January 2007 RAE - Start time: 9:00 a.m., Monday, Jan. 8.

There are three problems shown below, each on a separate page. Each student has to choose one and let Kathy Lopresti (lopresti@umd.edu) know by e-mail by **1 p.m. today.** You have until **Wednesday, Jan. 17, at 5 p.m.,** to complete and submit a written report. The written report should be e-mailed to Kathy Lopresti and a hard copy delivered to her by the due time.

The requirements for the written report, as explained on the ChBE website (http://www.chbe.umd.edu/grad/phd-aptitude.html) are:

The solution to the exam problem is to be in the form of a document not exceeding 10 double-space pages using a 12pt font. The 10 pages must include the title page, proposal body, and all figures; the number of pages used for references is unlimited.

The report **must** follow the following format:

1. It should include a single title page with a project summary.
2. It should include at most 5 pages dedicated to background information relevant to the particular RAE problem (including the figures of this section).
3. The remainder of the 10 page report must focus on proposed approach to solving the stated problem, any preliminary calculations or research results, the expected outcomes of the project, and a summary of the laboratory equipment and computational resources necessary to carry out the project.

The 10 page limit will be strictly enforced.

Prof. Zafiriou will be available to answer questions Jan. 8 through Jan. 11 and again on Jan. 18. For questions during Jan. 12 through Jan. 17, please contact either Prof. Dimitrakopoulos or Prof. Raghavan. You are reminded that students are not allowed to consult with anyone during the RAE, including with faculty members. For procedural questions, you should contact the designated faculty members.

The oral exams will take place on **Friday, Jan. 19**. Each student should plan on a brief (under 30 minutes) oral presentation. The presentation file can be brought to the examination room by the student on a memory stick. If this is not possible, please contact Kathy Lopresti prior to the examination time for alternate arrangements for transfering the file.

A schedule with the exact times and room numbers for each student is given below. If unforeseen factors necessitate any changes, you will be informed by e-mail.

Schedule for January 19, 2007 oral Research Aptitude Examinations.

Chacko, George; Time: 9:00 a.m. - 10:30 a.m.; Room: 2145
Choi, Jong Hoon; Time: 10:30 a.m. -12:00 noon; Room: 2136
George, Elijah; Time: 1:30 p.m. - 3:00 p.m.; Room: 2136
Kuriakose, Shugi; Time: 9:00 a.m. - 10:30 a.m.; Room: 2136
Lee, Hee Young; Time: 1:30 p.m. - 3:00 p.m.; Room: 2145
Palathra, Thomas; Time: 3:00 p.m. - 4:30 p.m.; Room: 2136
Walker, Justin; Time: 10:30 a.m. -12:00 noon; Room: 2145

Problem 1

More that half of drugs prescribed today are chiral molecules, for which pure enantiomers are required. For example, the thalidomide that caused many birth defects in the 1960's was the (+)-thalidomide, while the the (-)-thalidomide is a safe sedative. Thus methods of separating enantiomeric mixtures are worth pursuing.

Common methods for chiral separations include high-pressure liquid chromatography and electrophoresis. Consider that you want to try to devise some new methods of chiral separation.

1) Review and discuss the two or three most common methods of chiral separation that are currently in use.[1] What are their advantages, disadvantages, and limitations?

2) Review the thermodynamics of enantiomeric mixtures and discuss the features that might be used for new methods of chiral separation.[2]

3) Design an experimental test of your proposed new method.

References

1 T. J. Ward, Chiral separations, Anal. Chem. **78**, 3947-3956 (2007).

2 J. C. Wheeler, On the Gibbs phase rule for optical enantiomers, J. Chem. Phys. **73**, 5771-5777 (1980).

Problem 2

Many drugs and pharmaceutical formulations are administered in the solid state as pills or tablets. Often, the pill mostly consists of an inert substance containing a small amount of an active pharmaceutical ingredient (API). In the manufacturing process the API is purified via crystallization and then filtered and dried to form a powder or granular material. A few kilograms of solid API is then blended into a large amount of solid inert. To insure reproducible dosage rates, the API must be uniformly distributed within the inert or matrix material. This presents a significant and important challenge, particularly for cohesive powders (those that tend to agglomerate).

Solid-solid mixing is a practiced industrial art that has recently gained the attention of academics in Engineering, Physics and Pharmacology. As a result, there is an emerging body of literature on solid-solid mixing fundamentals and the equally important question of how to acquire and test a representative sample of blended material. Two Chemical Engineering groups worth checking out are those headed by F. J. Muzzio ant Rutgers and J. M. Ottino at Northwestern. There are several others that should also be considered.

Discuss the state of the art for solid - solid mixing and sampling. Explain how current research findings can be adapted to current pharmaceutical practice. Suppose that we wanted to uniformly blend a small amount of API into an inert on a typical manufacturing scale. Propose an efficient way to do this.

Problem 3

In the first step of manufacturing the most common form of photovoltaic cell, ingots of crystalline silicon are sliced into thin wafers that are then doped, metalized, and packaged to complete the solar cell panel. The wafers are sliced in parallel, much like a loaf of bread, using a high speed stainless steel wire and a silicon carbide slurry cutting fluid.

Because of the increasing demand for solar cells, the current manufacturing bottleneck is the availability of the raw silicon, which is only slightly less pure than that used for microelectronic device substrates. Therefore, there is a strong incentive to reduce the thickness of the wafers and to investigate the potential for recycling the silicon removed in the cutting process. Much remains to be understood of the cutting process, and so the goal of this exam question is to develop an approach to mathematically model the cutting process. For this RAE problem, please consider the following:

1) What are the time and length scales of this process? Is it a steady state or dynamic process?

2) Develop the modeling equations describing the two-phase flow of cutting fluid as it flows between the wire and silicon; also consider the the size distribution of the SiC and Si particles and assess whether the modeling techniques used for chemical-mechanical polishing (CMP) in semiconductor manufacturing can be used to describe the cutting process.

3) Describe the numerical techniques to be used to solve the modeling equations; discuss the overall strategy for cutting process optimization.

4) Consider whether it would be feasible to separate the silicon removed in cutting from cutting solution and recycled.