Kinetic Analysis of Food Systems

Alejandro G. Marangoni

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Alejandro G. Marangoni
Department of Food Science
University of Guelph
Guelph
Ontario
Canada

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Dedicated to my colleagues who remind me that the scientific endeavor is a privilege and an honor.

Introduction: Trials and Tribulations in the Study of Complex, Multicomponent, Multiphasic, Nonequilibrium Systems

> The computer model is to the mind what the telescope and microscope are to the eye. (Heinz Pagels)

Food systems encompass anything from whole organisms and living tissue to nanostructured soft materials: potatoes to cheese. One characteristic all these systems share is complexity. All food materials are multicomponent, multiphasic, and mostly nonequilibrium systems, while living matter is ephemeral. It is thus very difficult to use a thermodynamic approach to predict system behavior. However, at the same time, this makes food systems amenable to kinetic analysis, where researchers try to catch a fleeting glimpse at the dynamics of living processes, structure formation, structure breakdown, state transformations, and the energetics involved in these processes. At the end of the exercise, we talk about free energies of activation, partition functions, orders of processes, and rate constants instead of free energy, enthalpy, and entropy of standard states.

The complexity of a food system might discourage some; however, many of these complex systems are amenable to "coarse-graining," which means that structural or functional averages of ensembles of molecules, higher-order structural units, or entire metabolic pathways can be used to model whole system behavior – a mean field approach. Engineers have known this for a while and carry out phenomenological finite-element and finite-difference analysis; however, there are many approaches available, limited only to the imagination and skill of the researcher. Here is where art meets science, where creativity is key. How do we succeed in describing the behavior of a complex system?

Should we use a deterministic or a stochastic approach? Deterministic processes (cause-effect) follow an exact mathematical rule, while in stochastic processes, the time evolution of a system is represented by a variable whose change is subject to random variation. Deterministic modeling utilizes the tools of differential equations, assuming that the time evolution of a system can be modeled exactly. According to Laplace, "The state of the world at a given instant is defined by an infinite number of parameters, subject to an infinite number of differential equations. If some 'universal' mind could write down all these equations and integrate

them, it could then predict with complete exactness the entire evolution of the world in the infinite future." Features common to all deterministic mathematical formulations include that the system is completely defined by mathematical entity ω (can be a set of real numbers, one or more functions, etc.) and that values of ω in the future $t > t_o$ are uniquely determined by ω_o, the initial state of ω, namely, $\omega = F(t_o,\omega_o,t)$. For phenomena described by differential equations, the process of finding their solution involves the integration of these differential equations with the initial conditions $\omega = \omega_o$ and $t = t_o$. Such formulations are exact and direct expressions of the deterministic character of the actual phenomena, of the physical principle of causation. However, this quantitative infinity is coarse compared to the qualitatively inexhaustible character of the real world, and this approach sometimes does not adequately represent the infinite complexity of actual events.

Stochastic modeling, on the other hand, uses probabilities to analyze the time evolution of a system. A Markov chain is probably the most famous example of stochastic modeling, aside from random walks. In a time-discrete Markov process, the probability of each event depends only on the state attained in the previous event in time. Interestingly, most deterministic modeling deals with nonlinear functions, while probabilistic modeling relies on first- and higher-order polynomial functions. This is a consequence of the mathematics used in either approach. Is the world nonlinear and deterministic or linear and probabilistic?

Regardless of the approach, the art of an investigation consists in finding a very simple space Ω (i.e., a set of values of ω or different possible states of the system) such that if we replace the actual process by varying the point ω in a determinate way over this space, we can include all the *essential* aspects of the actual process. In the words of *J.W. Gibbs*, "One of the principal objects of theoretical research in any department of knowledge is to find the point of view from which the subject appears in its greatest simplicity."

