Dialog on Balancing Chemical Reactions

Bette: Excuse me, Prof, we need a little help.

Prof: Oh, hi Bette, Alf. What's the problem?

Bette: We want to talk about chemical reactions—I mean—this stuff must really be important and we don't want to miss out—

Alf: Yeah, the truth is, Prof, we're having trouble balancing reactions and you didn't really talk about that in class.

Prof: Ah.

Bette: Sure. We've been balancing reactions in chemistry courses since high school, but I've never been comfortable with it. I mean, it seems so arbitrary—how you do it.

Alf: Sometimes I can do a balance and sometimes I have a lot of trouble.

Prof: Ok. Let's look at an example. Let's burn methane:

$$CH_4 + O_2 \rightarrow ?$$

What are the products here?

Bette: Water and carbon dioxide.

Alf: Right.

Prof: Good. So we have this:

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

Is this balanced?

Alf: Nope.

Prof: Ok. So how are you going to balance this, Bette? Tell me what you're going to do first.

Bette: In chemistry we were taught to balance carbon first.

Prof: Ok, so?

Bette: The carbon is ok. I mean, we already have one carbon atom on the left and one on the right.

Prof: Good. Now what do you want to do?

Bette: I'm not sure.

Alf: I think we should do the hydrogen next.

Prof: Ok. Why?

Bette: Oh, I remember. Because we want to save the oxygen for last.

Prof: Right. Why?

Bette: Is it because the oxygen is by itself?

Prof: Exactly. It's something like a free variable—the stoichiometric number on the oxygen does not affect the balance of any other atom.

Alf: Ok. So we look at the hydrogens—we have four on the left, but only two on the right. We can fix that by writing this:

$$CH_4 + O_2 \rightarrow CO_2 + 2\,H_2O$$

Prof: Good. Now what Bette?

Bette: Now we have two atoms of oxygen on the left and four on the right, so we balance the oxygens by this:

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$$

Prof: Good. Are we done now?

Bette: Yes.

Prof: Ok. So what's you're problem?

Alf: That was a simple one, Prof. We can do those. But what if the reaction has several molecules with the same atoms and what if none of the molecules are atomic? Things get complicated.

Prof: It sounds like you have an example in mind.

Alf: Yeah, I wrote it down. Here it is:

$$C_2H_6 + CO_2 + H_2O \rightarrow C_2H_5OH$$

Prof: Goodness. Where did you find that?

Alf: Well, I made it up.

Prof: Did you indeed?

Bette: It doesn't matter, does it, Prof? You're always telling us that a good way to study is to make up problems.

Prof: No, Bette, in the context of practicing a balancing procedure, it doesn't matter whether the reaction is feasible. This as good as any to practice on. So, can you balance this?

Alf: We haven't been able to, Prof. If we start with carbon, like before, we have three on the left and two on the right. We can fix that with a three halves on the right,

$$C_2H_6 + CO_2 + H_2O \rightarrow \frac{3}{2} C_2H_5OH$$

Bette: But now everything else is really messed up.

Alf: We don't know what to do next, and if we get, say, the hydrogens balanced, then the carbon goes out of balance.

Bette: We're stuck.

Prof: Ok, what I hear you asking for is a systematic procedure that always works for obtaining a balance. The usual procedure, which we did for the methane combustion, is trial-and-error. Many reactions are so simple that we can do the trial-and-error process in our heads and get the balance. But you're right; other reactions are so involved that the mental trial-and-error process can be frustrating.

Bette: You mean we're not dumb?

Prof: Certainly not. Let's back up and ask, what are we really doing when we balance a reaction?

Alf: I don't get it.

Prof: Ok, what does "balance" mean?

Bette: Some things are equal.

Prof: Good. What things are equal in a reaction?

Alf: Oh. The atoms are equal.

Prof: Can you be more precise?

Bette: The number of each kind of atom in reactants must equal the number of each in products.

Prof: Good. So atoms are conserved during chemical reactions. What about molecules? Are molecules conserved?

Alf: No, Prof, you said that in class.

Prof: Ok, I said it. But is it true? Do you believe it?

Alf: You wouldn't tell us something that isn't true.

Prof: I might make a mistake, though. You shouldn't accept anything just because some Professor says it.

Bette: Then what's the point of school?

Prof: One point is to direct your attention to things that may be important to you later; another is to give you an opportunity to practice certain kinds of mental exercises that foster intellectual growth. You won't grow much if you just accept what others tell you.

