Lectures on Chemical Reaction Networks

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Contents

This lecture is divided into two parts. In the first part I shall try
to provide some motivation for everything that follows. In particular,
I shall try to explain, at least in an informal way, how chemists and
chemical engineers arrive at the differential equations they work with and
how these differential equations are tied to reaction network structure.
Once this is done we can begin to understand why a reasonably general theory
of chemical reaction networks is necessary. Moreover, we can begin to
understand why, despite the great complexity of the differential equations
involved, such a theory should even be possible in principle. In the
second part of this lecture I shall discuss the important but more mundane
subject of notation.

1.A. Motivation

These lectures will be about a special but rather large class of
ordinary differential equations — those that derive from chemical reaction
networks. In order that I might provide some sense of how these equations
come about it will be useful if I write down an example of a reaction net-
work and indicate informally how it induces a system of ordinary differential
equations. Then I can discuss the kinds of problems we will want to
consider.

Suppose that A, B, C, D and E are chemical species, and suppose I
believe that the chemical reactions occurring among these species are
reasonably well reflected in the following diagram:

$$
\begin{array}{c}
A \rightleftharpoons 2B \\
A + C \rightleftharpoons D \\
\nwarrow \quad \swarrow \\
B + E
\end{array}
\tag{1.1}
$$

What I have written down is a diagram of a chemical reaction network. It indicates that a molecule of A can decompose into two molecules of B, that two molecules of B can react to form one molecule of A, that a molecule of A can react with a molecule of C to form a molecule of D, and so on.

Now suppose that I throw various amounts of my species into a pot. I am going to presume that the pot is stirred constantly so that its contents remain spatially homogeneous for all time, and I shall also suppose that the contents of the pot are forever maintained at fixed temperature and total volume. This, of course, is not to say that the chemical composition of the mixture within the pot will remain constant in time, for the occurrence of chemical reactions will serve to consume certain species and generate others. In fact it is the temporal evolution of the composition that we wish to investigate. With this in mind we denote the (instantaneous) values of the molar concentrations of the species by $c_A(t)$, $c_B(t)$, $c_C(t)$, $c_D(t)$ and $c_E(t)$, and we abbreviate this list of numbers by the "composition vector" $c(t)$.[*] Thus the picture we are thinking about, at least for the moment, looks something like that shown in Figure 1.1.[†]

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[*] A molar concentration, say c_A, specifies the number of A molecules per unit volume of mixture. More precisely, c_A is the number of A molecules per unit volume divided by Avogardro's number, 6.023×10^{23}. We shall be somewhat more precise about what we mean by the "composition vector" in Section 1.B.

