y)]\varphi \frac{\partial}{\partial \varphi} = \omega_1(y)\varphi \frac{\partial}{\partial \varphi}. \tag{113}$$

This implies that

$$\tilde{M}_1 = -\frac{by}{y+a}\frac{\partial}{\partial y} + \left[-\frac{a(y+a-b)}{(y+a)^2} + \omega_1(y)\right]\varphi \frac{\partial}{\partial \varphi}, \tag{114}$$

$$\tilde{S}_1 = S_1 + S_1^* = \left[\omega_1(y) - \frac{y+a-b}{y+a}\varphi\right]\frac{\partial}{\partial y} + \left[\frac{aby}{(y+a)^4} + \omega_2(y)\varphi - \frac{y+a-b}{(y+a)^2}\varphi^2\right]\frac{\partial}{\partial \varphi}. \tag{115}$$

This result shows that M_1 can contain an arbitrary function $\omega_1(y)$. There may be different considerations for the choices of $\omega_i(y)$. One of these considerations is to choose $\omega_i(y)$ such that $M_2=0$. As other high order terms $M_i(i\geqslant 3)$ containing high powers of small number ϵ are very small and can be omitted,

$$M = A_0 + \epsilon M_1 \tag{116}$$

will be a good approximation if $M_2=0$. The details of the calculation of $\omega_i(y)$ and the corresponding S_2 can be found in Appendix B.

Using this approach, we obtain the corresponding differential equation system for M,

$$\frac{dy}{d\tau} = -\epsilon \frac{by}{y+a}, \tag{117}$$

$$\frac{d\varphi}{d\tau} = -\left\{(y+a) + \epsilon\left[\frac{(a+b)y + a(a-b)}{(y+a)^2} - \left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\right\}\varphi. \tag{118}$$

From Sec. III, we know that y and φ in Eqs. (117) and (118) are not the original y and φ, but functions of them given by

$$\hat{y} = y + \epsilon S_1 y + \epsilon^2(S_2 + \tfrac{1}{2}S_1^2)y + \cdots, \tag{119}$$

$$\hat{\varphi} = \varphi + \epsilon S_1 \varphi + \epsilon^2(S_2 + \tfrac{1}{2}S_1^2)\varphi + \cdots. \tag{120}$$

Here, to distinguish them, we use $\hat{y}$ and $\hat{\varphi}$ to represent the variables in Eqs. (117) and (118). If the above expressions contain only the terms with powers of ϵ equal to and less than l, we say that the resultant $\hat{y}$ and $\hat{\varphi}$ by Eqs. (119) and (120) are lth order approximation from the original exact solution. When we want to solve Eqs. (117) and (118), the initial values must be chosen by using Eqs. (119) and (120).

From this simple example, we can draw some general conclusions. First, the right-hand side of Eq. (117) is only a function of y. In general, the right-hand side of the differential equations in M for the variables corresponding to the invariants ω_i $(i=1,2,\ldots,m)$ of A_0 are only functions of these variables. Therefore, they compose an m-dimensional approximately lumped system for the original differential equations corresponding to A. Especially, when the dimension of the lumped system is one, it is an approximation of the differential equation for a generalized eigenfunction of A.[7]

Second, the right-hand side of Eq. (118) is a linear function of φ with a coefficient $\omega(y)$ which is only a function of the invariant y of A_0. As ϵ is a small positive number, Eqs. (117) and (118) imply that y changes slowly, but φ changes quickly. As $-(y+a)$ is negative, when $\epsilon \to 0$, we will obtain a stable equation for φ. Therefore, we call φ a *purely fast variable*. Thus one can find its approximate solution by a singular perturbation method.[9,11]

Using the singular perturbation method, we can solve the equation separately in the inner region $\tau \geqslant 0$ and in the outer region $\epsilon\tau \geqslant 0$ and match them at the edge of the boundary layer.

Let the outer solution $\Phi(\epsilon\tau)$ be an expansion

$$\Phi(\epsilon\tau) = \sum_{i=0}^{\infty} \epsilon^i \Phi_i. \tag{121}$$

It can be obtained by solving the following equation:

$$\epsilon \frac{d\Phi}{d(\epsilon\tau)} = -\left\{(y+a) + \epsilon\left[\frac{(a+b)y + a(a-b)}{(y+a)^2} - \left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\right\}\Phi. \tag{122}$$

Comparing the terms with like powers of ϵ in both sides of the equation will give some equations to determine Φ_i. As $-(y+a)$ is negative, the outer expansion is trivial, i.e., $\Phi_i \equiv 0$ for every i.

The inner solution $\phi(\tau)$ can be obtained by solving the following equation under setting $y=y(0)$:

$$\frac{d\phi}{d\tau} = -\left([y(0)+a] + \epsilon\left\{\frac{(a+b)y(0) + a(a-b)}{[y(0)+a]^2} - \left(1-\frac{b}{a}\right)\frac{y(0)}{y(0)+a}\ln\frac{y(0)}{y(0)+a}\right\}\right)\phi. \tag{123}$$

It gives

$$\phi(\tau) = \phi(0)\exp\left[-\left([y(0)+a] + \epsilon\left\{\frac{(a+b)y(0) + a(a-b)}{[y(0)+a]^2} - \left(1-\frac{b}{a}\right)\frac{y(0)}{y(0)+a}\ln\frac{y(0)}{y(0)+a}\right\}\right)\tau\right], \tag{124}$$

where $\phi(0)$ can be given by Eq. (120), which is a function of $y(0)$ and $\varphi(0)$, i.e., $\phi[y(0),\varphi(0)]$. Considering $\varphi(0) = \varphi[y(0),z(0)]$ and $z(0)=0$ yields $\phi(0) = \phi[y(0), z(0)] = \phi[y(0)]$.