Alf: Ok, Prof, you've told us that before. Anyway, molecules are not conserved in reactions.

Prof: Can you give an example, Alf?

Alf: Well . . .

Prof: Look back at the methane combustion. Is methane conserved during the reaction?

Alf: Well . . .

Prof: There are methanes on the right; are there any on the left?

Alf: No.

Prof: So, during the combustion, methane molecules are converted into other molecules—carbon dioxide and water. Methane is not conserved.

Bette: But that's obvious!

Prof: Yes, most things are obvious, once they're pointed out to us. My point is that we balance atoms not molecules; and "balancing" a reaction means that we impose a conservation law on atoms:

$$\begin{pmatrix}\text{number of atoms of} \\ \text{kind i in reactants}\end{pmatrix} = \begin{pmatrix}\text{number of atoms of} \\ \text{kind i in products}\end{pmatrix}$$

Bette: So, when we balance a reaction in the usual way, we're really satisfying this equation?

Prof: Right, Bette. And how many such equations can we write?

Alf: Must be one for each kind of atom.

Bette: Say, I'm starting to get an idea . . .

Prof: Ok, Bette, can you run with it?

Bette: Maybe. Look, let's take Alf's reaction,

$$C_2H_6 + CO_2 + H_2O \rightarrow C_2H_5OH$$

We're looking for the coefficients, which we don't know yet. But let's give them symbols, like in algebra,

$$a\,C_2H_6 + b\,CO_2 + d\,H_2O \rightarrow e\,C_2H_5OH$$

Prof: Very good, Bette. Now, can you state the problem?

Bette: Sure. The problem is to find the values of a, b, d, and e that satisfy the conservation law for each kind of atom in the reaction.

Prof: Good. How many conservation equations must be obeyed?

Bette: Well, we have carbon (C), hydrogen (H), and oxygen (O). So, three.

Alf: Hey, I get it! Look, here's the equation for carbon:

$$2a + b = 2e$$

Prof: Great, Alf.

Bette: And here are the ones for hydrogen: $6a + 2d = 6e$,
and oxygen: $2b + d = e$.

Prof: Good. Let's look at them all together:

$$\begin{aligned} 2a + b &= 2e \\ 6a + 2d &= 6e \\ 2b + d &= e \end{aligned}$$

Alf: Wait a minute, Prof. We've got a problem.

Prof: That should be, Houston, we've got a problem.

Alf: Say what?

Prof: Never mind. What's the problem?

Alf: We've got four unknowns, but only three equations. We can't solve it. We're stuck again.

Prof: What do you think, Bette?

Bette: We need another equation.

Prof: Are there more equations to be had? We've applied a balance to each kind of atom in the reaction. Can we balance molecules?

Bette: No, I guess we've written all the equations.

Prof: I guess so. Let me ask this: Are stoichiometric coefficients unique?

Alf: Say that's right. They're not unique.

Prof: Good. And that lack of uniqueness shows up by having more unknowns than equations. In other words, we can pick the value of one variable arbitrarily, then solve our equations for the others.

Bette: Really?

Prof: Well, let's test it. Pick a value for one of your unknowns, Bette.

Bette: Does it matter which?

Prof: It doesn't affect our analysis; but some choices may simplify subsequent calculations. Often, calculations are simplified if you assign a value to the unknown that appears in the most equations.

Bette: Ok, that would be "e" in our problem; let's set e = 1.

Prof: Fine, then we have this:

$$\begin{aligned} 2a + b \quad\quad &= 2 \\ 6a + \quad\quad 2d &= 6 \\ 2b + d &= 1 \end{aligned}$$

Can you solve these, Alf?

Alf: Sure, Prof. I can eliminate an unknown by combining these in pairs, then solve for the one that's left.

Prof: Yes, you can do that. But we wanted a completely general, systematic procedure, remember? So let's note that these equations are linear in the unknowns. The atom balances are always linear. So we can write them in matrix form:

$$\begin{bmatrix} 2 & 1 & 0 \\ 6 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix} \begin{pmatrix} a \\ b \\ d \end{pmatrix} = \begin{pmatrix} 2 \\ 6 \\ 1 \end{pmatrix}$$

Can you solve this, Alf?

Alf: There's something about determinants, we did it in high school.