[†] The reactor depicted in Figure 1.1 is closed with respect to the exchange of matter with its environment. Our focus on such reactors is temporary and is merely intended to illustrate in a simple context how chemists and engineers formulate differential equations based upon a set of reactions believed to approximate the true chemistry. We will begin to consider "open" reactors in the next lecture (Section 2.E). There we shall indicate how open reactors can be modelled in terms of reaction networks and how the appropriate differential equations, like those for closed reactors, bear a definite relationship to reaction network structure.
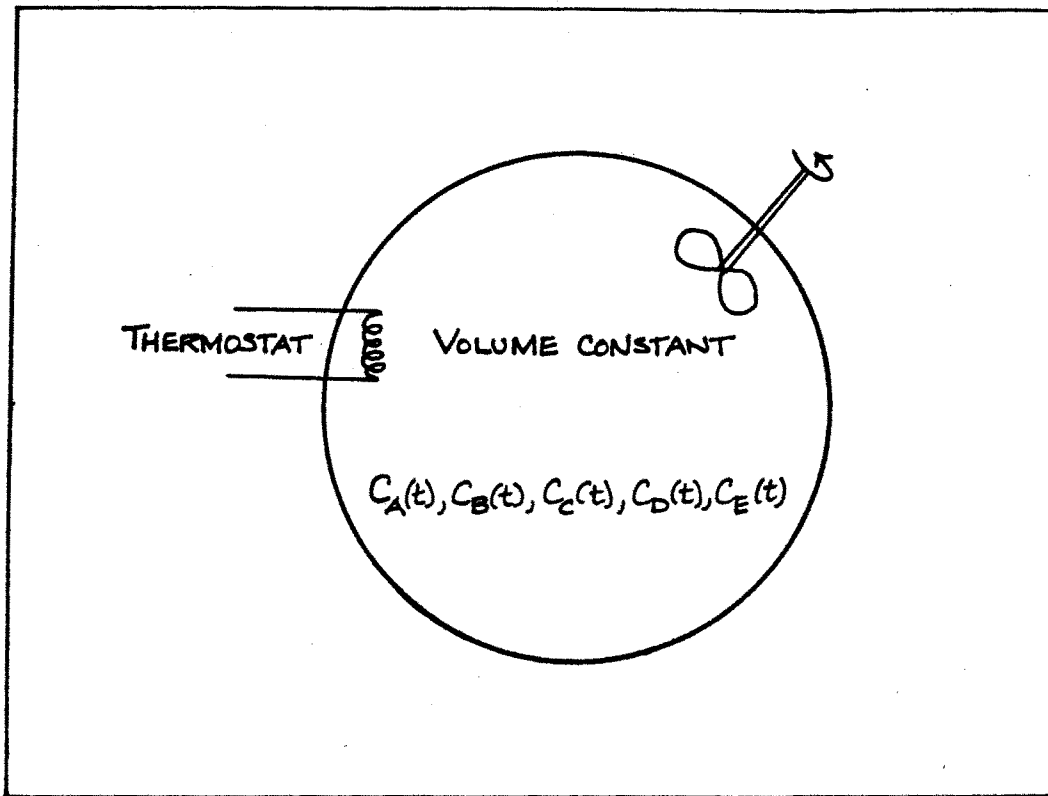
Figure 1.1

We would like to write down differential equations that describe the evolution of the five molar concentrations. Since chemical reactions are the source of composition changes, the key to understanding how to write down differential equations lies in knowing how rapidly each of the several reactions occurs. What is generally assumed is that the instantaneous occurrence rate of each reaction depends in its own way on the instantaneous mixture composition vector, c. Thus, we presume, for example, the existence of a non-negative real-valued rate function $\mathcal{K}_{A \to 2B}(\cdot)$ such that $\mathcal{K}_{A \to 2B}(c)$ is the instantaneous occurrence rate of reaction $A \to 2B$ (per unit volume of mixture) when the instantaneous mixture composition is given by the

vector c.[**] Similarly, we presume the existence of a rate function $\mathcal{K}_{2B \to A}(\cdot)$ for the reaction $2B \to A$, a rate function $\mathcal{K}_{A+C \to D}(\cdot)$ for the reaction $A+C \to D$, and so on. A <u>kinetics</u> for a reaction network is an assignment of a rate function to each reaction in the network.

Once we presume that network (1.1) is endowed with a kinetics we are in a position to write down the system of differential equations that govern our reactor. Suppose that, at some instant, the reactor is in some composition state c. Let us begin by thinking about the instantaneous rate of change of c_A. Every time the reaction $A \to 2B$ occurs we <u>lose</u> a molecule of A, and that reaction has an occurrence rate $\mathcal{K}_{A \to 2B}(c)$. On the other hand, every time the reaction $2B \to A$ occurs we <u>gain</u> a molecule of A, and that reaction occurs at rate $\mathcal{K}_{2B \to A}(c)$. Similarly, the reactions $B+E \to A+C$ and $D \to A+C$ produce a molecule of A with each occurrence, while each occurrence of the reaction $A+C \to D$ results in the loss of a molecule of A. Thus we write

$$\dot{c}_A = -\mathcal{K}_{A \to 2B}(c) + \mathcal{K}_{2B \to A}(c) - \mathcal{K}_{A+C \to D}(c) + \mathcal{K}_{D \to A+C}(c) + \mathcal{K}_{B+E \to A+C}(c). \quad (1.2)$$