As $y(\tau)$ changes slowly and the inner solution is valid only for a very small time, we can simply replace $y(0)$ by y without introducing a significant error. Thus

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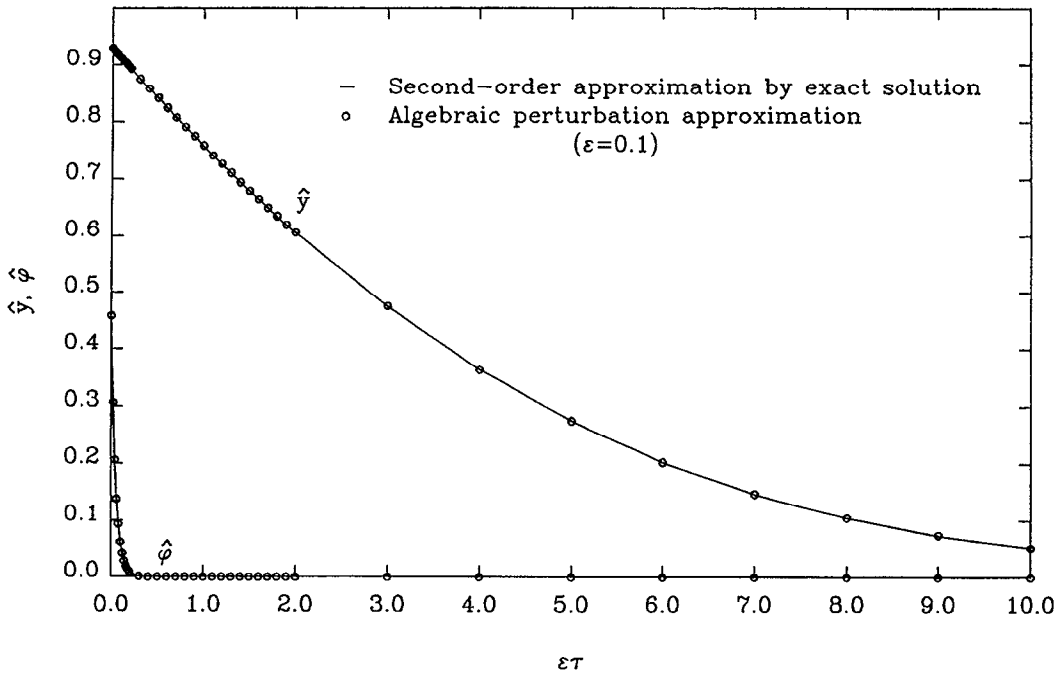

FIG. 1. A comparison between the solutions $\hat{y}(\epsilon\tau)$ and $\hat{\varphi}(\epsilon\tau)$ given by the second order approximation of the original differential equation system [Eqs. (98) and (99)] and the lumped differential equations (117) and (126) for $\epsilon=0.1$.

$$\phi(\tau)=\phi(y)\exp\left(-\left\{(y+a)+\epsilon\left[\frac{(a+b)y+a(a-b)}{(y+a)^2}-\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\right\}\tau\right). \tag{125}$$

When $\tau\to\infty$, $\phi(\tau)\to 0$. Then the inner solution $\phi(\tau)$ matches the trivial outer solution $\Phi(\epsilon\tau)\equiv 0$ as $\tau\to\infty$. Therefore, the solution of φ only consists of the inner solution

$$\varphi(\tau)=\phi(\tau)=\phi(y)\exp\left(-\left\{(y+a)+\epsilon\left[\frac{(a+b)y+a(a-b)}{(y+a)^2}-\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\right\}\tau\right). \tag{126}$$

Then Eqs. (98) and (99) can be approximately represented by a simple differential equation (117) and an exponential function (126). Generally speaking, when A_0 is diagonal for the variables φ_i $(i=1,2,\ldots,k)$ which are eigenfunctions of A_0 with negative eigenvalues, one may obtain k purely fast variables φ_i, and their transformed differential equations are of the form

$$\frac{d\varphi_i}{d\tau}=-\Omega_i(\omega)\varphi_i \quad (i=1,2,\ldots,k), \tag{127}$$

where Ω_i are some positive valued functions. The solutions of these equations can be given approximately by

$$\varphi_i(\tau)=\varphi_i(0)e^{-\Omega_i(\omega)\tau} \quad (i=1,2,\ldots,k). \tag{128}$$

When A_0 is Jordan, the solution of the lumped variable $\varphi_i(\tau)$ is a sum of exponential functions with the form given in Eq. (128). The proof is left to the reader.

