Modeling problems related to our environment

organized by
Ali Nadim and Ami Radunskaya

Workshop Summary

What do green buildings, environmental toxins, sources of ozone pollution in the atmosphere, and infrastructure planning for electrical power have in common? They were all topics of intense study at a workshop called "Modeling Problems Related to our Environment" which took place at the American Institute of Mathematics in Palo Alto, CA during the week of January 14, 2013. This workshop operated in a format similar to the Math-in-Industry Study Groups in which the problems are introduced on the first day by liaisons from industry. The participants then divide into teams and spend the week working on the problems. Each team presents its "solution" to the problem on the last day. Four projects were considered in the present workshop. These are briefly described below with a listing of the liaisons and participants in each group. Detailed technical reports on each project are available by contacting the workshop organizers.

Project 1:: Thermal Management of Green Buildings, introduced by the architectural firm EHDD of San Francisco [Liaison: Scott Shell, Participants: Jan Baetens, Chiu-Yen Kao, Eun Heui Kim, Ali Nadim, Remy Ndangali & Ami Radunskaya] A frontier in design and manufacture of houses is the so-called "passive house" or its original European counterpart "passivhaus" movement where, through a combination of air-tight construction and smart insulation, residential houses as well as office and lab buildings can be designed that use minimal (nearly zero) energy for heating and cooling. Just the presence of a few warm bodies (i.e., people) and the typical lighting and appliances in the house are enough to heat it to a comfortable temperature, even in the relatively cool northern European climate. The group at the workshop put together a mathematical model of such a house, accounting for heating by the incident sunlight and the internal sources (appliances and people), as well as for the controlled ventilation, convection to the outside air, and heat transfer through windows and to/from the ground. Perhaps not surprisingly, it turned out that for a well-insulated house, it was indeed possible to achieve a comfortable indoor temperature without needing an actual furnace or heater. The team also investigated the use of phase-change materials as part of the insulation to see their effect on increasing the thermal mass of the house without impacting its actual physical mass. The thermal simulator developed at the workshop can potentially be used by designers to better assess the thermal characteristics of a given house, given its solar exposure, wall and window materials, etc.

Project 2:: Source Apportionment for Atmospheric Ozone, brought by the US Environmental Protection Agency [Liaisons: Sergey Napelenok & Rohit Mathur, Participants: Joseph Fehribach, Natali Hritonenko, Antonio Palacios, S. T. Rao & Xiaoming Wang] It turns out that the amount of ozone in the troposphere is dictated by the amounts of multiple precursor chemicals (mainly nitrogen oxides and volatile organic compounds), each originating at distributed locations in space and time, as well as by exposure to sunlight during the daytime hours. The series of chemical reactions leading to ozone formation are extremely complex and nonlinear, and are coupled to atmospheric transport by convection and turbulent diffusion. The goal of the EPA as a regulating agency is to assess which of the many potential sources of the precursor chemicals (emissions from cars, factories, etc.) is the contributor to the measured ozone levels at various locations and times. This is a very challenging inverse problem. The team at the workshop proposed various approaches to this problem using Proper Orthogonal Decomposition and sensitivity analysis methods, and it also studied ways of further simplifying the mathematical description of the complex nonlinear chemistry by trying to identify and eliminate (from the model) those intermediaries that do not play as big a role in the overall kinetics of ozone production.

Project 3:: Characterization of Toxic Chemicals in the Environment, also brought by the US Environmental Protection Agency [Liaison: Richard Judson, Participants: Vijay Chickarmane, Cymra Haskell, Felicia Maria Magpantay, Nessy Tania & Jean Taylor] Hormones, and estrogen in particular, interact with receptor molecules and trigger a cascade of molecular reactions in the body, called the estrogen pathway. In this problem the group tried to determine whether man-made chemicals affect this chain of reactions, thereby disrupting the natural balance of chemicals in our body. In order to test the action of various chemicals, *in vitro* tests have been developed which are far more efficient and cheaper than live animal testing. However the reactions that take place in these tests are themselves complex, and so a positive reading on one of these tests could also be due to activity that is unrelated to the estrogen cascade. For this reason, several different tests are performed on each chemical in order to determine its effect on the estrogen pathway. The EPA provided the team with data from multiple tests on 1800 chemicals. The problem was to determine from this data which chemicals activated the estrogen pathway, hence causing imbalance in the body. Previous attempts to solve this problem used statistical analyses based only on the data. In contrast, the AIM team used knowledge of the chemical reactions involved in the estrogen pathway, along with the data, to formulate a constrained optimization problem whose solution indicates each chemical's tendency to interfere with these reactions. The team's method was tested on a group of thirty-five reference chemicals that are well understood, yielding good results. The method can be refined so that the EPA can use it to effectively test chemicals on other hormonal pathways.

Project 4:: Infrastructure Planning Based on Weather Sensitivity, introduced by Southern California Edison (SCE) [Liaisons: Frank Gonzales & Robert Tucker, Participants: Barbara Bailey, Joseph Biello, Gabe Chandler & Wenling Shang] Understanding the dynamics of electrical demand is important in planning power infrastructure in order to optimize our energy resources. One important feature to understand is how energy use depends on weather conditions. SCE brought the group historical data of the demand at different distribution stations. The problem was to understand which stations were winter-peaking (i.e., peak demand at low temperature), which were summer-peaking (peak demand at high temperature) and which locations were temperature-independent (i.e., no correlation). The AIM team developed several statistical tests to understand these correlations. In particular, they found that a linear regression was not sufficient to capture significant correlations; rather, piecewise linear regressions were much more effective. One interesting discovery was that winter-peaking stations were more important in terms of energy demand than SCE had previously thought. The AIM team was also able to give SCE advice on how to improve data collection and recording. These predictive models have the potential to enable energy companies to plan effectively, and to accurately evaluate the benefits of the use of solar panels and other types of renewable energy that depend on weather conditions.