If we turn our attention to species B we notice that whenever the reaction $A \to 2B$ occurs we gain <u>two</u> molecules of B, and whenever $2B \to A$ occurs we lose <u>two</u> molecules of B. When $D \to B+E$ occurs we gain <u>one</u> B, and when $B+E \to A+C$ occurs we lose <u>one</u> B. Thus, we write

$$\dot{c}_B = 2\mathcal{K}_{A \to 2B}(c) - 2\mathcal{K}_{2B \to A}(c) + \mathcal{K}_{D \to B+E}(c) - \mathcal{K}_{B+E \to A+C}(c) \quad (1.3)$$

Continuing in this way we can write down equations for $\dot{c}_C$, $\dot{c}_D$, $\dot{c}_E$ to generate the full system of differential equations that govern our reactor:

[**] More precisely, $\mathcal{K}_{A \to 2B}(c)$ is the number of occurrences of $A \to 2B$ per unit time per unit volume divided by Avogadro's number.

$$\dot{c}_A = -\mathcal{K}_{A\to 2B}(c) + \mathcal{K}_{2B\to A}(c) - \mathcal{K}_{A+C\to D}(c) + \mathcal{K}_{D\to A+C}(c) + \mathcal{K}_{B+E\to A+C}(c)$$

$$\dot{c}_B = 2\mathcal{K}_{A\to 2B}(c) - 2\mathcal{K}_{2B\to A}(c) + \mathcal{K}_{D\to B+E}(c) - \mathcal{K}_{B+E\to A+C}(c)$$

$$\dot{c}_C = -\mathcal{K}_{A+C\to D}(c) + \mathcal{K}_{D\to A+C}(c) + \mathcal{K}_{B+E\to A+C}(c) \qquad (1.4)$$

$$\dot{c}_D = \mathcal{K}_{A+C\to D}(c) - \mathcal{K}_{D\to A+C}(c) - \mathcal{K}_{D\to B+E}(c)$$

$$\dot{c}_E = \mathcal{K}_{D\to B+E}(c) - \mathcal{K}_{B+E\to A+C}(c) .$$

Thus far we haven't said anything about the nature of rate functions, and that is what we shall do now. More often than not chemists and engineers presume the kinetics to be of <u>mass action</u> type. With mass action kinetics one can merely look at a reaction and write down its rate function up to a multiplicative positive constant.

Here is the way things work: For the reaction $A \to 2B$ we presume that the more A there is in the reactor the more occurrences of the reaction there will be. In fact, we presume that the instantaneous occurrence rate of $A \to 2B$ is proportional to the instantaneous value of c_A . Thus, we write

$$\mathcal{K}_{A \to 2B}(c) = \alpha c_A ,$$

where α is a positive constant.

For the reaction $A+C \to D$ the situation is a little different. An occurrence requires that a molecule of A meet a molecule of C in the reactor, and we take the probability of such an encounter to be proportional to the product $c_A c_C$. Although we do not presume that every such encounter yields a molecule of D, we nevertheless take the occurrence rate of $A+C \to D$ to be given by

$$\mathcal{K}_{A+C \to D}(c) = \gamma c_A c_C ,$$

where γ is a positive constant. Similarly, an occurrence of the reaction $2B \to A$ requires that two molecules of B have an encounter, and we take

$$\mathcal{K}_{2B \to A}(c) = \beta (c_B)^2,$$

where β is a positive constant.

Thus, with mass action kinetics the rate functions for network (1.1) take the form

$$\mathcal{K}_{A \to 2B}(c) = \alpha\, c_A$$

$$\mathcal{K}_{2\bar{B} \to A}(c) = \beta(c_B)^2$$

$$\mathcal{K}_{A+C \to D}(c) = \gamma\, c_A c_C$$

$$\mathcal{K}_{D \to B+E}(c) = \varepsilon\, c_D \qquad\qquad (1.5)$$

$$\mathcal{K}_{D \to A+C}(c) = \delta\, c_D$$

$$\mathcal{K}_{B+E \to A+C}(c) = \xi\, c_B c_E$$

The positive numbers α, β, γ, ε, δ and ξ, called the rate constants for the corresponding reactions, are sometimes estimated on the basis of chemical principles or else one makes an attempt to deduce them from experiments. When a reaction network is presumed to be endowed with mass action kinetics it is the custom to indicate the rate constants (or symbols for them) alongside the corresponding reaction arrows in the network diagram. Thus for our example we might have a display like that shown in (1.6).