C. Results

To show the accuracy of the resultant approximately lumped differential equations (117) and (126), some calculations were done using the data from the hydrolysis of the benzoyl-*L*-arginine ethyl ester, catalyzed by trypsin.[10,13] $k_1=4\times10^6$, $k_{-1}=25$, and $k_2=15$ giving $a=1$, $b=0.375$ when s_0 is equal to the Michaelis constant $(k_{-1}+k_2)/k_1$. As Eqs. (117) and (118) are second order approximations, their initial values should be calculated by Eqs. (119) and (120) in second order. They give

$$\hat{y}(0)=y(0)+\epsilon S_1 y(0)+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)y(0)$$
$$=1-0.716\ 61\epsilon+0.040\ 953\epsilon^2, \tag{129}$$
$$\hat{\varphi}(0)=\varphi(0)+\epsilon S_1\varphi(0)+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)\varphi(0)$$
$$=0.5-0.427\ 67\epsilon+0.068\ 199\epsilon^2. \tag{130}$$

The solutions for $\epsilon=0.1$ and 1 are given in Figs. 1 and 2. For comparison, the second order approximations from solutions of the original differential equation system [Eqs. (98) and (99)] given by

$$\hat{y}(\tau)=y(\tau)+\epsilon S_1 y(\tau)+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)y(\tau), \tag{131}$$

$$\hat{\varphi}(\tau)=\varphi(\tau)+\epsilon S_1\varphi(\tau)+\epsilon^2(S_2+\tfrac{1}{2}S_1^2)\varphi(\tau), \tag{132}$$

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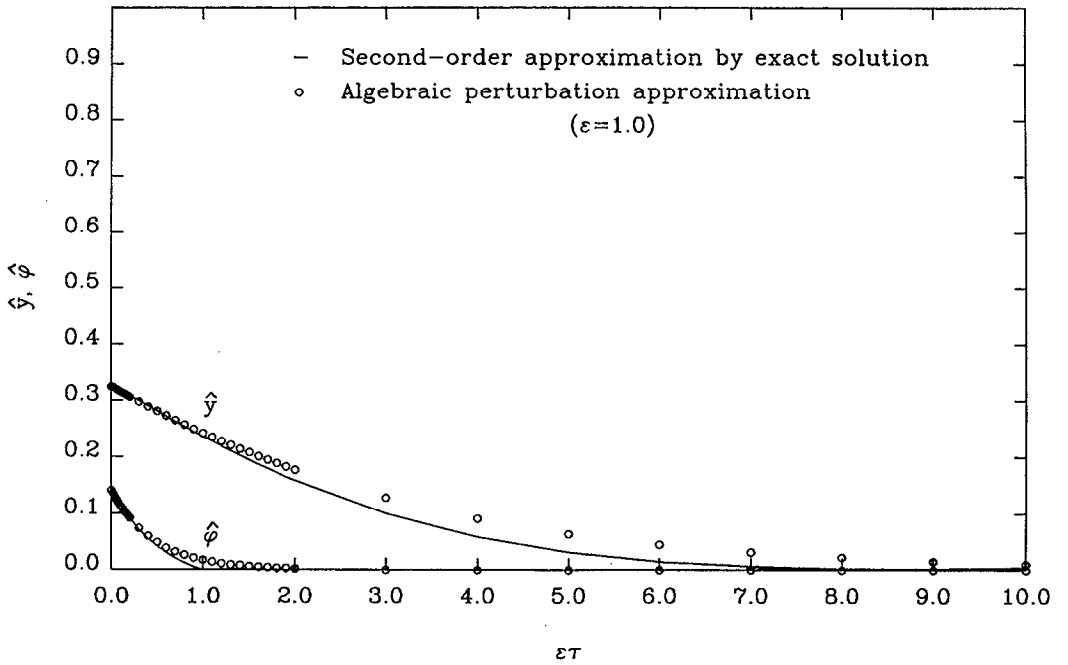

FIG. 2. A comparison between the solutions $\hat{y}(\epsilon\tau)$ and $\hat{\varphi}(\epsilon\tau)$ given by the second order approximation of the original differential equation system [Eqs. (98) and (99)] and the lumped differential equations (117) and (126) for $\epsilon=1$.

are also shown. For $\epsilon=0.1$, the solutions given by the two approaches are essentially the same. For $\epsilon=1$, the two solutions are very close. These results show that the algebraic method in nonlinear perturbation theory can be used successfully to construct unconstrained nonlinear lumped systems.

Moreover, the lumped system can be also used to inversely determine the solutions of the original variables $y(\tau)$ and $\varphi(\tau)$ by the second order inverse transformation

$$y(\tau)=\hat{y}(\tau)-\epsilon S_1\hat{y}(\tau)-\epsilon^2(S_2-\tfrac{1}{2}S_1^2)\hat{y}(\tau), \tag{133}$$

$$\varphi(\tau)=\hat{\varphi}(\tau)-\epsilon S_1\hat{\varphi}(\tau)-\epsilon^2(S_2-\tfrac{1}{2}S_1^2)\hat{\varphi}(\tau). \tag{134}$$

Then using Eq. (94), one can calculate $z(\tau)$. The results for $\epsilon=0.1$ and 1 are given in Figs. 3–5. For comparison, the first order approximations of the inverse transformation and the original exact solutions for y and z are also given. For $\epsilon=0.1$, even the first order approximation is almost exact. For $\epsilon=1$, the accuracy of the second order approximation is quite good except for the very beginning of the reaction course.

