Model Reduction in the Computational Modeling of Reaction Systems

Ronald G. Forsythe, Jr.[†]

Department of Engineering and Airway Science, University of Maryland Eastern Shore,
Princess Anne, Maryland 21853

Michael L. Mavrovouniotis*,[‡]

Chemical Engineering Department, Northwestern University, Evanston, Illinois 60208-3120

The underlying assumption for most lumping techniques is that the reduced models must be valid for the entire composition space. This is a harsh requirement that often limits the models that are generated. The scheme that is presented here uses the inherent structure of reaction systems to divide the composition space into regions. Within each region, the order-of-magnitude relationships that exist between terms in the rate equations are used to systematically reduce the order and coupling of the model. The full system is then described through piecewise combination of these simpler, region-specific models. Although these reduced models are based on assumptions that make them invalid globally, they are accurate within the regions for which they have been crafted.

INTRODUCTION

Model reduction of reaction systems has many applications in the study of chemical and biochemical systems. In order to completely model complex chemical reaction systems such as catalytic cracking, naphtha reforming, hydrosulfurination, and pyrolysis, it is necessary to generate the reactions and balance equations for hundreds or thousands of species. Current technology does not allow us to identify all of the species and reactions that are present in these systems, let alone monitor their concentrations through time. Even when the species and reactions are known, many of the parameters that describe the interactions of these complex reaction systems may not be well-defined. As a result, approximations for unknown parameters are used when generating simplified models for complex reaction systems. Since these reduced models are usually easier to understand than the full model, they provide insight into the dominant contributors in dynamic reaction systems. Furthermore, strategic use of reduced models can lead to more precise identification of system parameters. With these issues in mind, researchers have been seeking ways to algorithmically generate reduced order models for reactions systems.

The primary technique has been the identification of "lumped" models which combine compounds with similar behaviors into pseudo-species that track the overall behavior of the system.[1−3] Translation of the model into a smaller space results in a loss of physical and chemical information. Lumps that combine species based on similarities in physical properties lose detailed information about the physical properties and about the reaction rates of the species. Similarly, lumps that are based solely on reaction rates neglect information about the structures and physical properties of their components. As a result, current trends in lumping seek to manage both physical and chemical information of the system by defining classes of compounds, reactions, and structures.[4−6] These techniques provide more

accurate characterization of processes at the cost of using larger lumped models.

Another approach for reducing nonlinear models is based on a singular perturbation method using two time scales.[7−9] Van Breusegem and Bastin have developed an algorithm based on the assumption that a few reactions will dominate the system over the entire composition space (Figure 1).[8] Further analysis indicates that their lumped models are most accurate for the specific region of the composition space that corresponds to their basic assumptions.[10]

These efforts indicate that reduced models can be tailor-made to specific regions using information that is inherent in the structure of reaction systems. Within each region, the full model can be reduced through quasi-steady state analysis, singular perturbation analysis, and by identifying pools of materials that express similar reaction rates. These techniques lead to model reduction through replacement of some differential equations with algebraic relations and through reduction of the coupling of the system. In the worst case, a region will have to use the full model that has been specified for the composition space. The best model reduction occurs when the system can be assumed to be at steady state and the full model is described entirely by algebraic equations. Since species that are removed from the set of differential equations can still be determined through algebraic relations to those that remain, these techniques allow full or previously lumped models to be reduced without further information loss.

The following lumping scheme is applicable to proper, semiproper, and improper basis sets.[1] It shifts the emphasis of model reduction from describing the composition space with a single lumped model that is valid globally, to using piecewise combinations of simpler, region specific models.

REACTION SYSTEMS

The balance equations that are used to track the composition profile of a system of chemical compounds are shown in eq 1.

[†] email: ronjr@erika.umd.edu.
[‡] email: mlmavro@nwu.edu.

$$\Delta Mass_i = Mass_{in,i} - Mass_{out,i} +$$
$$Mass_{gen,i} - Mass_{con,i} \quad (1)$$

for each species i in the system. The total mass for the system is determined by summing the mass balances for all species in the system.

$$\Delta Mass = Mass_{in} - Mass_{out} \quad (2)$$

The generation and consumption terms of eq 1 can be condensed into a single set of reaction rate terms, $\sum \alpha_{ij} r_j$, such that each term r_j represents the rate of reaction j and α_{ij} represents the stoichiometric coefficient of species i in reaction j. The convention will be that r_j is positive when the reaction proceeds in the "forward" direction, and α_{ij} is positive for products, negative for reactants, and zero when a species does not occur in a reaction.