$$A \underset{\beta}{\overset{\alpha}{\rightleftharpoons}} 2B$$

$$(1.6)$$

$$A{+}C \underset{\delta}{\overset{\gamma}{\rightleftharpoons}} D$$
$$\xi \nwarrow \qquad \swarrow \varepsilon$$
$$B + E$$

If we assume mass action kinetics for the network we have been studying, the appropriate differential equations are obtained by inserting (1.5) into (1.4):

$$\dot{c}_A = -\alpha c_A + \beta (c_B)^2 - \gamma c_A c_C + \delta c_D + \xi c_B c_E$$

$$\dot{c}_B = 2 \alpha c_A - 2 \beta (c_B)^2 + \epsilon c_D - \xi c_B c_E$$

$$\dot{c}_C = -\gamma c_A c_C + \delta c_D + \xi c_B c_E \qquad\qquad (1.7)$$

$$\dot{c}_D = \gamma c_A c_C - (\delta+\epsilon) c_D$$

$$\dot{c}_E = \epsilon c_D - \xi c_B c_E \ .$$

We have arrived at a fairly concrete system of ordinary differential equations, and we can begin to pose questions about them. Here are some of the questions we might like to ask:

(a) Does the system (1.7) admit a positive equilibrium — that is, an equilibrium at which all species concentrations are positive?

(b) Does the system (1.7) admit multiple positive equilibria (in a sense to be made precise in the next lecture*)?

(c) Does the system (1.7) admit an unstable positive equilibrium?

(d) Does the system (1.7) admit a periodic (positive) composition trajectory?

These are not easy questions, and the answers to them might of course depend on the particular (positive) values taken by the rate constants α, β, γ, δ, ϵ, and ξ . Even if we could answer these questions for all positive values of the rate constants what would we have accomplished?

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*We shall want to know whether there can exist multiple positive equilibria within a stoichiometric compatibility class. In rough terms a stoichiometric compatibility class is a certain set of compositions which remains invariant under the flow given by (1.7).

We would have understood one model chemical system fairly well, at least with respect to certain qualitative issues.

There are, however, thousands of distinct reaction networks that might, on one occasion or another, command our attention. Each has its own system of differential equations, perhaps more complicated by far than the system we have been considering. How, then, are we to proceed? It is clear that we cannot rely forever on purely ad hoc studies of whatever systems might present themselves for examination. Even if we cast aside the long-term enormity of such an undertaking, there are still two problems that must be faced in the short run. First, questions of the kind we have posed will, for the most part, be confronted by engineers and chemists, not mathematicians. Second, it is by no means clear that mathematicians, even the most expert, are currently in a position to provide much help. The fact is that even moderately large systems of nonlinear differential equations — in particular polynomial systems like those displayed in (1.7) — remain poorly understood[*] in general.

It seems to me that what is required is a rather broad-based theory of those systems of differential equations that derive from reaction networks, a theory which would in some sense cuts across the fine details of individual problems to provide qualitative information about large classes of systems all at once. Moreover, we would like the results of such a theory to be of the kind that engineers and chemists can use easily in addressing questions like those we have posed.

This seems like a lot to ask, and I should try to explain why a theory of the kind I have in mind should even be possible in principle. Although we shall also be interested in the more general situation, let me temporarily restrict my attention to reaction networks endowed with mass action kinetics. Thinking back to the source of the system (1.7), we recall that it derived in a rather orderly way from the network (1.6). In fact, we knew how to write down the appropriate

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[*] Consider, for example, the remarkable complexity of the seemingly innocuous Lorenz system [L1], which is composed of three polynomial ordinary differential equations in three variables.

differential equations (up to values of the rate constants) merely from inspection of the reaction diagram. Had we begun with a different network we would have arrived at a different system of differential equations, but again the essential shape of those equations (up to values of the rate constants) would have derived from the reaction network in a precise way. Indeed, it is the close connection between reaction network structure and the shape of the induced differential equations that lends the subject of chemical reactor theory its coherency.

