A WEB-BASED LIBRARY OF LOW PRESSURE FLAME DATA

SAND2006-4926C

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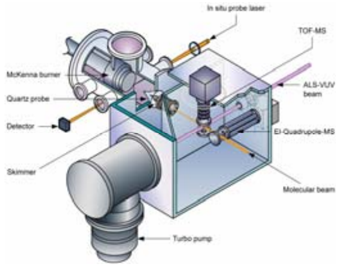
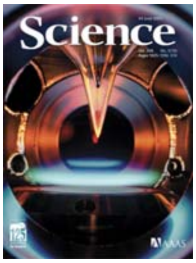
Introduction

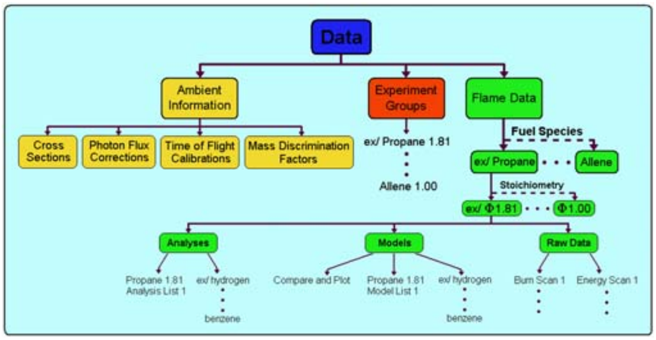
The elucidation of chemical mechanisms of combustion is a crucial element of our fundamental understanding of combustion processes. Our knowledge of chemical mechanisms is often succinctly represented by detailed chemical kinetic models derived from both theory and quantitative experiments based on state-of-the-art diagnostics. In particular, it has proven particularly valuable to compare experimental data from low pressure, one-dimensional laminar flames to models employing detailed chemical kinetics. These comparisons facilitate the determination of important species and chemical pathways in combustion, improving our understanding of pollutant formation, ignition, and other kinetically controlled phenomena and providing validation and improved accuracy for current models. Furthermore, advanced computers and algorithms are enabling the application of increasingly sophisticated models in computations of realistic systems. Validation of detailed chemistry models against a range of precise measurements under thoroughly characterized conditions increases the confidence with which flame models can be applied in scientific and engineering simulations.

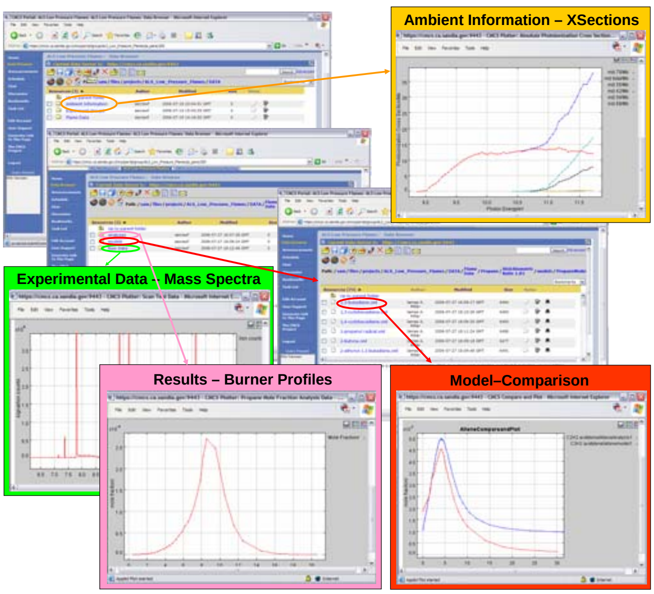
In collaboration with the groups of T. A. Cool of Cornell University and K. Kohse-Höinghaus of the Universität Bielefeld, Germany, significant data on the composition of complex flames has been obtained using flame-sampling photoionization mass spectrometry with a newly developed mass spectrometer and photons from the continuously tuneable synchrotron Advanced Light Source at Berkeley. Experimental results are available of a variety of different flames using fuels representing the major classes of chemicals appearing in modern fuel blends: alkanes, alkenes, alkynes, cyclic hydrocarbons, aromatics, alcohols, ether, and esters. In summary, a wealth of information for chemical kinetic modelling can be provided and we hope that combustion models can be made more accurate and more robust by considering the results.