In this way, the full set of balance equations for a system of species is

$$\Delta Mass_i = Mass_{in,i} - Mass_{out,i} + \sum \alpha_{ij} r_j \quad (3)$$

which can be reduced to

$$\Delta Mass_i = \sum \alpha_{ij} r_j \quad (4)$$

for a closed system. Thus, while the rate equations may be nonlinear with respect to individual compositions, they are linear with respect to the rate terms that they comprise. In order to simplify the analysis of reaction systems, only closed systems will be considered from this point forward. The treatment of open systems can be handled by including terms corresponding to flow rates in the balance equations.

REGIONAL ANALYSIS

A region is defined by specifying a set of relations for the characteristic parameters of the reaction system (Figure 2). The constraints that are considered for lumping of species are based on relationships between the relative magnitudes of the rates of reactions in the system. Reaction rates are used to define the relations because they capture not only the trends in individual species concentrations but also the relevant species interactions within a system. With the exception of monomolecular reaction schemes, it is difficult to write generalized model reduction rules when using relations based solely on species concentrations.

Regions can be continuous or discontinuous and range in size from the empty set, for which there are no points that satisfy the constraints of the region, to the full composition space, in which all points satisfy the regional constraints. When regions overlap, a new region is created whose boundaries are determined from the intersection of the constraints for the overlapping regions. It is also possible to identify regions that do not intersect. These disjoint regions are necessarily specified by constraints that cannot be satisfied simultaneously (for example, rate₁ > rate₂ *and* rate₂ > rate₁). The region formed by the intersection of two or more disjoint regions is a null region. The full composition space is represented by the union of all regions that are specified for it.
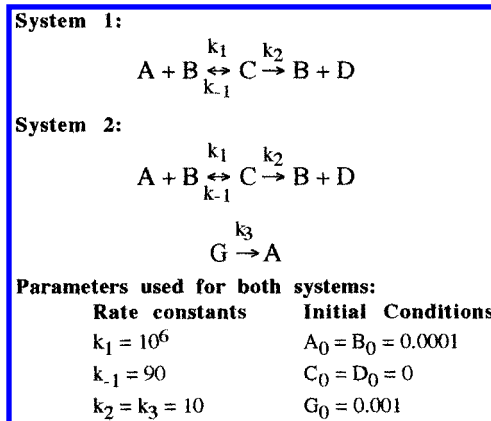
Figure 1. Enzymatic reaction systems used as examples. System 1 has been reduced by van Breusegem and Bastin. System 2 adds a reaction that feeds the original system.
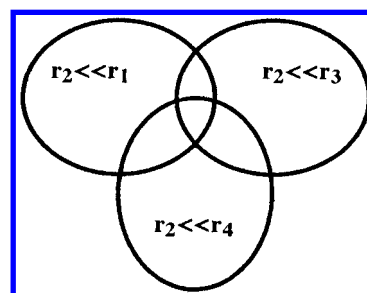
Figure 2. Specifying relationships between reaction rates is one way to decompose a composition space into regions.
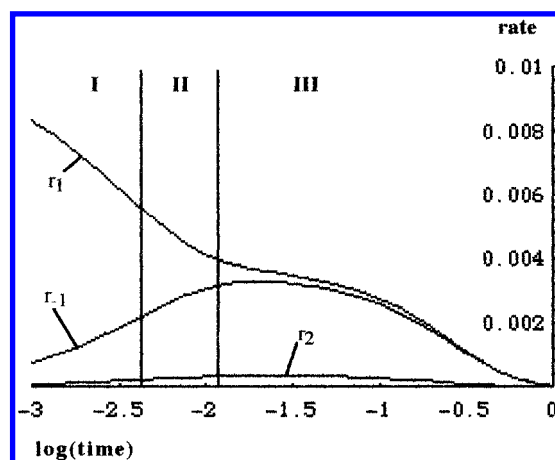
Figure 3. The relative magnitudes of reaction rates vary with time. The rates shown are for system 1 for the initial conditions described in Figure 1.