There are advantages in calculating the original variables through the lumped differential equations and the exponential functions of the purely fast variables. The lumped differential equation system has a lower dimension and is usually less stiff, so that longer time steps may be used in the integration. The formulas of S_i are usually quite complicated, as are the inverse transformations. However, they are only algebraic expressions and need only be calculated at selected output times rather than at each integration step. Compared to solving a higher dimensional and more stiff differential equation systems, using lumped systems may be computationally less expensive yet can still give the full information for all the variables.

V. CONCLUSIONS AND DISCUSSION

A general analysis of approximate unconstrained nonlinear lumping by the algebraic method in nonlinear perturbation theory is presented. There is a one-to-one relation between an n-dimensional ordinary differential equation system $d\mathbf{y}/dt=\mathbf{f}(\mathbf{y})$ and the linear partial differential operator $A=\Sigma_{i=1}^{n}f_i(\mathbf{y})/(\partial/\partial y_i)$. For the linear partial differential operator, some canonical forms such as diagonal, Jordan, blockwise diagonal, and quasilinear, were defined. The dependent variables in the corresponding ordinary differential equation system of these canonical forms are partly or completely separated. Thus the determination of nonlinear lumping schemes is equivalent to the determination of the canonical forms of A.

When the corresponding linear partial differential operator A possesses the form

$$A=A_0+\epsilon A_1+\epsilon^2A_2+\cdots,$$

where ϵ is a small positive number, and the leading operator A_0 is of some canonical form, the algebraic method in nonlinear perturbation theory can be used to find special transformations e^{-S} and e^{S}, where

$$S=\epsilon S_1+\epsilon^2S_2+\cdots,$$

which will transform A into a canonical form

$$M=e^{-S}Ae^{S}=A_0+\epsilon M_1+\epsilon^2M_2+\cdots$$

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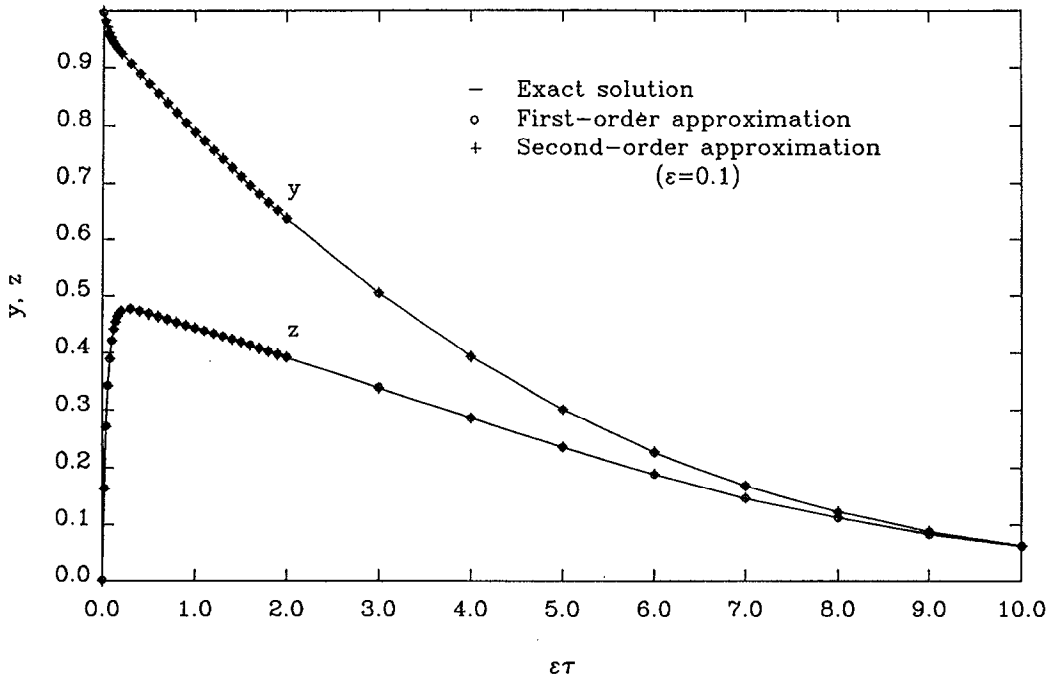

FIG. 3. A comparison between the exact solutions of $y(\epsilon\tau)$ and $z(\epsilon\tau)$ and the first and second order approximations of $y(\epsilon\tau)$ and $z(\epsilon\tau)$ given by the inverse transformation from the solutions of the lumped differential equations (117) and (126) for $\epsilon=0.1$.

similar to A_0. In practice, one only takes a few terms M_i to approximate M; the resultant ordinary differential equation system of M is then an approximately unconstrained lumped model.

The theoretical basis of the algebraic method in nonlinear perturbation theory was summarized. Two approaches to determine S_i and M_i were discussed. A simple reaction system was used to illustrate this method in the application for

