Research Aptitude Problem 1
Scavenging of aerosol particles by ice crystals

Ice crystals, also known as single snowflakes, can serve as scavengers of aerosol particles during snowfall precipitation events. Paleoclimate experts are very interested in the dynamics of this scavenging process because through chemical analysis of glacier ice core samples, it is possible to obtain information about the composition of past atmospheres. There are two main mechanisms of ice crystal growth: vapor diffusion and accretion of supercooled water droplets. Aerosol particles may serve as ice nucleation and cloud condensation nuclei or may be scavenged by other routes. For this research aptitude problem, please address the following questions:

1. Which mechanism (vapor phase vs. accretion of supercooled droplets) is generally more effective at scavenging and why? Another way to rephrase this is which method results in the dirtiest snow? Hint: thermophoretic diffusion and the thermodynamics of phase change play a role.
2. It is known that chemical composition is a factor in ice crystal and cloud droplet nucleation although the details are still under discussion. Are differences in aerosol chemical composition important when it comes to scavenging (which happens after the nucleation step).
3. After surveying the literature, develop an original testable hypothesis within the general area of effects of chemistry and/or aerosol microstructure (aerosol diameter, shape etc..) on removal of aerosol phase material by scavenging during snow precipitation events.
4. Develop an experimental plan as well as a simple modeling framework for testing your hypothesis. How would you measure scavenging rates? Given uncertainties in your experimental system, what level of detail in your model is reasonable? How would the model be solved?

A useful reference might be:
Baltensperger et al., Transfer of Atmospheric Constituents into an Alpine Snow Field, *Atmospheric Environment,* **27A** 1881-1890 (1993).

Research Aptitude Problem 2
Solar hydrogen production from methane

Methane gas is produced by the action of bacteria as they digest cellulose in the buried waste. The gas generally is a 50/50 mixture of methane and carbon dioxide and is saturated with water vapor.

A growing industry has developed to process that gas into useful energy products, instead of the more traditional practice of flaring the gas or letting it seep into the atmosphere. One company (shec-labs.com) has proposed a solar powered syngas/shift hydrogen production system in which the overall endothermic energy needs of the steam reforming and gas shift reactions are met with a concentrating solar reflector system.

The focus of this research aptitude exam is to develop a dynamic model of the tubular, heterogeneous catalytic reactor systems used to carry out the methane reforming and gas shift reaction. Special emphasis is to be placed on the thermal dynamics of the reactor systems, so that questions of how quickly the reactors can return to steady state can be answered. The motivation for the research is to assess the feasibility of using solar energy to heat the reactors, given the rapid changes that can take place when a cloud passes between the sun and the collectors, and that the reactors must be restarted every morning - an unusual operating mode for many industrial reaction processes.

Specific issues and questions that should be assessed in the solution to this RAE problem are the following:

1) Give a brief overview of the methane reforming and shift reactions, discussing the currently used catalysts and the design decisions that must be made in these equilibrium-limited reactions.

2) Propose how you would assess whether the landfill gas can be used as-is for feed to the reforming reactor, or whether most of the CO2 must first be scrubbed; given an overview of typical gas dehydration and CO2 scrubbing processes.

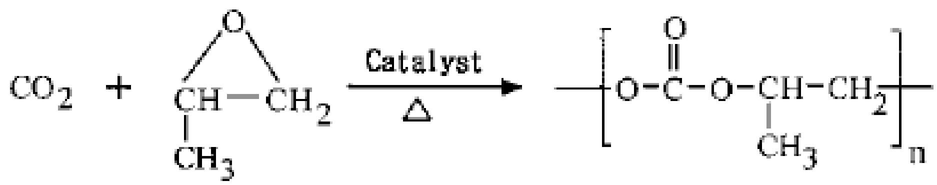
3) Describe the modeling equations needed for each reactor - what are the important chemical reactions, and the main chemical species and energy transport mechanisms? How is the solar heating aspect of the reactor to be modeled?

4) How would the modeling equations be solved? Describe the appropriate numerical methods.

5) Assess the process measurement and control strategies that would be required to operate these reactor systems.

Research Aptitude Problem 3
CO_2 Capture through chemical reactions

Carbon dioxide (CO_2) is the most well known greenhouse gas and its emission needs to be minimized or completely avoided in current and future chemical processes. CO_2 is a very stable compound but it reacts with cyclic ether compounds such as ethylene oxide, propylene oxide, and isobutylene oxide to form high molecular weight aliphatic polycarbonates.



Since CO_2 has low reactivity, high activity catalysts are needed for the copolymerization process. The examples of most widely used catalysts are $Zn_3[Fe(CN)_6]_2$, ZnO/glutaric acid, and $Zn(OH)_2$/glutaric acid.

1. Review recent literature on the properties and applications of aliphatic polycarbonates
2. Review literature on the current industrial polymerization processes, polymerization kinetics, and identify technical challenges.
3. Develop a kinetic model for the copolymerization of CO_2 and a chosen cyclic ether comonomer and apply it to the modeling of appropriate polymerization reactor systems (e.g., batch reactor, continuous reactor).
4. Perform model simulations and discuss the results. Propose what you would do to solve some technical challenges you have identified in (2).

Reference: M. Ree et al. *J. Polym. Sci.: Part A: Polym. Chem*. 37, 1863-1876 (1999).