Using the constraints that define each region, it is possible to make assumptions that can be used to generate model reductions that will be valid for all composition profiles that fall within its constraints. A composition space can be divided into regions based on relationships between the relative magnitudes of the reaction rates of the system (Figure 3). The constraints of each region allow simplifying assumptions to be made that are used to reduce the global model for that region. These reduced models are used to track the system while it is in its specified region. Tracking a system through the full composition space is done by piecewise combination of the reduced models through each of the regions that the system passes. In the event that two or more regions intersect, the model reductions for this intersection are determined from the union of the constraints for those regions.

ORDER-OF-MAGNITUDE RELATIONSHIPS

The structure of mass action kinetics allows equations to be analyzed according to relationships between their individual terms. For a known composition profile, it is possible to sort the reaction rates in nonincreasing order and identify the dominant reaction rates in each species balance. Those species that do not participate in terms that are dominant contributors in the rate equations for any other species can be considered for removal from the model. In this way fast and slow characterizations of species are region-specific rather than global assignments. However, care must be taken to ensure that species that participate in reactions that proceed very slowly relative to others are not mistakenly labeled as unimportant and removed from the system. A term that is slow for one or more species in a region is not necessarily unimportant globally. Toxins, pollutants, and contaminants are often monitored at small levels even though they may not achieve substantial concentrations.

Since the species balance equations are linear with respect to reaction rates, regional constraints are defined according to relationships between terms rather than concentrations. As a result, the information used for model reductions is stored within the definitions of the regional boundaries.

It is possible to create a matrix **C** whose rows correspond to the species of the system and whose columns reflect the terms that are summed in each of the species rate equations. Element c_{ij} takes one of three values:

0 term r_j does not occur in the rate equation for species i

1 the coefficient of term r_j is positive

−1 the coefficient of term r_j is negative

The concept of *term* rather than *rate* is used in these definitions because some models (such as previously lumped or reduced models) do not correlate directly to a physical system but are still capable of being reduced by this algorithm. For example, some reduced models use terms that have negative values. This is not observed in mass action kinetics in which each term is the product of rate constants and species concentrations; all of which are positive values.

At any given time, each rate equation will be dominated by a few terms, and model reductions are realized by selective replacement of inconsequential nonzero elements in **C** and by substituting algebraic relations for differential equations whose dominant terms are balanced (Figure 4). These terms are easily calculated from the model and can be sorted in a nonincreasing order based on order-of-magnitude relationships between them using the following relationships:

$\gg$ **Much Greater Than.** One rate is much greater than the other. The latter rate can be ignored in the case of a regular perturbation. For example, specifying that $r_i \gg r_j$ indicates that term r_j can be removed whenever it occurs in an equation with r_i. $r_i \gg r_j$ when $r_i > \alpha_1 r_j$.

In the case of a singular perturbation, the importance of the smaller rate is enhanced by the canceling effects of the dominant terms. Two or more terms may be large but cancel the effects of one another because they have opposite signs.

$>$ **Greater Than.** The magnitude of one rate is noticeably larger than the other. The smaller rate makes a significant
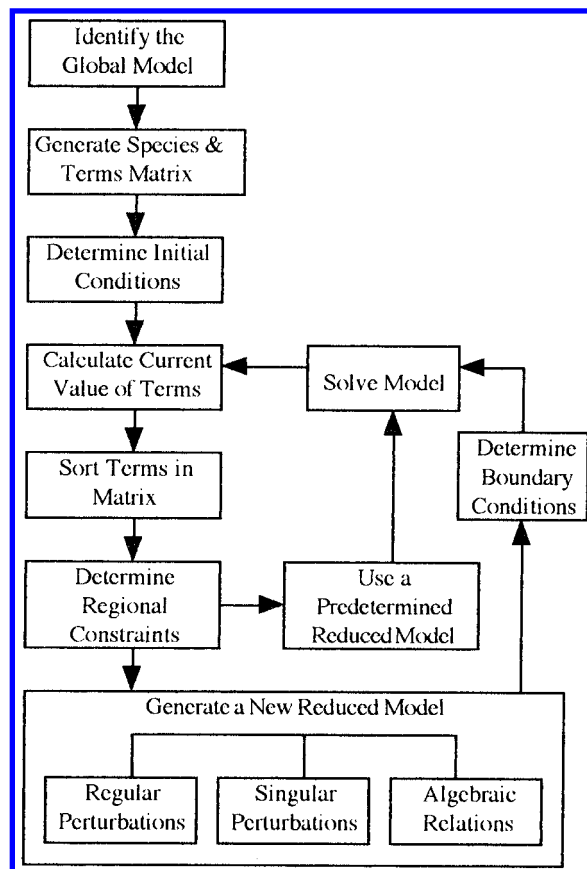