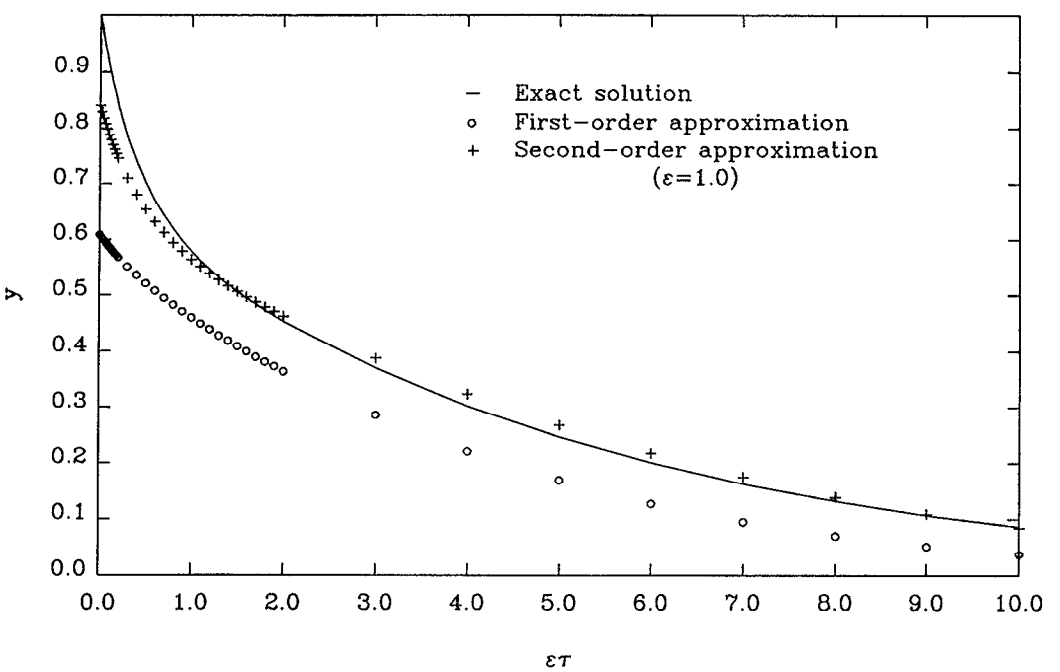

FIG. 4. A comparison between the exact solutions of $y(\epsilon\tau)$ and the first and second order approximations of $y(\epsilon\tau)$ given by the inverse transformation from the solutions of the lumped differential equations (117) and (126) for $\epsilon=1$.

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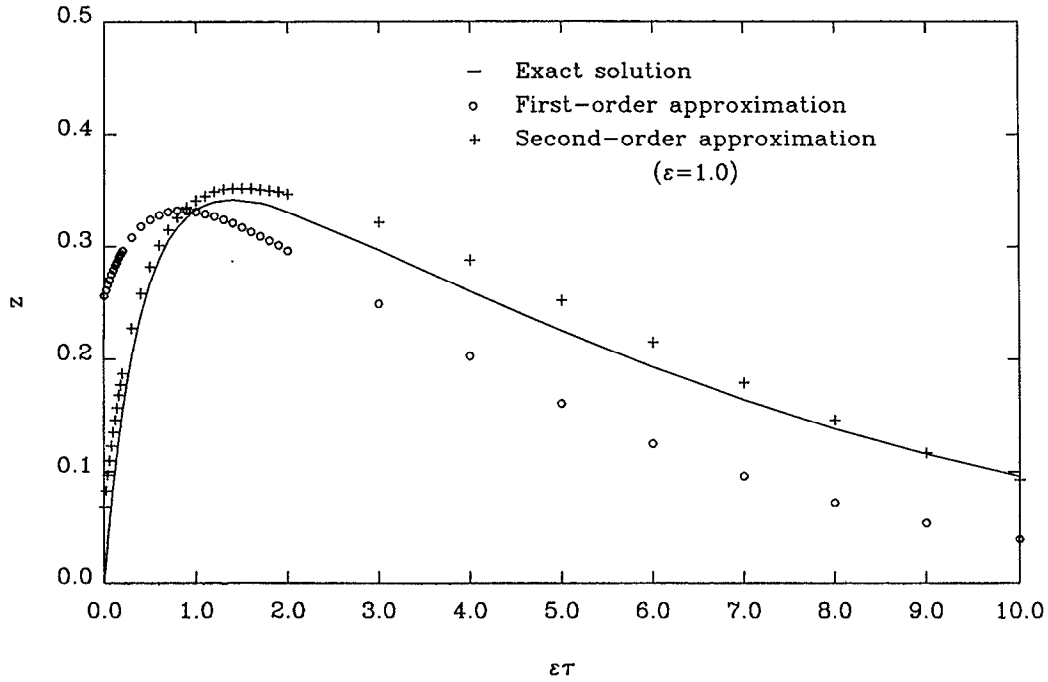

FIG. 5. A comparison between the exact solutions of $z(\epsilon\tau)$ and the first and second order approximations of $z(\epsilon\tau)$ given by the inverse transformation from the solutions of the lumped differential equations (117) and (126) for $\epsilon=1$.

unconstrained nonlinear lumping where the dependent variables of the lumped model are nonlinear functions of the original ones. This method supplies some purely fast variables without the requirement that the corresponding original variables must be linear in the original differential equation system, which is a requirement of another approach presented by the authors.[9] The solution of the purely fast variables can be approximately obtained by the singular perturbation method. In unconstrained nonlinear lumping, using the solutions of the purely fast variables and the lumped variables as well as the inverse transformation, one can find the solutions of all original dependent variables. Thus solving a higher dimensional differential equation system can be replaced by solving a lower dimensional and less stiff lumped differential equation system and calculating the algebraic expressions of the inverse transformation, which may reduce the computational effort. From the example, we see that sometimes time scale separation in the original equations might not be necessary in order to reduce the dimension of the system. In fact, although ϵ was present in the original equations, it was finally set to $\epsilon=1$ and the accuracy of the reduced scheme was still good. This makes the approach quite general. When $\epsilon=1$, the series $M_0+M_1+M_2+\cdots$ may not be convergent, however, the approximation by a finite terms of M_i may still be of great practical use.[11]

