

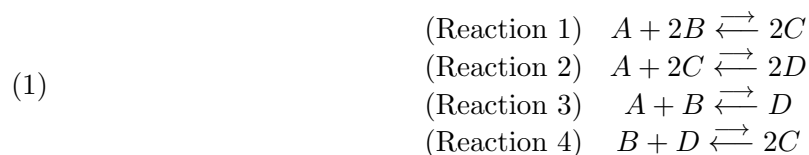
MATH3200: APPLIED LINEAR ALGEBRA
SELF-STUDY AND PRACTICE MODULE 45B: APPLICATIONS OF
LINEAR COMBINATIONS AND OF THE LINEAR SPAN TO SYSTEMS OF
CHEMICAL REACTIONS: THE STOICHIOMETRIC MATRIX

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This module is based on Conversation 23 and gives you additional information about this material. In particular, we will introduce here the important concept of the *stoichiometric matrix* of a system of chemical reactions.

Recall that in Conversation 23 we considered systems of chemical reactions between certain *chemical species* that could be compounds or chemical elements.

We will write here this system in simplified symbols for the chemical species as



The double arrows in each reaction indicate that in theory it can (simultaneously) occur both in the *forward direction* (from left to right) and in the *backward direction* (from right to left). The chemical species on the left of each equation are called the *reactants* (of the forward reaction) and the species on right are called the *reaction products*.

Recall that the vector of concentrations (in moles per liter) at time t of all species will be written as

$$\begin{bmatrix} [A]_t \\ [B]_t \\ [C]_t \\ [D]_t \end{bmatrix}$$

The vector of *net changes* in concentrations between times $t = 0$ and times $t = 1$ is then

$$\vec{\mathbf{w}} = \begin{bmatrix} [A]_1 - [A]_0 \\ [B]_1 - [B]_0 \\ [C]_1 - [C]_0 \\ [D]_1 - [D]_0 \end{bmatrix}$$

In particular, if only the first reaction occurs in the forward direction with a net consumption

of 1 mole per liter of the first reactant A , we get a net change of $\vec{\mathbf{v}}_1 = \begin{bmatrix} -1 \\ -2 \\ 2 \\ 0 \end{bmatrix}$

This vector is called the *reaction vector* of the first reaction. The reaction vectors for the other 3 reactions are:

$$\vec{v}_2 = \begin{bmatrix} -1 \\ 0 \\ -2 \\ 2 \end{bmatrix} \quad \vec{v}_3 = \begin{bmatrix} -1 \\ -1 \\ 0 \\ 1 \end{bmatrix} \quad \vec{v}_4 = \begin{bmatrix} 0 \\ -1 \\ 2 \\ -1 \end{bmatrix}$$

In a system of chemical reactions, all reactions occur simultaneously. Let k_i denote the net rate at which reaction i occurs. Then the observed vector \vec{w} will be the linear combination of the reaction vectors with coefficients k_i . Thus in a system with 4 reactions as in our example, we will have

$$(2) \quad \vec{w} = k_1 \vec{v}_1 + k_2 \vec{v}_2 + k_3 \vec{v}_3 + k_4 \vec{v}_4.$$

Note that $k_i > 0$ signifies that the forward direction of the reaction dominates, $k_i < 0$ signifies that the backward direction of the reaction dominates, and $k_i = 0$ signifies that the reaction does not occur or that the forward and backward direction exactly cancel each other out.

Thus a given vector \vec{w} can be a vector of net changes for a given reaction system if, and only if, \vec{w} is in the linear span of the reaction vectors. In our example this would mean that \vec{w} would need to be in $\text{span}(\vec{v}_1, \vec{v}_2, \vec{v}_3, \vec{v}_4)$.

The matrix whose columns are the reaction vectors for a given chemical reaction system is called the *stoichiometric matrix* of this system and will be denoted here by \vec{S} . While there is no universal agreement among chemists whether the reaction vectors should be written as the rows or the columns of the stoichiometric matrix, in this course *we always will write them as the columns of \vec{S}* . The reason is that when we use this convention, we can express the vector \vec{w} of net changes as the product of \vec{S} with the vector \vec{k} of net reaction rates:

$$(3) \quad \vec{S} \vec{k} = \vec{w}.$$

In particular, for a system with 4 reactions like in our example, (3) becomes:

$$(4) \quad \vec{S} \begin{bmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{bmatrix} = \vec{w}.$$

Notice that for our definition of \vec{S} , Equations (2) and (4) are two different ways of expressing the exact same thing. Moreover, notice that a given vector \vec{w} can be a vector of net changes for a given reaction system if, and only if, the corresponding linear system (3) is consistent.

Question 45.4: Find the stoichiometric matrix \vec{S} for the system in our example.

Question 45.5: Recall that in Conversation 23 Frank said that the vector $\vec{w} = \begin{bmatrix} 3 \\ -4 \\ 0 \\ 2 \end{bmatrix}$

could not be a vector of net changes for the system in our example. Was he right? How would you use the terminology introduced in this module to determine the answer?