MATH3200: APPLIED LINEAR ALGEBRA
SELF-STUDY AND PRACTICE MODULE 45A: APPLICATIONS OF LINEAR COMBINATIONS AND OF THE LINEAR SPAN TO SYSTEMS OF CHEMICAL REACTIONS: REACTION VECTORS

WINFRIED JUST, OHIO UNIVERSITY

This module is based on Conversation 23 and gives you additional information about this material.

Recall that in Conversation 23 we considered systems of chemical reactions between certain *chemical species* that could be compounds or chemical elements.
We focused on the example of the system

$$
\begin{array}{cc}
O_2 + C \overset{\longrightarrow}{\longleftarrow} CO_2 & O_2 + 2C \overset{\longrightarrow}{\longleftarrow} 2CO \\
O_2 + 2CO \overset{\longrightarrow}{\longleftarrow} 2CO_2 & C + CO_2 \overset{\longrightarrow}{\longleftarrow} 2CO
\end{array} \tag{1}
$$

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). Note that each of the first three reaction represents a process of carbon or carbon monoxide burning. Thus under normal conditions, only the reactions occur only in the forward directions. The backward directions are *energetically implausible,* but not outright impossible, so they are included in the description of the system for completeness.
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.* For the first reaction, the reactants are oxygen O_2 and carbon C, and the reaction product is carbon dioxide CO_2.
This system can be written in simpler symbols for the chemical species as

$$
\begin{array}{ll}
\text{(Reaction 1)} & A + 2B \overset{\longrightarrow}{\longleftarrow} 2C \\
\text{(Reaction 2)} & A + 2C \overset{\longrightarrow}{\longleftarrow} 2D \\
\text{(Reaction 3)} & A + B \overset{\longrightarrow}{\longleftarrow} D \\
\text{(Reaction 4)} & B + D \overset{\longrightarrow}{\longleftarrow} 2C
\end{array} \tag{2}
$$

However, in the process of the rewriting, the order of reactions got scrambled up and it is no longer immediately clear which letter represents which chemical specie.

Question 45.1: Match each of the letters A, B, C, D in the simplified notation to the chemical symbol among O_2, CO, CO_2, C that it represents.

From now on, we will work with the system written in the form (2). 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.

Question 45.2: Construct reaction vectors $\vec{\mathbf{v}}_2, \vec{\mathbf{v}}_3, \vec{\mathbf{v}}_4$ of the other three reactions in system (2), again assuming that 1 mole per liter of the first reactant is consumed.

Question 45.3: Suppose you have *any* chemical reaction that involves some or all of chemical species A, B, C, D but no other species. Which of the following would be *possible* reaction vectors?

$$\vec{\mathbf{v}}_1 = \begin{bmatrix} -1 \\ -2 \\ -1 \\ 4 \end{bmatrix} \qquad \vec{\mathbf{v}}_2 = \begin{bmatrix} 1 \\ 0 \\ 3 \\ 2 \end{bmatrix} \qquad \vec{\mathbf{v}}_3 = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad \vec{\mathbf{v}}_4 = \begin{bmatrix} -1 \\ 2 \\ 0 \\ 0 \end{bmatrix}$$