Theoretically, the algebraic method in nonlinear perturbation theory can be used for any mass action reaction system in the determination of unconstrained nonlinear lumping schemes with any desired accuracy. Unfortunately, in practice, the formulas for the higher order S_i and M_i are often too complicated to handle. The complexity of S_i and M_i depends on the choice of A_0. Obviously, the more terms of the original differential equation system contained in A_0, the better the accuracy of the lumped system and the fewer terms of M_i are needed. However, when A_0 contains more terms of the original differential equation system, transforming it to a canonical form may become a difficult problem. There may not be a general approach to choosing the best A_0. One has to treat this problem individually. For some problems, it may be required that the lumped system contain some of the original variables, so that the inverse transformation is not necessary to calculate their concentrations. Future work will therefore include the development of an approach to constrained nonlinear lumping, which will leave some species unlumped.

ACKNOWLEDGMENTS

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APPENDIX A

When conditions (1) and (2) for the mapping property of Y_i are not satisfied, i.e., Y_i transforms a Jordan basis function to non-Jordan ones, in some cases we can still transform Y_i to a canonical form M_i by the determination of an appropriate S_i. For example, when Y_i transforms a Jordan basis function $\varphi_\lambda(\mathbf{y})$ of A_0 to a set of Jordan basis functions $\phi_k(\mathbf{y})$ and other non-Jordan basis functions $\eta_l(\mathbf{y})$, i.e.,

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$$Y_i\varphi_\lambda(\mathbf{y})=\sum_{k\in I_{i,\lambda}}\phi_k(\mathbf{y})+\sum_{l\in I'_{i,\lambda}}\eta_l(\mathbf{y}), \tag{A1}$$

Eq. (63) becomes

$$M_i\varphi_\lambda(\mathbf{y})=A_0S_i\varphi_\lambda(\mathbf{y})-\lambda S_i\varphi_\lambda(\mathbf{y})+\phi_\lambda(\mathbf{y})$$
$$+\sum_{\gamma\in I_1}\phi_\gamma(\mathbf{y})+\sum_{\delta\in I_2}\eta_\delta(\mathbf{y}), \tag{A2}$$

where $I_{i,\lambda}$, $I'_{i,\lambda}$, I_1, and I_2 are all sets of positive integers. We can still find suitable S_i if $\eta_\delta(\mathbf{y})$ possess some special forms, for instance,

$$f(\omega,\varphi_\lambda),\quad \phi_\gamma f(\omega,\varphi_\lambda),\quad \varphi_\lambda f(\omega,\phi_\gamma).$$

Actually, such forms commonly occur in chemical kinetics.

In order to have M_i in a canonical form, we should choose $S_i\varphi_\lambda(\mathbf{y})$ such that all terms in $\Sigma_\gamma\phi_\gamma(\mathbf{y})$ and $\Sigma_\delta\eta_\delta(\mathbf{y})$ will be deleted by canceling them with terms given by $A_0S_i\varphi_\lambda(\mathbf{y})$ and $\lambda S_i\varphi_\lambda(\mathbf{y})$. As $\phi_\gamma(\mathbf{y})$ are Jordan basis functions of A_0, we can choose some terms of $S_i\varphi_\lambda(\mathbf{y})$ by Eq. (66) to eliminate them. To cancel $\eta_\delta(\mathbf{y})$, we need to choose other special terms for $S_i\varphi_\lambda(\mathbf{y})$. We will discuss the above three cases separately for $\varphi_\lambda(\mathbf{y})$ and $\phi_\gamma(\mathbf{y})$ being eigenfunctions of A_0.

Suppose $\Sigma_\delta\eta_\delta(\mathbf{y})$ contains a term $f(\omega,\varphi_\lambda)$. In order to delete it, $S_i\varphi_\lambda(\mathbf{y})$ must contain a term x_1 such that

$$A_0x_1-\lambda x_1+f(\omega,\varphi_\lambda)=0. \tag{A3}$$

Let

$$x_1=x_1(\omega,\varphi_\lambda). \tag{A4}$$

Then Eq. (A3) can be written in the following form:

$$\lambda\varphi_\lambda\frac{dx_1}{d\varphi_\lambda}-\lambda x_1=-f(\omega,\varphi_\lambda), \tag{A5}$$

or

$$\frac{dx_1}{d\varphi_\lambda}-\frac{x_1}{\varphi_\lambda}=-\frac{f(\omega,\varphi_\lambda)}{\lambda\varphi_\lambda}. \tag{A6}$$

This is a first order linear differential equation for x_1 with respect to the independent variable φ_λ. The solution is

$$x_1=\varphi_\lambda\left(c-\int\frac{f(\omega,\varphi_\lambda)}{\lambda\varphi_\lambda^2}\,d\varphi_\lambda\right), \tag{A7}$$

where c is an arbitrary constant. If we choose $c=0$, then

$$x_1=-\varphi_\lambda\int\frac{f(\omega,\varphi_\lambda)}{\lambda\varphi_\lambda^2}\,d\varphi_\lambda. \tag{A8}$$

When the integral can be given explicitly, x_1 is obtained. Sometimes, the implicit solution (A8) is enough for the determination of a lumped differential equation system.