Figure 4. Procedures for implementing region-specific model reductions.

contribution to the rate equation but not enough to create a singular perturbation. The assumption $r_i > r_j$ can be made when $\alpha_1 r_j > r_i > \alpha_2 r_j$.

$\approx$ **Approximately Equal.** The magnitudes of the terms are approximately the same. $r_i \approx r_j$ when $r_i < \alpha_2 r_j$.

Although typical values for α_1 and α_2 are 10 and 4, respectively, these cutoffs are arbitrary and can be adjusted to improve the quality of the reduced models. As α_1 increases, it becomes more difficult for a term to be removed from the system. Similarly, decreasing α_2 makes it harder for two reactions to be considered to be at equilibrium. These actions lead to reduced models that are more similar to the full model.

REGIONAL REDUCTIONS

The full composition space can be divided into distinct regions based on relationships between the orders-of-magnitudes of the terms. Defining the regions in this way provides reduced models that are valid for specific regions of the composition space and as long as the system satisfies the regional constraints.

Another advantage is that the regional boundaries are not determined by the individual species, but by the terms of the equations which may be nonlinear with respect to concentrations, but are linear with respect to the individual terms.

Modeling the full system is accomplished through piecewise combination of reduced models as the system passes from region to region (Figure 5). In the event that species are deemed negligible in a region, the species concentrations

MODEL REDUCTION OF REACTION SYSTEMS

J. Chem. Inf. Comput. Sci., Vol. 37, No. 2, 1997 **261**
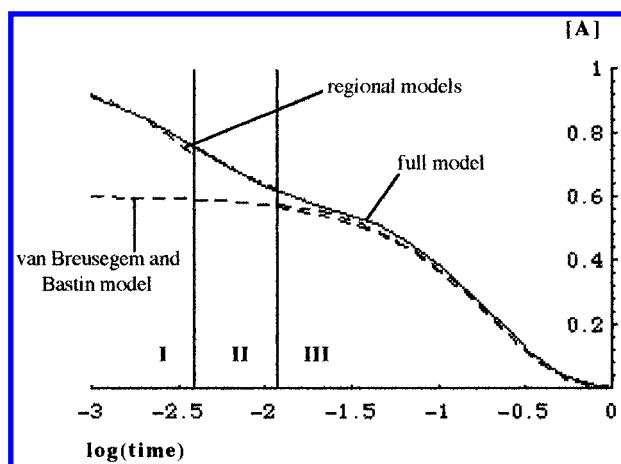
Figure 5. Comparison of full model to regional results and to the reduced model predicted by van Breusegem and Bastin for system 1.
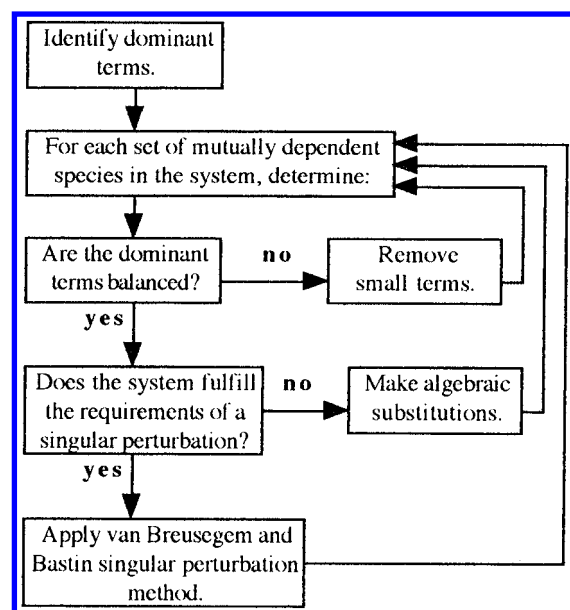
Figure 6. Algorithm for generating reduced models by reducing the coupling and order of models.

will have to be reconciled with a real process when moving into a region in which they are again included in the model.

