My research activities are in separative chemical reactors, detailed chemical kinetics modeling of complex reaction systems, and the chemistry of air pollution. In the first subject we are investigating simulated countercurrent moving bed reactors. These are continuous flow reactors in which chemical reactions are carried out in the presence of solid adsorbents so that both separation by adsorption and chemical reaction are integrated into a single process unit. Carrying out separation during chemical reaction can overcome reactant conversion limitation because of chemical equilibrium. Furthermore, the integration of reactor and separator can lead to considerable savings in capital and operating costs.

Detailed chemical kinetics models (DCKM) are a fundamentals based approach to describing complex chemical reactions and reactive flows. They incorporate elementary reactions (the individual molecular interactions by which chemical change occurs), coupled with transport of matter and heat. Kinetics and thermodynamic data bases, and molecular theories of kinetics assist the determination of individual reaction rates. Computational quantum chemistry is a powerful tool when kinetic and thermodynamic data are not available. Good DCKM provide predictive models for chemical reactors, and they provide a rational basis for accurate model reduction and for reactor optimization. Industrial chemical processing, combustion, and atmospheric chemistry, among others, are areas where DCKM can be used to good advantage.

Our work on air pollution chemistry is currently focused on the chemical reactivity of halogenated alkoxy radicals. These species are intermediates in the atmospheric degradation of halogenated compounds, some of which occur naturally, and many of which make their way into the atmosphere through human activity. Many aspects of haloalkoxy radical chemistry are not well understood. Haloalkoxy radicals are key intermediates in determining where the fluorine, chlorine and bromine from atmospheric pollutants finally reside in the environment. We do laboratory studies of haloalkoxy reaction kinetics and mechanisms, complementing the experimental work with computational methods for molecular structure and energetics, and with molecular reaction rate theories, to address environmental concerns.

Selected Publications
Ab Initio Molecular Orbital and RRKM Calculations of the Thermal Unimolecular Dissociation of the CH2ClO Radical (with F. Wu), J. Phys.


