A New Web Archive
For TNF Workshop Data

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Abstract

Much current scientific data is understandable by humans but is not in an inter-operable format that is easily searchable and translatable by computers. To remedy this, a prototype of a new web based archive for the publication of TNF Workshop data has been established. In addition, piloted flames C, D, E, and F data has been re-released in an interoperable format that takes advantage of this new web based archive to display online views of the data and automatic translations of the data into useful, downloadable formats (e.g. plots, tabular views). The archive also allows for data to be browsed in a hierarchical folder structure or viewed on an automatically updated webpage. The ability to accept TNF data from any institution, including modeling and simulation data, is envisioned. Currently, a TNF group has been established on the Collaboratory for Multi-scale Chemical Science (CMCS) Web Portal. TNF Workshop participants can join this group to learn more about the tools and see examples regarding the sharing of data through the new prototype web archive.

Data File Formats

For data to take advantage of the new web based archive's capabilities, it must adhere to a few conditions. To use the provided Java tool, the data must first be in a plain text file with white-space delimitation (see Figure 1). The text file is allowed to contain metatag headers (Figure 2) to provide a title, abstract, authors, collaborators, date, type of data, etc. Once the data file is in this format, the Java conversion tool may be used to convert the plain text file into an Extensible Markup Language (XML) file (Figure 3). Once in XML, the data can be uploaded to CMCS, providing the ability to share data and view it in a variety of formats.
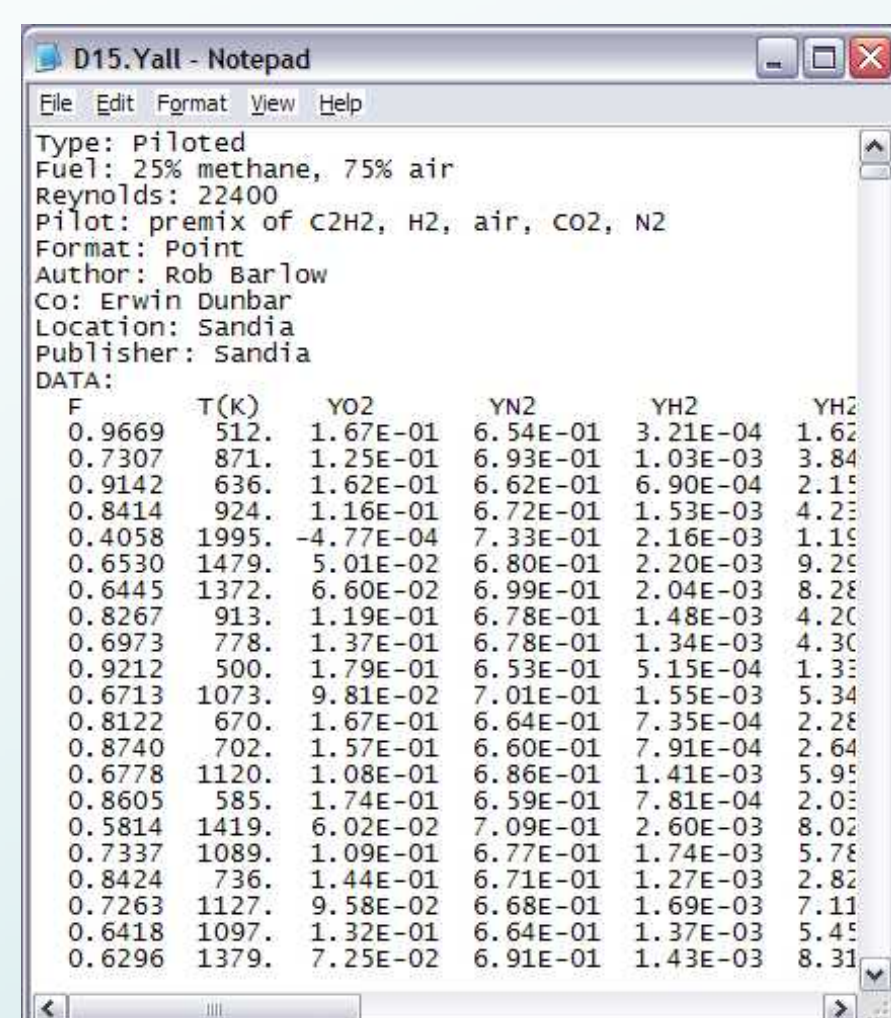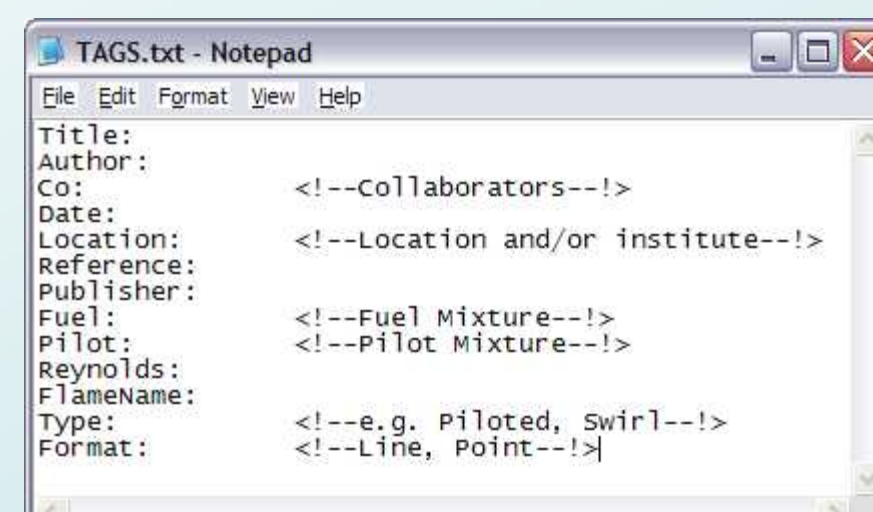

