Chemistry 471/671
Introduction to Green Chemistry

Thoughts About Problem Set #1 (6 points)
Due Tuesday, September 13, 2011

Due to the abstract nature of this week's lecture material, we present an abstract problem set. For this week's assignment only, no answer can truly be wrong, so long as you can back up your answer with a logical argument. However, answers presented without the "work" of a logical thought process can be considered wrong. Show how you arrived at the answers you have given. Note that these sorts of open-ended questions are regular occurrences in the real world, and learning to make good assumptions is a valuable skill.

1) Approximately how much fuel (in gallons or liters, your choice) is consumed during the morning rush hour for an American city of approximately 1 million people? How does your answer change if we name a specific city, rather than a generalization? How does your answer change if the city isn't American?

The class's answers ranged from 150,000 gallons to 2,600,000 gallons with an average of 600,000 gallons. I suspect the "correct" answer is a bit lower than that average – I'm inclined to side with the 4 or 5 people who put it between 250,000 and 350,000. But again, I don't know the right answer. Some things that you should have considered in your answers:

- How many workers are there in a population of 1,000,000? (Housewives, children, students, retirees… might not be part of rush hour)
- How many workers work outside the home?
- How many of them drive solo?
- How many carpool?
- How many take public transportation?
- How long is the average commute (in distance or time)?
- How much gasoline gets burned in the average car in that distance/time?
- How much fuel gets used by public transportation?

Once we start considering a specific city, a few more things come in to play:

- What if public transportation is much better/worse than the "average"? Consider LA or Atlanta vs. Boston or New York
- What if the city is spread out, rather than compact? Again, Atlanta is very different than Manhattan. The Manhattan commute lasts longer, but is a much smaller distance, on average.
- What role does climate play? If a city is hot, A/C will burn a lot of fuel in idling cars.
- How well-planned is the town? Older cities tend to have tangled road systems and unplanned growth, which lead to longer commuting distances AND times.

Foreign cities tend to have a lot more public transportation and a lot fewer drivers. But foreign cities outside of Europe and Japan also tend to have much older cars, which consume a lot more fuel as a function of time.

2) Approximately how many liters of organic solvent waste are produced each semester during undergraduate chemistry labs at Boston's colleges and universities?

The class's answers ranged from 855 L to 130,000(!) L with an average of about 25,000L… 9,500 L if we exclude that very large maximum value. Again, I suspect the "correct" answer is a bit lower than the average – I'm inclined to side with the people who put it in the low thousands, but so much here depends on how many schools you declare to be "in Boston;" Harvard and MIT would **really** change your answer. Again, I don't claim to know the right answer. Some things that you should have considered in your answers:

- How many schools teach undergraduate labs?
- Which lab courses are likely to generate significant amounts of waste? (Not just orgo?)
- How many students take each lab course? (Lots more in bio labs and freshman labs than in orgo)
- How much waste does each student generate?
- Do they work in pairs? Threes?
- Do all schools have the same patterns of waste generation? (Hint: NO!)
- Keep in mind – if you're using UMB data to represent Boston, you're overcounting – we have MANY more students than a lot of Boston schools

3) Choose ONE of the two scenarios above. Discuss the ways in which this use of resources is a poor example of Green Chemistry. Be specific: which principles are being violated? What might be done to remedy the situation? Consider that any changes will need to be economically as well as philosophically sound if they are to be implemented.

Principles to consider in Scenario #1:

- 1 – prevent waste
- 4 – chemical products should minimize toxicity
- 6 – energy requirements should be minimized
- 7 – feedstock should be renewable
- 10 – minimize the use of persistent environmental pollutants
- 12 – minimize the potential for chemical accidents, including fires and spills

Solutions to consider for Scenario #1:
This one's actually quite difficult. If there were an economic and political solution, it would be in place. Some random thoughts (by no means exhaustive)...

- Alternative fuel vehicles are a great idea, but they're costly
- Americans hate public transportation, and they hate buses in particular
- Renewable fuel sources have yet to be developed

The cities with congestion problems have **already** grown, so suggesting intelligent growth patterns hits the problem 100 years or more too late
How do we convince people to carpool?
Where does the money come from to offer better AND cheaper public transportation?

Principles to consider in Scenario #2:

1 – prevent waste
2 – atom economy
3 – use and generate products with little or no toxicity
5 – minimize auxiliary substances
12 – minimize the potential for chemical accidents, including fires and spills

Solutions to consider for Scenario #2:
This one's a lot easier. There are any number of ways to reduce the use of solvents in organic labs, which are the prime contributor to the problem: microscale reactions, solvent-free reactions, solid-state reactions, water as a solvent. The thing is that practically none of Boston's schools DO teach the subject this way. Why not? What sort of things should be done to encourage them to change the historical teaching approach? Who should be responsible for encouraging those changes? Where does the money come from?

For those of you teaching the undergraduate labs here at UMB… why not work these concepts in? Shouldn't we expect our graduates to be as familiar with this as they are with significant figures?

Reading Analysis #1 (4 points – with 2 points reserved for Discussion)
Due Tuesday, September 13, 2011

1) Which of the Presidential Green Chemistry Award winners do you think is the **most** likely to have an economic impact on a global scale? Which is the **least** likely? Explain your choices.

Obviously, this is really an opinion question. What I was looking for was a *reason* for your answers. Some of the reasons provided weren't very compelling, but overall this went pretty well. The votes were actually fascinating:

Most Likely: 4 for Sherwin-Williams water-based paint
3 for TPGS
2 for bioamber
2 for bio-bdo
1 for the nexar membrane

Least Likely: 6 votes for the nexar membrane
4 for TPGS
1 for water-based paints
1 for bioamber

Note that TPGS is the second most likely and the second least likely to be an economic success. Neat how that worked out.

2) Which of the 12 Principles are being observed in Journal of Organic Chemistry paper on TPGS-750-M? Which aren't? Can you think of any ways to address those "missing" Principles? If so, why didn't the authors?

Principles most of us agree are observed: 1 – preventing waste, 2 – Atom Economy, 4 – preserving efficacy, and 8 – reducing unnecessary derivatization.

After that, there's a lot of disagreement. Some are quite tricky to apply. Using TPGS in place of solvents is definitely addressing 5 – reducing auxiliary substances, 6 – minimizing energy requirements, and 9 – using catalytic reagents (although the metal catalysts are already part of the reactions studied). BUT the method by which they actually synthesize the TPGS itself doesn't really address any of these principles.

Ones that we generally agree are NOT observed: 3 – using non-toxic reagents (toluene isn't awful, but it's not good), 7 – use renewable feedstocks (we have options for succinic acid, but I don't know of any non-petroleum sources for ethylene glycol), 10 – environmental persistence, 11 – in-line monitoring and 12 – minimizing possibility of accidents.

So, if we can (mostly) identify the things they didn't do… why didn't they? Well, for one thing, they're not using the 12 Principles as a check list. They have a specific goal, and they meet that goal. Moreover, their job is to publicize what they DID do. In true JOC fashion, there's no telling what they've tried that didn't work. Maybe they've tried to address ALL the remaining principles, and they didn't work?