This is our source of hope. If reactor behavior is determined by a system of differential equations which, in turn, is determined by the underlying reaction network in a precise way, then perhaps one can prove theorems which tie qualitative aspects of reactor behavior directly to reaction network structure.

Can this in fact be done? I hope that these lectures will help to demonstrate that one can proceed surprisingly far in this direction. In Lecture 3 I will state two theorems, one of which will <u>immediately</u> answer all four questions that we posed about the system (1.7). The answers are <u>yes</u>, <u>no</u>, <u>no</u>, and <u>no</u>; these answers hold <u>for all positive values of the rate constants</u> α, β, γ, δ, ϵ, and ξ. Moreover, <u>these answers can be obtained merely from inspection of the reaction diagram</u> (1.6); one need not even write out the differential equations. The fact is that one can delineate a large class of networks — some extremely complicated — for which the corresponding differential equations admit solutions of a very limited variety, regardless of the (positive) values the rate constants take.

Our objectives will be rather broad, and I should try to make clear what these are. Results of the kind I have just described are typical of those we are after. <u>We seek to classify reaction networks according to their capacity to induce differential equations which admit behavior of a specified type</u>. When we restrict our attention to networks endowed with mass action kinetics we will <u>not</u> ask, for example, whether the differential equations for a particular network taken with <u>specified</u> rate constants admit periodic orbits. Rather, we will ask if the network is such that the induced differential equations admit periodic orbits for <u>at least one</u> set of rate constants — that is, if the <u>network</u> has the capacity to

admit periodic orbits. The network itself will be our object of study,
not the network endowed with a particular set of rate constants.*

1. B. Notation

It is not difficult to see that the differential equations induced
by a reaction network can be rather cumbersome. With this in mind I want
to spend a little time talking about notation. Although the notation
I shall use is quite natural to the problems we shall address, it is not
entirely traditional.

With each reaction network we can associate three sets. The first is
the set $\mathscr{S}$ of chemical <u>species</u> — {A, B, C, D, E} in network (1.1).
The second is the set of objects that appear before and after the reaction
arrows — {A, 2B, A+C, D, B+E} in (1.1). These objects are called
the <u>complexes</u> of the network, and the set of complexes will be denoted by
the symbol $\mathscr{C}$. The third is the set $\mathscr{R}$ of <u>reactions</u> — {A→2B, 2B→A,
A+C→D, D→A+C, D→B+E, B+E→A+C} in network (1.1).

With each of these sets we shall want to associate a (finite-dimensional)
vector space so that we can, for example, speak of a "vector of species
concentrations" or a "vector of reaction rate constants." If m is the
number of species, if n is the number of complexes and if r is the
number of reactions in a network we can, of course, work in the vector
spaces $\mathbb{R}^m$, $\mathbb{R}^n$, and $\mathbb{R}^r$. In this way we can speak of the "composition
vector $c \in \mathbb{R}^m$," c_i being the molar concentration of the ith species,
i = 1, 2,...,m. And we can speak of the "rate constant vector $k \in \mathbb{R}^r$,"
k_j being the rate constant of the "j^{th} reaction," j = 1,2,...,r. This is
what tradition would seem to require.

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*It is perhaps worth mentioning here that, in practice, complete sets of
rate constants for intricate networks are hardly ever known with great
precision. It is often the case that chemists have a very good sense of
what reactions are occurring but can estimate or measure rate constants
only to within a considerable margin of uncertainty. For a discussion
of the relationship between reaction network structure and the extent to
which rate constants can be determined uniquely from certain classes of
experiments see [F3] and, for more detail, [F1] and [K]. In [F1] there
is also a discussion of how information about the reaction network itself
can, in principle, be inferred from near-equilibrium experiments.

It turns out, however, that $\mathbb{R}^m$, $\mathbb{R}^n$, and $\mathbb{R}^r$ are somewhat awkward media in which to work. At the very least these spaces require that we number everything in sight so that we can speak of the "i^{th} species," the "j^{th} reaction," or the "k^{th} complex." Thus, we must impose an artificial ordering on each of the three sets of objects even before we begin to work, and we must carry that order around thereafter, suppressing or rearranging it whenever it becomes intrusive. There is a much better and far more natural way to do things, and that is what we shall discuss now.