Prof: Ok, there is Cramer's rule, which works well enough here. First we get the determinant of the coefficient matrix,

$$\begin{vmatrix} 2 & 1 & 0 \\ 6 & 0 & 2 \\ 0 & 2 & 1 \end{vmatrix} = (0 + 0 + 0) - (0 + 6 + 8) = -14$$

Then we solve for each unknown,

$$a = \frac{\begin{vmatrix} 2 & 1 & 0 \\ 6 & 0 & 2 \\ 1 & 2 & 1 \end{vmatrix}}{-14} = \frac{(0 + 2 + 0) - (0 + 6 + 8)}{-14} = \frac{-12}{-14} = \frac{6}{7}$$

$$b = \frac{\begin{vmatrix} 2 & 2 & 0 \\ 6 & 6 & 2 \\ 0 & 1 & 1 \end{vmatrix}}{-14} = \frac{(12 + 0 + 0) - (0 + 12 + 4)}{-14} = \frac{-4}{-14} = \frac{2}{7}$$

$$d = \frac{\begin{vmatrix} 2 & 1 & 2 \\ 6 & 0 & 6 \\ 0 & 2 & 1 \end{vmatrix}}{-14} = \frac{(0 + 0 + 24) - (0 + 6 + 24)}{-14} = \frac{-6}{-14} = \frac{3}{7}$$

Bette: Say, I remember that.

Prof: Good. So Alf's reaction

$$a\,C_2H_6 + b\,CO_2 + d\,H_2O \rightarrow e\,C_2H_5OH$$

can be balanced like this:

$$\tfrac{6}{7}\,C_2H_6 \;+\; \tfrac{2}{7}\,CO_2 \;+\; \tfrac{3}{7}\,H_2O \;\rightarrow\; C_2H_5OH$$

And we can multiply through by 7 to get integer coefficients:

$$6\,C_2H_6 \;+\; 2\,CO_2 \;+\; 3\,H_2O \;\rightarrow\; 7\,C_2H_5OH$$

Alf: Wow! Does this always work?

Prof: Every time, Alf. It's the analytic version to balancing by trial-and-error. If you have more than three equations in three unknowns, you may want to use a software package to solve the linear algebra problem. But the conservation equations are always linear in the unknown stoichiometric coefficients, so trial-and-error is never required.

Bette: Say, Prof, can the difference between the number of equations and number of unknowns be greater than one?

Prof: Yes it can. Remember, the number of unknowns is the number of different molecular components; call that number C. The number of equations is the number of atoms (elements); call it E. In Alf's reaction we had

$$C - E = 1$$

So we picked the value of one unknown. Now you're asking whether the numbers of molecules and atoms can differ by more than one, and certainly, they can,

$$C - E \geq 1$$

Bette: Then what do we do?

Prof: You have options, Bette. You can merely choose values for (C – E) unknowns, just as we did for Alf's reaction. Alternatively, there is this interpretation: if (C – E) > 1, then there is more than one independent balance for the reaction. This suggests the given reaction is actually a sum of simpler, mutually independent reactions. So, perhaps you can find those reactions and balance them separately. Ideally, each has (C – E) = 1.

Bette: Then it seems we need a way to decide how many independent reactions can be formed from a particular group of molecules.

Prof: Right, Bette. I'll show you that test when we study multiple reactions. It involves another tool from linear algebra. (See Balancing Act.pdf at www.macatea.com/workshop)

Alf: So, linear algebra is useful.

Prof: Indeed, Alf, much of mathematics is useful to engineers.

Bette: Wait a minute, Prof. Can C = E? If so, then we have a situation where the stoichiometric coefficients are unique—so I guess not?

Prof: Actually, the answers to your questions are "yes" and "no". A reaction can have C = E; for example,

$$a\ NO_2 \ \rightarrow\ b\ N_2O_4$$

Here, the number of components is C = 2 and the number of elements is also E = 2. So we can write two balance equations; one for nitrogen

$$a = 2b$$

and one for oxygen

$$2a = 4b$$

Alf: But those are really the same equation.

Prof: Right, Alf. We really have only one independent equation with two unknowns, and we still get to choose one unknown arbitrarily. So the stoichiometric coefficients of this reaction are not unique, even though C = E.

Bette: Thanks, Prof, this helps a lot.

Alf: Yeah, Prof. We need to practice this process for balancing reactions.

Prof: Ok, Alf, practice is good—but remember—part of an engineer's job is to fit the right tool to the problem at hand.

Alf: Meaning?

Prof: There's no sense in hitting a problem like (a $NO_2 \rightarrow$ b N_2O_4) with the machinery of linear algebra when you can easily balance it in your head.

Alf: So, part of the practice is in deciding which *process* we should use for a given problem.

Prof: Now you're getting it!