Professor McCready

Research/Projects for undergraduates 2016-2017

CO2 absorption into 400-600 μm "capsules" containing reactive ionic liquids using a fluidized bed flow.

We[1] have collaborators at Lawrence Livermore National Laboratory[2] who have invented a microfluidic co-extrusion process to manufacture "capsules" consisting of a polymer shell which contains an ionic liquid that reacts reversibly with carbon dioxide. The capsules are nominally 300-600 μm in diameter and spherical in shape. Our work is to use these in a "fluidized bed" to absorb carbon dioxide from a simulated flue gas stream. We need to verify that the particles are suitable for a fluidized bed (i.e., they don't stick together and that they have good structural integrity when subjected to the collisions that occur with fluidization), exactly how fast the absorption rates are and the overall effectiveness of the process. We will also regenerate the capsules in either a fluidized bed or packed bed flow using a hot vapor or gas.

To achieve high capacities of CO2 absorption, a chemical reaction is needed (e.g., with MEA) but the reactions are exothermic so that heat must be somehow removed in the process or a rather extreme increase in temperature would occur for the gas stream. In the MEA process, there is some increase in temperature but the large quantity of otherwise inert water carries away the heat. When no liquid is present, some sort of cooling will be necessary in the absorber and this is much easier to accomplish in a fluidized bed than a packed bed.

We have an engineer and a graduate student working on this project but there are useful tasks for an undergraduate.

Development of a new vapor compression cycle experiment for the undergraduate lab.

This is not research project.

Several years ago, we had company in Champaign Illinois, build a device to test a vapor-compression refrigeration cycle that used carbon dioxide and and ionic liquid. This project, while intellectually interesting, didn't lead to the "hoped-for" new cooling technology that used less power while not containing those nasty HFC's that have such large infrared absorption signatures.

However, the device still exists and I don't want to discard it. It has lot of instrumentation and could be turned into a nice undergraduate laboratory experiment employing a single fluid, (no IL). I am looking for someone with mechanical skills to see if we can accomplish this.

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[1] This project is a joint effort of Professors Brennecke, Stadtherr and McCready

[2] https://www.llnl.gov/news/microcapsules-capture-carbon-safely

The following projects are of a much more speculative nature (i.e., they may not reach a positive conclusion). I am curious about what could be done on them that has not be done before so I would like to "take a shot". Note also that these are information gathering and then modeling; there are laboratory experiments to be done.

"Big Data" to discern (known) physical laws.

You may be aware of the term "Big Data" which is nominally use of large sets of information (usually quantitative or semi-quantitative) to either engage in marketing (if I shop for an "cabin air filter", I must also need a car air freshener or a cargo net so my browser blasts these adds) discern specific quantitive association for processes that are not (obviously) governed by fundamental physical laws.

The ability to do these studies is a result of the continual expansion in both computational power for the analysis as well increased, essentially ubiquitous electronic inter-connectedness that enables acquiring the data in the first place.

No doubt, large retailers have been able to make better decisions (at least some of the time) from technologies using big data and personal and public security is enhanced when the facial recognition systems at major airports identify me before I get to the security checkpoint.

With the life sciences, I am sure that there are many efforts aimed at determining what could the termed "the laws of biology", that is, general relations analogous to Newton's Laws of Motion. This seems like a noble and interesting quest which is probably extremely hard. I would like to propose a somewhat different tact that would involve examining what "data" on what length and time scales could be analyzed with a "fair" optimization algorithm and produce, say, well know relations (for want a better example) for the pressure drop — flow rate relations for laminar and turbulent flow. For example, from the population density of a city and some knowledge of the total length of water pipes, then use this information for 100 cities, produce the Blassius relation? We could see. How about caloric intake, and size for different animals, I would be pretty certain that we would find a heat transfer correlation that matched something analogous to Dittus-Boelter. Many possibilities exist.

The big question to ultimately ask is when can this approach be expected to give a valid result and for which situations is it not possibly going to work (which could save a lot of wasted effort.)

Declining productivity and GDP growth, why is it happening?

There is a relatively new book "The Rise and Fall of American Growth" by Robert Gordon who explains the declining rates of productivity increase (I am simplifying quite a bit so you could read his book for more nuance.) to the claim that most of the inventions that transformed humans from single agrarian groups with only limited domesticated animals to do work, have already been invented (e.g., the steam engine, the existence of microbes, the telephone, the automobile, computers and the internet). His prediction that productivity will decline down to

levels of the medieval ages within several decades. (I would imagine this book would quite fun to discuss with people of different political views… To throw down the gauntlet, I am pretty sure I know his political leanings…)

So rather than argue about technology, I was thinking one Saturday morning while cooking my favorite breakfast "invention": A pumpkin/pumpkin pie spice waffle, toppled with sweetened cream cheese, granola, Golden-Crisp apples and of course whipped cream! …. isn't the counter to lack of really big inventions the incredible pallet of possible pieces of technologies that can be combined together if sufficient need, justification and (say) free market incentives exists. Could the lack of grow be caused by something stopping it. (Hence the comment about me guessing his political slant while revealing mine!!)

So back to food, and the arts. Could we study the rate of innovation in something that is not affected by politics to see if big creativity gains only follow big innovations (how did they cook without immersion heaters and flash coolers?) Food might be easier to get a quantitive read on it. The arts might be harder but fun. If we compare "Miss Saigon" to "King and I", (with full knowledge of previous literature and other art forms), does the existence of more different kinds of music and dance forms and improved lighting and audio/electronic tech, (and better musicians!) add to the overall impact or not?

Modeling of antibiotic resistant bacteria.