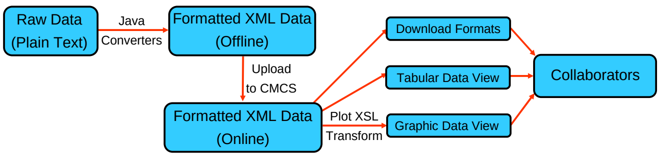
Organization of ALS Data on CMCS



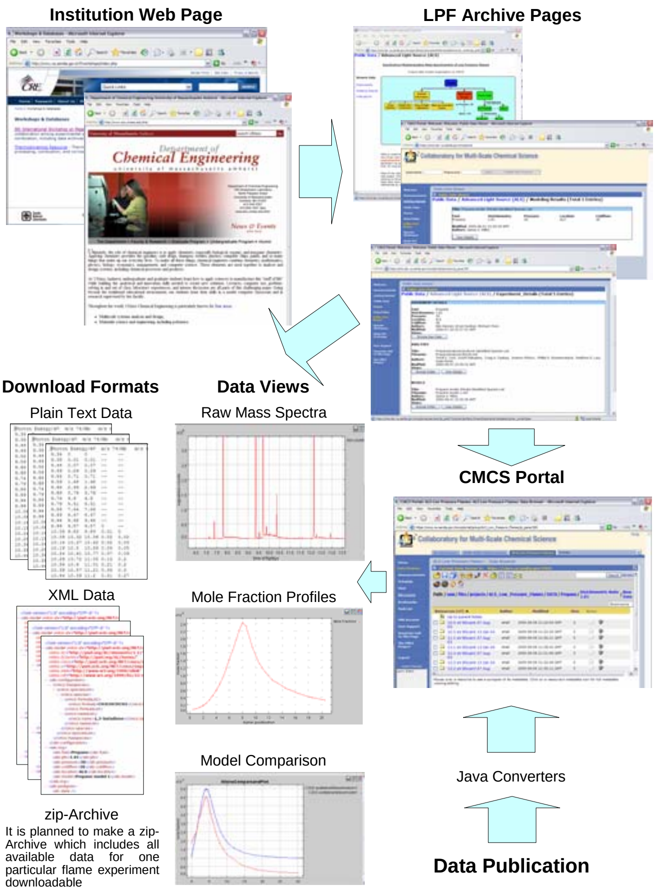


Rapid Data Conversion and Publishing

There are two obvious infrastructure challenges: (1) Making storage, reprocessing, and retrieval of results straightforward and (2) Developing procedures to make the data archival. To this end, we have made use of the collaborative data sharing and XML technologies offered by the CMCS infrastructure. This work includes the development of a data schema that includes important metadata previously locked away in handwritten laboratory notebooks. Use has been made of automated XML translations that allows easy visualization of data files according to their type. These same technologies are now being applied with some new interfaces to facilitate the public release of the data to the combustion community.



Data Access From CMCS Archive



Conclusions

- ✓ A web based library of well-documented flames is currently under construction using the Collaboratory for Multi-scale Chemical Science (CMCS) at www.cmcs.org.
- ✓ Raw data, processed data, and the codes and methods to go from one to the other will all be archived for direct use or for reanalysis as new information appears.
- ✓ A functional prototype (based on a subset of the available data) is presented to obtain feedback from the combustion research community.
- ✓ The goal is to advance basic scientific understanding of flame chemistry by facilitating the development and validation of more accurate chemical models, and models for new fuels and related reactants, that are appropriate for model validation.

Acknowledgements

This work is supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, and by the Office of Advanced Scientific Computing Research, Mathematical, Information, and Computational Sciences, U. S. Department of Energy. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the National Nuclear Security Administration under contract DE-AC04-94-AL85000. The authors also gratefully acknowledge contributions by Eric Hall, Michael Chen, Scott Crawford, and Erwin Dunbar.