For the second case $\phi_\gamma f(\omega,\varphi_\lambda)$, $S_i\varphi_\lambda(\mathbf{y})$ must contain term x_2 such that

$$A_0x_2-\lambda x_2+\phi_\gamma f(\omega,\varphi_\lambda)=0. \tag{A9}$$

Let

$$x_2=\phi_\gamma g(\omega,\varphi_\lambda). \tag{A10}$$

Then Eq. (A9) can be written in the following form:

$$\lambda\varphi_\lambda\phi_\gamma\frac{dg}{d\varphi_\lambda}+\gamma\phi_\gamma g-\lambda\phi_\gamma g=-\phi_\gamma f(\omega,\varphi_\lambda), \tag{A11}$$

or

$$\frac{dg}{d\varphi_\lambda}-\frac{\lambda-\gamma}{\lambda\varphi_\lambda}g=-\frac{f(\omega,\varphi_\lambda)}{\lambda\varphi_\lambda}. \tag{A12}$$

This is a first order linear differential equation for g with respect to the independent variable φ_λ. The solution is

$$g=\varphi_\lambda^{(\lambda-\gamma)/\lambda}\left[c-\int\frac{f(\omega,\varphi_\lambda)}{\lambda}\varphi_\lambda^{(\gamma-2\lambda)/\lambda}d\varphi_\lambda\right], \tag{A13}$$

where c is an arbitrary constant. Choosing $c=0$ yields

$$x_2=-\phi_\gamma\varphi_\lambda^{(\lambda-\gamma)/\lambda}\int\frac{f(\omega,\varphi_\lambda)}{\lambda}\varphi_\lambda^{(\gamma-2\lambda)/\lambda}d\varphi_\lambda. \tag{A14}$$

For the third case, $\varphi_\lambda f(\omega,\phi_\gamma)$, $S_i\varphi_\lambda(\mathbf{y})$ must contain term x_3 such that

$$A_0x_3-\lambda x_3+\varphi_\lambda f(\omega,\phi_\gamma)=0. \tag{A15}$$

Let

$$x_3=\varphi_\lambda g(\omega,\phi_\gamma). \tag{A16}$$

Then Eq. (A15) can be written in the following form:

$$\lambda\varphi_\lambda g+\gamma\phi_\gamma\varphi_\lambda\frac{dg}{d\phi_\gamma}-\lambda\varphi_\lambda g=-\varphi_\lambda f(\omega,\phi_\gamma), \tag{A17}$$

or

$$\frac{dg}{d\phi_\gamma}=-\frac{f(\omega,\phi_\gamma)}{\gamma\phi_\gamma}. \tag{A18}$$

The solution is

$$x_3=\varphi_\lambda\left[c-\int\frac{f(\omega,\phi_\gamma)}{\gamma\phi_\gamma}\,d\phi_\gamma\right], \tag{A19}$$

where c is an arbitrary constant. Choosing $c=0$ gives

$$x_3=-\varphi_\lambda\int\frac{f(\omega,\phi_\gamma)}{\gamma\phi_\gamma}\,d\phi_\gamma. \tag{A20}$$

For different functions of $\eta_\delta(\mathbf{y})$, one may find different ways to choose S_i.

APPENDIX B

We will choose $\omega_i(y)$ such that $M_2=0$. From Eq. (38), we know that when $A_2=0$,

$$M_2=[A_0,S_2]+[A_1,S_1]+\tfrac{1}{2}[[A_0,S_1],S_1]. \tag{B1}$$

It can be readily verified that when $A_2=0$, we also have

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$$M_2=[A_0,S_2]+\tfrac{1}{2}[[M_1+A_1],S_1]. \tag{B2}$$

Equation (B2) implies that

$$Y_2=\tfrac{1}{2}[[M_1+A_1],S_1]. \tag{B3}$$

As shown in Eqs. (114) and (115), M_1 and S_1 can contain arbitrary functions $\omega_i(y)$ $(i=1,2)$. Then Y_2 and consequently M_2 might be nonunique and are functions of $\omega_i(y)$. Actually, the calculation gives

$$\begin{aligned}Y_2=&\left\{\left[\frac{aby(y+a-b)}{(y+a)^4}-\frac{by}{y+a}\omega_1'+\frac{ab}{(y+a)^2}\omega_1\right]+\left[\frac{b^2y+a(y+a-b)(y+a-2b)}{(y+a)^3}+\frac{(y+a-b)(\omega_2-\omega_1')+\omega_1}{2}\right.\right.\\&\left.-\frac{y+a-b}{2(y+a)}\omega_1\right]\varphi-\left.\frac{(y+a-b)^2}{(y+a)^2}\varphi^2\right\}\frac{\partial}{\partial y}+\left(\left\{\frac{aby[a(y+a-b)-b(y+a)+4by]}{(y+a)^6}+\frac{ab(y+a)-4aby}{2(y+a)^4}\omega_1\right.\right.\\&\left.-\frac{aby}{2(y+a)^3}\omega_2\right\}+\left[\frac{ab(3.5y-a)(y+a-b)}{(y+a)^5}-\frac{by}{(y+a)}\omega_2'+\frac{2ab-a(y+a)}{(y+a)^3}\omega_1-\frac{1}{2}\omega_1\omega_1'\right]\varphi\\&+\left\{\frac{(y+a-2b)[a(y+a-b)-by]+a(y+a-b)^2}{(y+a)^4}-\frac{y+a-b}{2(y+a)^2}\omega_1+\frac{y+a-b}{2(y+a)}\omega_1'-\frac{y+a-b}{2}\omega_2'\right\}\varphi^2\\&\left.-\frac{(y+a-b)(y+a-2b)}{2(y+a)^3}\varphi^3\right)\frac{\partial}{\partial\varphi}.\end{aligned} \tag{B4}$$