Reduced models are determined by matching a current composition profile to the constraints of a region for which a reduced model has already been generated or by generating an entirely new reduced model from the full model using the following procedures (Figure 6).

1. Identify Insignificant Terms. Van Breusegem and Bastin use two time scales to provide *global* definitions for fast and slow species and reactions.[8] This is acceptable for smaller systems; however, complex reaction systems require more flexibility and benefit from slow and fast term definitions that are specific to individual rate equations. A term that is inconsequential for one species may be a dominant term in another rate equation and set standards to which even slower terms will be compared. When a similar situation is encountered by the van Breusegem and Bastin algorithm, the small terms in the rate equation for slower species are not removed.

When the dominant terms in an equation are unbalanced, it is possible to identify inconsequential terms in each row in **C** by comparing them to the term with the largest

magnitude. At the completion of this step, all elements in **C** that correspond to inconsequential terms in each regular perturbation are replaced by zeros. In this way fast and slow term classification is dependent on the species balances in which they are found. A term that is slow in one equation may be identified as fast or dominant in the equation for another species. The case in which the dominant terms are balanced is considered in the singular perturbation discussion that follows.

2. Identify the Singular Perturbations and Algebraic Reductions. When the dominant terms in a rate equation are balanced, the differential equations for some species can be replaced by algebraic equations that relate them to other species in the system. Care must be used when implementing the van Breusegem and Bastin technique. The nature of their singular perturbation results is such that they provide useful model reductions for reverse reactions that are at quasi-steady-state. Furthermore, these singular perturbation reductions require that reactions feeding the system will be zero and that those draining the reactants will be slow compared to the fast reactions at equilibrium. In order for the van Breusegem and Bastin technique to be useful, all species in a chain of equilibrium reactions must meet the requirements that they are balanced and dominant reactions for all species balances in which they are involved. When this occurs, the van Breusegem and Bastin technique will provide a useful reduced model for the system.

The cases for which the dominant terms in the rate equations are balanced and the van Breusegem and Bastin technique is not beneficial are handled by using a quasi-steady-state assumption. Species in chains of reactions can be reduced by replacing the differential equations with algebraic relations that relate the species to others in the system based on a quasi-steady-state assumptions. These algebraic substitutions allow regional reductions to be made for sequential reactions that occur in chains or pathways as well as reactions at equilibrium that do not meet the conditions for a van Breusegem and Bastin reduction.

It is also possible to identify species or pools of species that are at quasi-steady-state. The differential equations that represent the mass balances for these species can be replaced by algebraic equations that relate their concentrations to other species in the system. In complex reaction systems, many intermediates will quickly reach quasi-steady-state. Although a set of quasi-steady-state assumptions may not be valid for the entire composition space, each one is valid for a specific region. Regional analysis allows each assumption to be used as it is encountered.

The model reductions that result from singular perturbations do not result in a loss of information in the system. All species that are removed from the set of differential equations can be determined through algebraic relations to remaining species.

3. Identify Insignificant Reactions. After all of the insignificant terms have been removed from the set of modeling equations, some terms may no longer participate in any species balances. These zero columns can be removed from **C**. Furthermore, when all terms that a reaction is involved no longer play dominant roles in any species balance, the reaction can be removed from further consideration in this region.