Figure 1: Text Data Schema

Figure 2: Currently Allowed Data File Metatag Headers (can be expanded to fit new headers)
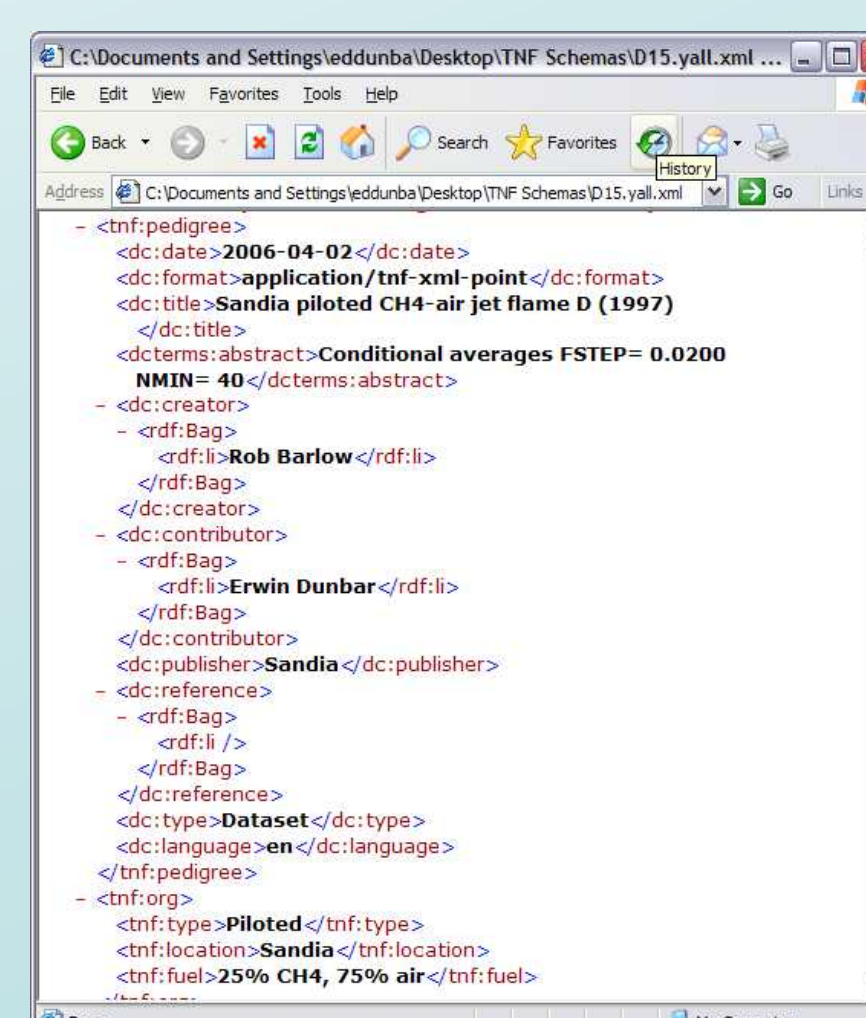
Figure 3: XML Data Schema