Following the same procedure as in the determination of M_1 and S_1, we obtain

$$\begin{aligned}M_2=&\left[\frac{aby(y+a-b)}{(y+a)^4}-\frac{by}{y+a}\omega_1'+\frac{ab}{(y+a)^2}\omega_1\right]\frac{\partial}{\partial y}+\left[\frac{ab(3.5y-a)(y+a-b)}{(y+a)^5}-\frac{by}{(y+a)}\omega_2'\right.\\&\left.+\frac{2ab-a(y+a)}{(y+a)^3}\omega_1-\frac{1}{2}\omega_1\omega_1'\right]\varphi\frac{\partial}{\partial\varphi},\end{aligned} \tag{B5}$$

and

$$\begin{aligned}S_2=&\left\{\left[\frac{b^2y+a(y+a-b)(y+a-2b)}{(y+a)^4}+\frac{(y+a-b)(\omega_2-\omega_1')+\omega_1}{2(y+a)}-\frac{(y+a-b)}{2(y+a)^2}\omega_1\right]\varphi-\frac{(y+a-b)^2}{2(y+a)^3}\varphi^2\right\}\frac{\partial}{\partial y}\\&+\left(\left\{-\frac{aby[a(y+a-b)-b(y+a)+4by]}{(y+a)^7}-\frac{ab(y+a)-4aby}{2(y+a)^5}\omega_1+\frac{aby}{2(y+a)^4}\omega_2\right\}\right.\\&+\left[\frac{-by(y+a-3b)+2a(y+a-b)(y+a-2b)+a(y+a-b)^2}{(y+a)^5}-\frac{y+a-2b}{2(y+a)^3}\omega_1+\frac{y+a-b}{2(y+a)^2}\omega_2-\frac{y+a-b}{2(y+a)}\omega_2'\right]\varphi^2\\&\left.-\frac{(y+a-b)(y+a-1.5b)}{2(y+a)^4}\varphi^3\right)\frac{\partial}{\partial\varphi}.\end{aligned} \tag{B6}$$

Here, ω_i' denotes the derivative of ω_i with respect to y.

In order to give $M_2=0$ from Eq. (B5), we set

$$\frac{aby(y+a-b)}{(y+a)^4}-\frac{by}{y+a}\omega_1'+\frac{ab}{(y+a)^2}\omega_1=0 \tag{B7}$$

and

$$\frac{ab(3.5y-a)(y+a-b)}{(y+a)^5}-\frac{by}{(y+a)}\omega_2'+\frac{2ab-a(y+a)}{(y+a)^3}\omega_1-\frac{1}{2}\omega_1\omega_1'=0. \tag{B8}$$

Equation (B7) is equivalent to a first order linear differential equation

$$\omega_1'-\frac{a}{y(y+a)}\omega_1=\frac{a(y+a-b)}{(y+a)^3}. \tag{B9}$$

The general solution is

$$\omega_1(y)=\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}-\frac{by}{(y+a)^2}+c\frac{y}{y+a}, \tag{B10}$$

where c is an arbitrary constant. Taking $c=0$ gives a special solution

$$\omega_1(y)=\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}-\frac{by}{(y+a)^2}. \tag{B11}$$

Substituting $\omega_1(y)$ into Eq. (B8) and integrating gives

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$$\omega_2(y)=\frac{2.5ab}{(y+a)^3}-\frac{17a+3b}{8(y+a)^2}+\frac{-2a^2+ab+b^2}{4ab(y+a)}+\left[\frac{-2a^2+ab+b^2}{4a^2b}+\frac{(a-b)(2a^2-3ab+2ay+4by)}{4ab(y+a)^2}\right]\cdot\ln\frac{y}{y+a}+\frac{(-a+b)^2y}{2a^2b(y+a)}\left(\ln\frac{y}{y+a}\right)^2. \tag{B12}$$

For the chosen $\omega_i(y)$, we have

$$\tilde{M}_1=-\frac{by}{y+a}\frac{\partial}{\partial y}+\left[-\frac{(a+b)y+a(a-b)}{(y+a)^2}+\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\varphi\frac{\partial}{\partial\varphi}. \tag{B13}$$

If we approximate M by

$$M=A_0+\epsilon\tilde{M}_1, \tag{B14}$$

the corresponding differential equation system for M is the following:

$$\frac{dy}{d\tau}=-\epsilon\frac{by}{y+a}, \tag{B15}$$

$$\frac{d\varphi}{d\tau}=-\left\{(y+a)+\epsilon\left[\frac{(a+b)y+a(a-b)}{(y+a)^2}-\left(1-\frac{b}{a}\right)\frac{y}{y+a}\ln\frac{y}{y+a}\right]\right\}\varphi. \tag{B16}$$

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