4. Identify Insignificant Species. After all insignificant reactions are removed, some species will no longer be

participants in the remaining reactions and terms. Before species are eliminated, it is important to distinguish between species that must be tracked (terminal products, toxins, pollutants, etc.) and those that can be eliminated from the set of modeling equations. It is generally a good idea to avoid using this step when reducing proper lumping schemes because it may be difficult to distinguish between species that can be ignored and those that are required. This step is very useful when analyzing the improperly lumped systems that are achieved through Li and Rabitz[3] model reductions. Many of the generated vectors in a Li and Rabitz reduced model are linearly independent and usually do not correlate directly to objects in the physical space.[3]

After the reduced model is solved, the values that are obtained can be reintroduced to step 2. A system is modeled by tracking it from region to region where each region is described by a specific reduced model. Since the regions can use different basis sets of pseudo-species, the boundary conditions must be rectified by sampling the system as the model passes from one region to the next.

The regions that a model encounters depend on the initial conditions and the internal structure of the reaction system. For example, if $r_1 = k_1 C$, $r_2 = k_2 C$, and $k_1 \gg k_2$, then the only allowable regional constraint relating r_1 and r_2 will be $r_1 \gg r_2$. Similar relationships that exist between terms help to remove many regions from consideration.

Example: An Enzymatic Reaction. Reaction system 2 that is described in Figure 1 is used as an example. This system adds a reaction to the example studied by van Breusegem and Bastin and extends the time required for their singular perturbation model to become valid.

Step 1: Identify the Global Model. This system is assumed to follow mass action kinetics so that the species balances for this reaction system are as follows:

$$\frac{d[A]}{dt} = k_3 G - k_1 AB + k_{-1} C = r_3 - r_1 + r_{-1}$$

$$\frac{d[B]}{dt} = -k_1 AB + k_{-1} C + k_2 C = -r_1 + r_{-1} + r_2$$

$$\frac{d[C]}{dt} = k_1 AB - k_{-1} C - k_2 C = r_1 - r_{-1} - r_2$$

$$\frac{d[D]}{dt} = k_2 C = r_2$$

$$\frac{d[G]}{dt} = -k_3 G = -r_3 \tag{5}$$

The relative magnitudes of the rates are illustrated in Figure 7. The remaining steps discuss the generation of reduced models for the four regions through which the system passes.

Step 2: Sort Terms and Generate Relations. The constraints that follow are indicative of the four significant regions. All of the acceptable relations have not been listed because each region change only affects some of the equations. A region change based on two terms that do not both occur in a species balance has no affect on its rate equation. Similarly, a rate equation is only affected when a region change correlates with its terms. For example, the same reduced model is used for species G in all regions. Its concentration is independent of other species, and its reduced
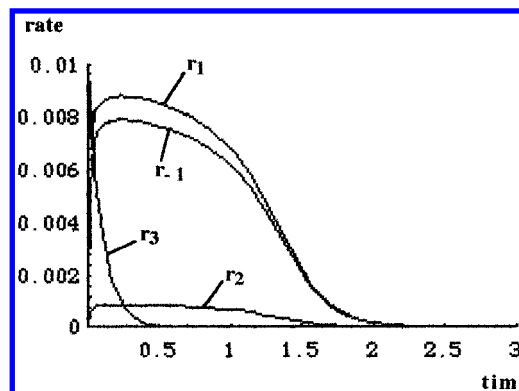
Figure 7. Comparison of reaction rates for system 2 based on the initial conditions listed in Figure 1.

model is always identical to the full model.

$$\textbf{Region I: } \{r_3 \gg r_{-1}, r_1 \gg r_{-1}, r_3 \gg r_2, r_1 \gg r_2\}$$

$$\textbf{Region II: } \{r_1 > r_{-1}, r_1 \gg r_2\}$$

$$\textbf{Region III: } \{r_1 > r_{-1}, r_1 \gg r_2, r_1 \gg r_3\}$$

$$\textbf{Region IV: } \{r_1 \approx r_{-1}, r_1 \gg r_2, r_1 \gg r_3, r_{-1} \gg$$
$$r_2, r_{-1} \gg r_3\}$$