We denote the real numbers by $\mathbb{R}$, the positive real numbers by $\mathbb{P}$ and the non-negative real numbers by $\overline{\mathbb{P}}$.

If I is a set we denote by $\mathbb{R}^I$ the vector space of real-valued functions with domain I . (Addition of functions and multiplication of a function by a real number are defined in the usual way.) By $\mathbb{P}^I$ [resp., $\overline{\mathbb{P}}^I$] we mean the subset of $\mathbb{R}^I$ consisting of those functions which take exclusively positive [resp., non-negative] values.

Henceforth in this section we shall suppose that I is a _finite_ set. In this case if x is a vector in $\mathbb{R}^I$ we shall almost always use the symbol x_i to denote the number that x assigns to $i \in I$. If x and y are vectors in $\mathbb{R}^I$ we use the symbol xy to denote the vector in $\mathbb{R}^I$ such that

$$(xy)_i = x_i y_i \ , \qquad \forall \ i \in I. \qquad (1.8)$$

If x is a vector in $\mathbb{R}^I$ we denote by e^x the vector of $\mathbb{P}^I$ such that

$$(e^x)_i = e^{x_i} \ , \qquad \forall \ i \in I . \qquad (1.9)$$

For $z \in \mathbb{P}^I$ we denote by $\ln z$ the vector of $\mathbb{R}^I$ such that

$$(\ln z)_i = \ln z_i \ , \qquad \forall \ i \in I. \qquad (1.10)$$

By the _support_ of $x \in \mathbb{R}^I$ (denoted supp x) we mean the subset of I assigned non-zero values by x. That is,

$$\text{supp } x: = \{i \in I: x_i \neq 0\}. \tag{1.11}$$

If J is a subset of I we reserve the symbol ω_J to indicate the characteristic function on J; that is, ω_J is the vector of $\mathbb{R}^I$ such that

$$(\omega_J)_i = \begin{cases} 1 \text{ if } i \in J \\ \\ 0 \text{ if } i \notin J \end{cases} \tag{1.12}$$

In particular, if J is the singleton $\{j\}$ then $\omega_{\{j\}}$ is the vector of $\mathbb{R}^I$ such that

$$(\omega_{\{j\}})_i = \begin{cases} 1 \text{ if } i = j \\ \\ 0 \text{ if } i \neq j \end{cases} \tag{1.13}$$

In this case _we shall write_ ω_j _in place of the more formal_ $\omega_{\{j\}}$.[*]

By the _standard basis_ for $\mathbb{R}^I$ we mean the set

$$\{\omega_j \in \mathbb{R}^I : j \in I\}. \tag{1.14}$$

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[*]This practice raises a minor possibility of confusion: While x_j is a number — the value assigned to $j \in I$ by $x \in \mathbb{R}^I$ — ω_j is a _vector_ in $\mathbb{R}^I$. No confusion should result if it is remembered that a subscripted ω is _always_ a vector. The symbol ω will never appear without a subscript.

This set is clearly linearly independent; and, moreover, each $x \in \mathbb{R}^I$ has a representation

$$x = \sum_{j \in I} x_j \omega_j \; . \tag{1.15}$$

Thus, (1.14) is in fact a basis for $\mathbb{R}^I$, and we have that the dimension of $\mathbb{R}^I$ is just the number of elements in the (finite) set I . Note that, for $J \subset I$, we have

$$\omega_J = \sum_{j \in J} \omega_j \; ; \tag{1.16}$$

in particular,

$$\omega_I = \sum_{j \in I} \omega_j \; . \tag{1.17}$$

We define the <u>standard scalar product</u> in $\mathbb{R}^I$ as follows: If x and z are vectors of $\mathbb{R}^I$ then

$$x \cdot z \; := \; \sum_{i \in I} x_i z_i \; . \tag{1.18}$$

Note that, with respect to this scalar product, the standard basis for $\mathbb{R}^I$ is orthonormal. Unless stated otherwise we shall always take $\mathbb{R}^I$ to be endowed with its standard scalar product. Moreover, we shall always take $\mathbb{R}^I$ to be equipped with the usual finite-dimensional vector space topology (for example, that given by the norm deriving from the standard scalar product).