At this point, we should discuss other considerations in the modeling process. Are we going to adopt a reductionist view or a wholistic view of the system? A reductionist approach would attempt to describe the behavior of a system from the behavior of the smallest structural unit in that system. In this bottom-up approach, whole system behavior can be predicted from the behavior of ensembles of the smallest structural units. A wholistic approach would seek to describe the behavior of the whole system as a unit, separate from its individual building blocks. In this top-down approach, correlations would be established between macroscopic behavior and particular length scales in a system in an attempt to correlate function to biological or physical structure and their interactions. The approach could also be mechanistic or phenomenological in nature. Mechanistic approaches are based on theory that describes the physical and chemical behavior of a system. A phenomenological approach just utilizes a convenient function which describes system behavior without addressing the reason for that behavior. Finally, I would like to mention the difference between interpolation and extrapolation. A simple phenomenological modeling exercise such as obtaining a least squares estimate of a straight line by linear regression generates a function which can only predict unknown values within the bounds of the data set. It should never be used outside these limits.

This is interpolation. A more sophisticated mechanistic modeling exercise should be able to predict unknown states of the system beyond the data set used to create such model. This is true prediction and constitutes extrapolation from the experimental data set.

In my experience, the modeling process of a complex system involves the following necessary steps for maximum impact:

1. *Write down all the variables that you believe affect the behavior of your system.*
2. *Design the experiment properly, with particular attention to replication. The experiment has to have at least three determinations of three replicates. They are not the same thing!*
3. *Try to control or monitor as many variables as possible during experiments.*
4. *Carry out proper statistical analysis. Any proposed effects or trends need to be statistically significant at least at the 5% level. Determine which variables significantly affect the system and which ones do not;* i.e.*, is the variability attributed to a treatment greater than the one attributed to random experimental error?*
5. *Model the system's behavior using a mechanistic or phenomenological model and test its validity.*
6. *Attribute mechanistic significance to the parameters derived from the model.*

Any discussion about modeling eventually digresses into the realm of the philosophy of carrying out research. Research is the systematic search for new knowledge, while scientific research takes place when research involves a testing step of carefully formulated ideas. Types of research include (a) fact finding, information gathering not intended to derive generalizations or solve problems; (b) critical interpretation, arriving at conclusions through logical reasoning (critical reviews), which is not scientific research; and (c) complete research, solving problems and arriving at generalizations after a thorough search for existent pertinent facts, analysis and logical classification of these facts, and development of a reasonable case using inductive reasoning. The scientific method is a form of complete research plus the development of a hypothesis and controlled experimentation. An essential element of the scientific method includes model building, which has to do with the creation of a hypothesis. Models are central to the scientific method and complete research. Models allow us to explain and create understanding and maybe even predict behavior. These days there is way too much information and not enough knowledge created in research. Moreover, nobody has time to look back and possibly accumulate wisdom (and share it) gathered from new and old knowledge.

This book takes a "stream of consciousness" approach to the subject and is not meant to be exhaustive by any stretch of the imagination. Section 1 is an introduction to the topic of kinetic analysis assuming no prior knowledge of the subject. Section 2 includes nine examples of kinetic modeling that illustrate many techniques and approaches to problems such as color loss, oil migration, biodiesel manufacture, crystallization, nucleation, and protein aggregation. The examples

provide a practical handle on how to carry out kinetic analysis, while each chapter is designed to cover a major mathematical technique such as Fourier series analysis and solutions to coupled ordinary differential equations. Examples include both phenomenological and mechanistic modeling. The book is also meant to be a standard reference in the use of the specific models presented for research. The student of modeling should always remember that a model is "entertained" since it is just an attempt to catch a glimpse at the workings of nature. Experimental evidence must always be gathered, which will support or not support the model in the long term. A model is a sophisticated hypothesis.

I finish this brief introduction with two of my favorite quotations which are very relevant to modeling and scientific research, one by a famous scientist and one by a famous wilderness adventurer:

> If nature were not beautiful it would not be worth knowing, and if nature were not worth knowing life would not be worth living. (Henri Poincare)

> Only those who have had the experience can know what a sense of physical and spiritual excitement comes to one who turns his face away from men and towards the unknown. (Bill Mason)

Alejandro G. Marangoni
Guelph, ON, Canada
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Contents

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