Step 3: Generate Model Reductions. Region I. After removing the inconsequential terms from the full model, the following set of rate equations were obtained:

$$\frac{d[A]}{dt} = r_3 - r_1$$

$$\frac{d[B]}{dt} = -r_1$$

$$\frac{d[C]}{dt} = r_1$$

$$\frac{d[D]}{dt} = r_2$$

$$\frac{d[G]}{dt} = -r_3 \tag{6}$$

Region II. Removing the small terms from the full model yields that following set of equations:

$$\frac{d[A]}{dt} = r_3 - r_1 + r_{-1}$$

$$\frac{d[B]}{dt} = -r_1 + r_{-1}$$

$$\frac{d[C]}{dt} = r_1 - r_{-1}$$

$$\frac{d[D]}{dt} = r_2$$

$$\frac{d[G]}{dt} = -r_3 \tag{7}$$

Region I is actually a subset of region II. The constraints of the former are much more specific than those of the latter. As a result, region I is actually described with more accuracy by the reduced model that is specified for region II. However, since region I is more specific, more information can be extracted from its constraints in order to produce a simpler model.

Region III. This region has terms balanced, but the **G** still provides enough influence to prevent the singular perturbation model from being applicable.

$$\frac{d[\mathbf{A}]}{dt} = -r_1 + r_{-1}$$

$$\frac{d[\mathbf{B}]}{dt} = -r_1 + r_{-1}$$

$$\frac{d[\mathbf{C}]}{dt} = r_1 - r_{-1}$$

$$\frac{d[\mathbf{D}]}{dt} = r_2$$

$$\frac{d[\mathbf{G}]}{dt} = -r_3 \qquad (8)$$

Region IV. The equation set is identical to those that were found for region III. The difference is that the concentration of **G** can be assumed to be zero and the van Breusegem and Bastin technique can be applied to obtain the following model:

$$[\mathbf{A}] = \frac{k_2\mathbf{C}}{k_1\mathbf{B}}$$

$$\frac{d[\mathbf{B}]}{dt} = \frac{k_1 k_2 \mathbf{B}^2 \mathbf{C}}{[k_1\mathbf{B}^2 + k_2(\mathbf{B} + \mathbf{C})]}$$

$$\frac{d[\mathbf{C}]}{dt} = -\frac{k_1 k_2 \mathbf{B}^2 \mathbf{C}}{[k_1\mathbf{B}^2 + k_2(\mathbf{B} + \mathbf{C})]}$$

$$\frac{d[\mathbf{D}]}{dt} = r_2$$

$$\frac{d[\mathbf{G}]}{dt} = -r_3 \qquad (9)$$

Step 4: Solve the Reduced Model for the Next Time Step. The composition profile of the system is tracked through piecewise combinations of its reduced models (Figure 8).

Since the time required to reach the region in which a singular perturbation model is valid varies, it is beneficial to use regional analysis techniques to generate reduced models for the preceding regions. It is also possible to achieve further model reduction by specifying algebraic relations between species with similar rate equations. This allows the order of the system to be reduced by at least one in all regions, and, in region IV, the order is reduced by two. The model reductions that have been illustrated here allow complete characterization of all species that have been
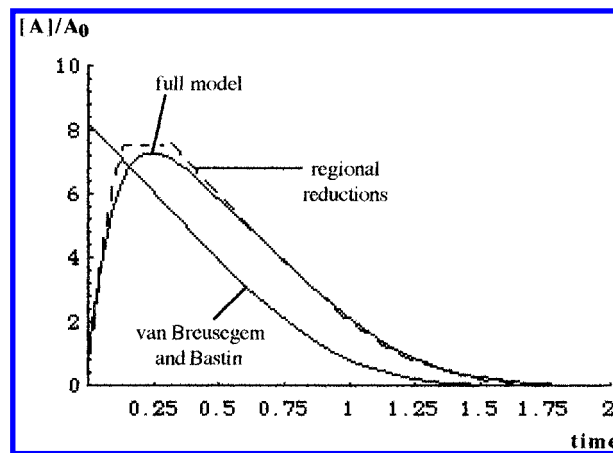
Figure 8. Predicted concentration for species **A**. The van Breusegem and Bastin model assumes that the concentration of G is zero globally. This causes the model to be shifted to time zero. Regional analysis effectively captures the kinetics that occur before this assumption becomes valid.

removed from the differential equation set through the use of algebraic relationships.

