Modeling Desulfurization of Natural Gas for Fuel Cells

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Commercial energy systems based on fuel cells run off of pipeline natural gas supplied by public utility companies. Impurities are often introduced into the gas by the utility companies, either by design or as a result of processing and/or transmission. For example, various sulfur compounds are introduced to provide an odor for the purpose of leak detection. These impurities are harmful for fuel cells, and must be removed by desulfurization systems. A typical desulfurization system consists of a series of canisters packed with absorbing materials (e.g. activated carbon pellets) through which the natural gas flows prior to entering the fuel cells, see Figure 1. The concentration of impurities in the pipeline gas is very low, typically around 1–5 parts per million (by volume), but this is still too high for fuel cell systems, which require a much cleaner gas feed with an impurity concentration less than 5 parts per billion.

![Figure 1: Schematic of a fuel cell energy system with a series of desulfurization vessels designed to remove impurities in the natural gas feed prior to entering the fuel cells.](image)

The basic task of the student team working on this problem will be to model the sulfur concentration of the gas feed passing through a desulfurization vessel consisting of a packed bed of absorbing pellets. Of particular interest is the so-called break-through time, i.e. the time it takes for the vessel to become sufficiently fouled so that the natural gas exiting the vessel does not meet the low-impurity threshold of the fuel cell system. Mathematical models can provide a predictive capability of the break-through time, and may also suggest improvements in the design. This problem is rich in techniques of applied mathematics, including multiscale modeling, asymptotic analysis and numerical methods for differential equations, and it will likely provide a fun challenge for the students on the team. It is expected that the team will begin with simplified “toy” models of the desulfurization vessel to get warmed up and to understand the basic modeling issues and analysis, prior to considering more complex models.