Exposition

The problem of treating bacterial infections associated with surgical procedures and even common skin wounds has been getting considerable publicity as the number of cases and types of situations where resistance has been encountered increases. The *standard* stories, that bacterial infections were considered to not be a problem for a couple of decades and thus drug research and fundamental research ebbed, that there still is little incentive for the drug industry to develop new molecules because the financial payback is not nearly what can be obtained for drugs that treat chronic conditions, that existent is enhanced because antibiotics (ABs) are over-prescribed for illnesses for which they have no efficacy and that feeding ABs in large quantities to chickens, pigs and cows to increase weight gain and prevent at least some of the effects of overly-crowded conditions, are all probably true to some extent. However, evidence of resistance to penicillin was observed within a two years from its introduction (Appelbaum 2007, Clinical Infectious Diseases, 45:S165-70) which is perhaps due as much to the probability (Chen et al. 2013, Env. Sci. Tech. 47: 12753-12760) that at least some types of bacteria that were present in people who were treated even in these early years already had the genetic code for an enzyme to de-activate the β-lactam ring. In fact bacteria obtained from an isolated cave show considerable *multi-drug* resistance (Bhullar et al., PLOS One Vol. 7, April 2012, e34953) and even display a resistance mechanism that was not previously identified in "modern" bacteria.

Currently about 1 out 25 patients in US hospitals get nosocomial infections and the death rate is close to 10% of these patients. The types are split between pneumonia, surgical site, urinary tract, GI, central line and other infections. If the reason for hospitalization was nonelective, the

threat of infection may be acceptable. However the problem of infection from resistant bacteria would seem to actually have a real "tipping point" if the surgery is not absolutely essential. For the past few decades significant advances in surgical techniques have made treatment of many conditions routine and outcomes (e.g., ACL reconstruction, "Tommy John", aortic valve replacement) very much better than the past and the associated hazard dropping continuously due to improved anesthesia drugs and techniques (among other reasons). While we have all probably known of someone, who has had the complication of a bacteria infection (e.g., Tom Brady, Rob Gronkowski,…) from routine surgery for a non life-threatening condition , in most cases, these people have fully recovered. However, if the infection rate for "elective" surgery reaches a critical value, perhaps 5% would be enough and if the death rate of these cases reaches a second critical value (again perhaps 5-10%), there would be a crisis in the surgical community. Of course physicians are smart and hospitals diligent so there has been considerable ramping up of procedures to prevent such infections. Still as the threat increases and the last line of defense weakens, the tipping point could be reached.

Possible topics to explore:

1. Mathematical modeling rate of resistance growth. While no doubt some work exists within biology that attempts to quantify the number and kinds of mutations that would be necessary to match a current animal (e.g., the development of modern dogs) from the ancestor species or explain how Japanese beetles have become almost completely resistant to *Sevin* (1-naphthyl methylcarbamate) in 40 years, has there really been useful research to explain the rate of MRSA development in the modern clinical environment? We know that some strains of bacteria likely to have been present in our guts had the genetic code for this, so was intra-species transmission of DNA the most important step or has it been evolution of *SA* strains? If different degrees of strain clearance occur, in various numbers of patients, is the number of predicted cases increased. How about assumptions about community and nosocomial origins of particular cases. There would seem to be almost unlimited numbers of problems that could be considered.
2. Analysis of multi, simultaneous treatments. Last fall a paper appeared in *Science Translational Medicine* (Imamovic and Sommer, 2013, Vol5 204ra132 1-10) that noted that two different drugs given simultaneously in certain circumstances worked better than either one individually. The study did not specifically identify mechanisms but it could be speculated that either that opening channels to pump one molecule out made it easier for another molecule to diffuse in, or that causing the bacterium to spend energy to defeat one mechanism left it with less energy to fight the other "battle". This work was not really all that new but apparently physicians don't know how to quantify this effect or what dose of pharmaceutical "A" that would be just enough to allow "B" to be increasingly effective. This effort would be data collection combined with mathematical modeling.
3. Most effective utilization of future drugs How should a new drug be used to (a) preserve its efficacy and (b) preserve the revenue stream that could lead to future drugs? (Actual research on monetization may not be out of bounds!) Should it be used only when a profile of the pathogens confirms that other treatments won't work, should it be treated as a "controlled-

substance", should it only be given for an active infection or would it actually be more effective prophylactically?

4. Environmental incidence of antibiotics and transmission/ spread of resistant bacteria. This is an active research area elsewhere. To the extent that ABs are eluted through the kidneys of patients in a still active form and similarly through use in agricultural settings, what is the influence on environmental bacteria in terms of resistance? How do "they" get back into the human or animal infection cycle? Do they transmit genetic material that does come back? Or, for the bacteria within treated patients, are these really transmitted other than through acute symptoms (sneezing?) Many claims are made but which are the key steps?
5. Can we use thermodynamics in our favor to control virulent bacteria? It would be interesting to look at bacterial colonies and ultimately infected tissue in terms of the energy (i.e. nutrient and waste) fluxes to see if there is a way to put harmful bacteria at an *energetic* disadvantage — meaning that they are not as efficiently using available food sources as healthy tissue or non deleterious bacteria.? Will "turning off quorum sensing, if it can be done, contribute to this?

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I really have to add disclaimers to the following three projects. Many different research groups, in the specific fields of interest, are working on these topics. I find the topics interesting and would like to see if there is "anything" that I could contribute, as a complete outsider, but with substantial knowledge of all of the tools of chemical engineering.

I could write more, but if you are interested, let me know and we could talk about any of these.

1. Model for overall brain connectivity and memory/learning.

2. Model for the "tissue" where a bacterial infection occurs. Plus some of the surrounding body.

(Would like to have a nonliving model experimental system eventually.)

3. Exact issues with heart monitoring post-surgery

4. Match up of evolution rates to reality — go after antibiotic resistance in bacteria.