Figure 8 provides a comparison of the reduced models obtained through regional analysis to those obtained by using the method described by van Breusegem and Bastin for species A. The reduced model obtained by applying the van Breusegem and Bastin method is valid when the concentration of species *G* can be approximated to be zero. This technique ignores all kinetics that occur in the system before this is true and shifts the reduced model to time zero. Regional analysis captures the kinetics that occur in the system before this reduced model becomes valid so that the van Breusegem and Bastin model will be applied at the appropriate time.

CONCLUSION

A methodology has been provided for finding region-specific reduced models of a composition space. A composition space is divided into regions based on relationships between the orders-of-magnitudes of terms in the modeling equations. Since the assumptions used to reduce a full model are inferred directly from the constraints that define region boundaries, each reduced model will be valid for a specific region. Furthermore, since the regional boundaries are based on the magnitudes of terms, they are easily linked to the physical system, and a reduced model remains valid as long as the composition profile of the physical system falls within the specified boundaries. Reduced models can be derived directly and systematically from the full model based on information gained from the composition profile of the physical system.

The benefits of region specific reduced models include providing desired accuracy for the regions they are intended to model; being less coupled and having smaller orders than the original models from which they are derived; emphasizing important contributions of species and reactions in each of the regions; maintaining the connection to the initial physically meaningful models; and the potential for automatic generation from the structures of the full model and the composition profiles of a system.

Using regional analysis also enhances the performance of existing model reduction techniques. Region-specific models

eliminate time shifts that limit the application of van Breusegem and Bastin models. The reduced models that are produced by the Li and Rabitz techniques[3] are often fully coupled, improper lumpings that characterize a limited (but specific) scope of the physical system. Dividing the composition space into regions allows further reductions in order and coupling, while maintaining the level of accuracy and the relationship to the physical system.

Since each of the reduced models inherently focuses on the parameters that are important in a region, the procedure can be adapted to facilitate the estimation of parameters from raw data. Insight into the relationship between the terms within a model allows the focus to be placed on finding values for those parameters that make significant contributions in a region. As a result of smaller order and less coupling, the simplified models require fewer parameters to be fit to experimental data.

REFERENCES AND NOTES

(1) Wei, J.; Kuo, J. C. W. A Lumping Analysis in Monomolecular Reaction Systems: Analysis of the Exactly Lumpable System. *I&EC Fundamentals* **1969**, *8*, (1), 114−123.

(2) Coxson, P. G.; Bischoff, K. B. Lumping Strategy. 1. Introductory Techniques and Applications of Cluster Analysis. *Ind. Eng. Chem.* **1987**, *26*, 1239−1248.

(3) Li, G.; Rabitz, H. Determination of Constrained Lumping Schemes for Nonisothermal First-order Reaction Systems. *Chem. Eng. Sci.* **1991**, *46*, 583−596.

(4) Boock, L. T.; Klein, M. T. Lumping Strategy for Modeling the Oxidation of C1-C3 Alcohols and Acetic Acid in High-Temperature Water. *Ind. Eng. Chem. Res.* **1993**, *32*, 2464−2473.

(5) Liguras, D. K.; Allen, D. T. Comparison of Lumped and Molecular Modeling of Hydropyrolysis. *Ind. Eng. Chem.* **1992**, *31*, 45−53.

(6) Quann, R. J.; Jaffe, S. B. Structure-Oriented Lumping: Describing the Chemistry of Complex Hydrocarbon Mixtures. *Ind. Eng. Chem. Res.* **1992**, *31*, 2483−2497.

(7) Martinez, E. C. Lumping of Components and Reactions in Complex Reaction Networks. *Chem. Eng. Comm.* **1990**, *43*, 1−24.

(8) van Breusegem, V.; Bastin, G. Reduced Order Mathematical Modeling of Reaction Systems: A Singular Perturbation Approach (full version). Technical report, Laboratoire d'Automatique, Dynamique et Analyse des Systémes, University of Louvain, 1991.

(9) Kokotovic, P. V.; Khalil, H. K.; O'Reilly, J. Singular Perturbation Methods in Control: Analysis and Design; Academic Press: London, 1986.

(10) Forsythe, R. G.; Mavrovouniotis, M. L. An Object Oriented Package for Chemical Reactor Design and Analysis; 1995 Annual Conference Proceedings, American Association for Engineering Education, ASEE, Washington, DC, June 1995; pp 1771−1774.

CI950184E