We now pause to illustrate how, in very simple examples, vector spaces of the kind we have been discussing provide perhaps the most natural media in which to work.

Example 1.B.1. Let us think again about the homogeneous reactor with
species A, B, C, D and E that we discussed earlier. We denote the set of
species by the symbol $\mathscr{S}$; that is,

$$\mathscr{S} = \{A, B, C, D, E\}.$$

At some fixed instant the reactor contents have some fixed composition:
With each species $\mathscr{s} \in \mathscr{S}$ there is associated a (non-negative) molar
concentration $c_{\mathscr{s}}$, and we would like to represent that composition state
in some vector space. But to say that there is a non-negative number
associated with each species is to say that there is a <u>function</u> $c: \mathscr{S} \to \overline{\mathbb{P}}$
that assigns to each species its molar concentration. Now c is an
element of $\overline{\mathbb{P}}^{\mathscr{S}}$, which in turn is a subset of the vector space $\mathbb{R}^{\mathscr{S}}$.
We need proceed no further; c is the vector we seek.

Suppose our reactor is in composition state $c \in \overline{\mathbb{P}}^{\mathscr{S}}$. How might
we interpret supp c? Recall that

$$\text{supp } c = \{\mathscr{s} \in \mathscr{S}: c_{\mathscr{s}} \neq 0\}.$$

Hence, supp c is just the set of species present in the reactor when
the reactor is in composition state $c \in \overline{\mathbb{P}}^{\mathscr{S}}$.

Example 1.B.2. Let $\mathscr{R}$ denote the set of reactions in network (1.1).
That is,

$$\mathscr{R} = \{A \to 2B, \ 2B \to A, \ A+C \to D, \ D \to A+C, \ D \to B+E, \ B+E \to A+C\}.$$

Now suppose that the network is endowed with mass action kinetics so that
with each reaction there is associated a (positive) rate constant, and
suppose also that we would like to have available a "vector of rate constants."
To say that with each reaction there is associated a positive rate constant
is to say that there is a <u>function</u> $k: \mathscr{R} \to \mathbb{P}$. Thus k is an element of
$\mathbb{P}^{\mathscr{R}}$, which in turn is a subset of the vector space $\mathbb{R}^{\mathscr{R}}$. In this sense
we have immediately that k is a vector of rate constants.

There is one final matter of notation we need to consider. Suppose that I is a (finite) set and that

$$\{\omega_i \in \mathbb{R}^I : i \in I\}$$

is a standard basis for $\mathbb{R}^I$. When the set I carries no algebraic structure it is sometimes the custom to replace the symbol ω_i by i itself. (See, for example, pp. 197-199 of [NSS] or pp.240-241 of [L2].) Thus, the symbol $i + j$ becomes an abbreviation for the vector $\omega_i + \omega_j \in \mathbb{R}^I$. Similarly, $2j$ becomes an abbreviation for the vector $2\omega_j \in \mathbb{R}^I$.[*]

We shall adopt this convention when (and only when) the set in question is the set $\mathcal{S}$ of chemical species. Thus if, as in our example, $\mathcal{S} = \{A,B,C,D,E\}$, we can regard the symbol $A+B$ as an abbreviation for $\omega_A + \omega_B \in \mathbb{R}^{\mathcal{S}}$, the symbol $2B$ as an abbreviation for $2\omega_B \in \mathbb{R}^{\mathcal{S}}$, and so on. In this way we can regard what we have called the complexes of a network — $2B$, A, $A+C$, D, and $B+E$ in network (1.1) — as vectors in $\mathbb{R}^{\mathcal{S}}$ (and, in particular, as vectors in $\overline{\mathbb{P}}^{\mathcal{S}}$). This view will permit an easy transition between our formal definition of a reaction network (given at the beginning of the next lecture) and the portrayal of a network in its usual diagrammatic form.

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[*] In this way we develop what is sometimes called the vector space of formal linear combinations of elements of I.