Math 232: Linear Algebra
Balancing Chemical Reactions

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In chemistry, we often know that some chemical compounds can turn into others, like how hydrogen gas (made of two hydrogen atoms, denoted H_2) can combine with oxygen gas (O_2) to produce water:

$$H_2 + O_2 \longleftrightarrow H_2O$$

However, this way of writing the chemical reaction is considered *unbalanced*, since there are two oxygen atoms on the left side and only one on the right side. (Chemical reactions can't change the number of atoms of each kind, although nuclear reactions can.) A *balanced* version would look something like this:

$$2H_2 + O_2 \longleftrightarrow 2H_2O,$$

showing two hydrogen molecules can combine with one oxygen molecule to form two water molecules. Now each side of the reaction has four hydrogen atoms and two oxygen atoms.

Balancing reactions with linear algebra

How do we figure out how many of each molecule we need in order to balance the reaction? With a small example like this one, we could do it by eyeballing, but here's a general method. We can start by making a variable coefficient for each molecule:

$$xH_2 + yO_2 \longleftrightarrow zH_2O$$

Then each type of atom gives us a linear equation relating x, y, and z. The total number of hydrogen atoms on the left side is $2x$, and the total number on the right side is $2z$, so these must be equal. Comparing the total number of oxygen atoms on the two sides gives us $2y = z$. So we get a linear system of equations:

$$\left| \begin{array}{c} 2x = 2z \\ 2y = z \end{array} \right|$$

Converting these equations to an augmented matrix gives us

$$\left[\begin{array}{ccc|c} 2 & 0 & -2 & 0 \\ 0 & 2 & -1 & 0 \end{array}\right]$$

which has reduced row-echelon form equal to

$$\left[\begin{array}{ccc|c} 1 & 0 & -1 & 0 \\ 0 & 1 & -1/2 & 0 \end{array}\right]$$

There's no pivot in the third column, so we can use z as a free parameter for the set of solutions:

$$x = z$$
$$y = \frac{1}{2}z$$

Choosing z to be the smallest positive integer that makes x and y integers too, namely $z = 2$, we get $x = 2$ and $y = 1$. So a balanced form of the reaction is

$$2H_2 + O_2 \longleftrightarrow 2H_2O.$$

Burning propane

Propane (C_3H_8), like most compounds made of hydrogen and carbon, is highly flammable: it reacts easily with oxygen to produce carbon dioxide and water vapor:

$$C_3H_8 + O_2 \longleftrightarrow CO_2 + H_2O.$$

Question 1. Try using linear algebra to find a balanced version of the propane reaction.

Question 2. What happens to the solution set if you try to balance the propane reaction without the H_2O term? How would you interpret that?

Question 3. What happens to the solution set if you are also burning methane (CH_4), like this?

$$C_3H_8 + CH_4 + O_2 \longleftrightarrow CO_2 + H_2O.$$

How would you interpret that?

Question 4. When we're balancing chemical reactions, we're not just looking for any solutions, we're looking for solutions that are positive integers. What could it mean if you found a solution with some of the variables negative, or equal to 0?