Future Expansion

This archive is intended to also present the data in a format that not only works well today but will also be compatible with the computer software of tomorrow. Since XML is a well established standard, viewable in any web browser, future support is guaranteed. Further, new plots and views can be produced without having to alter the data files. The Java program is being released as Open Source, providing the ability for future users to modify the program to fit specific needs.

There is also an expanding need for shared information within the TNF workshop. Participants are therefore encouraged to consider contributing their data to this new web archive– particularly simulation results, modeling results, and image data.
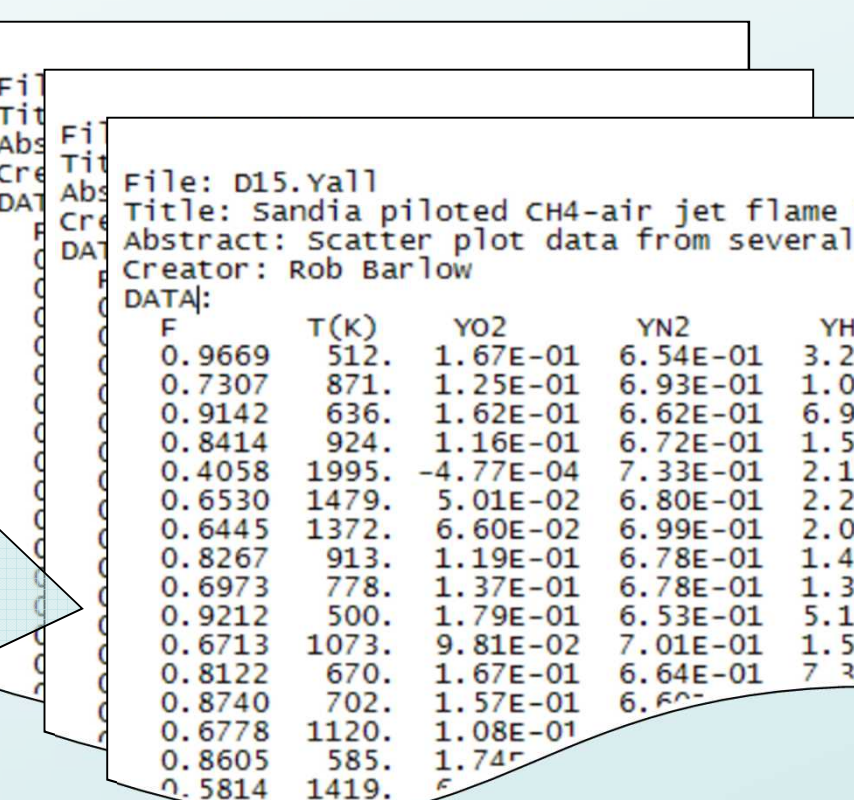
Implementation
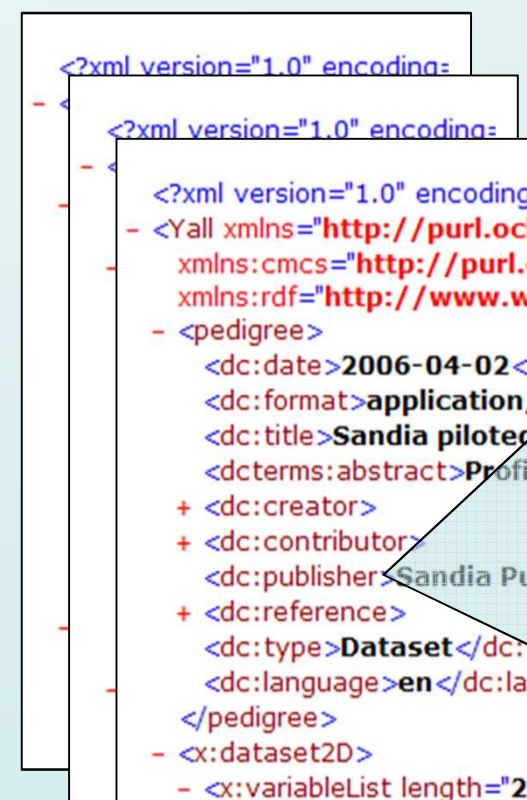
Institution Web Page
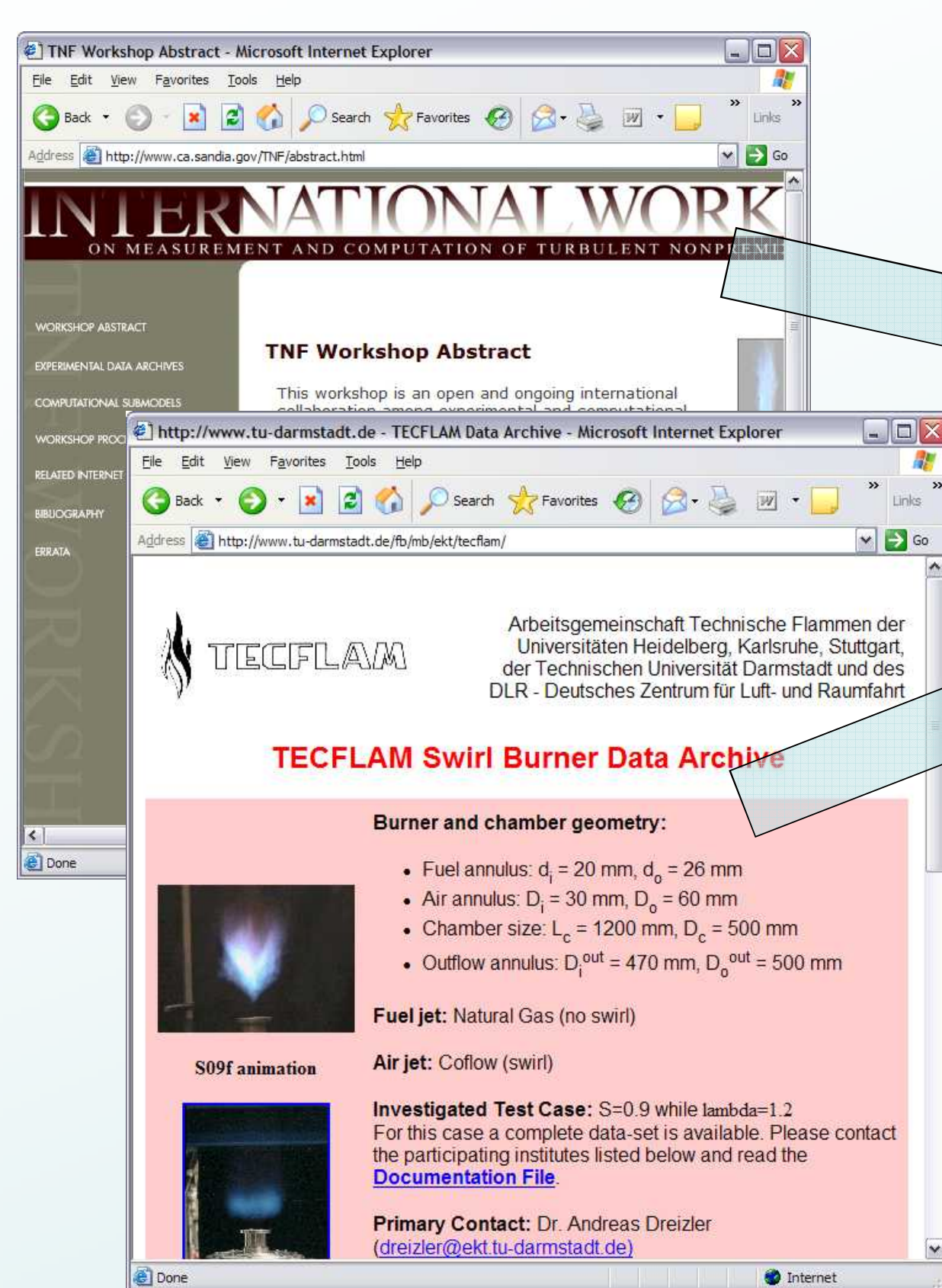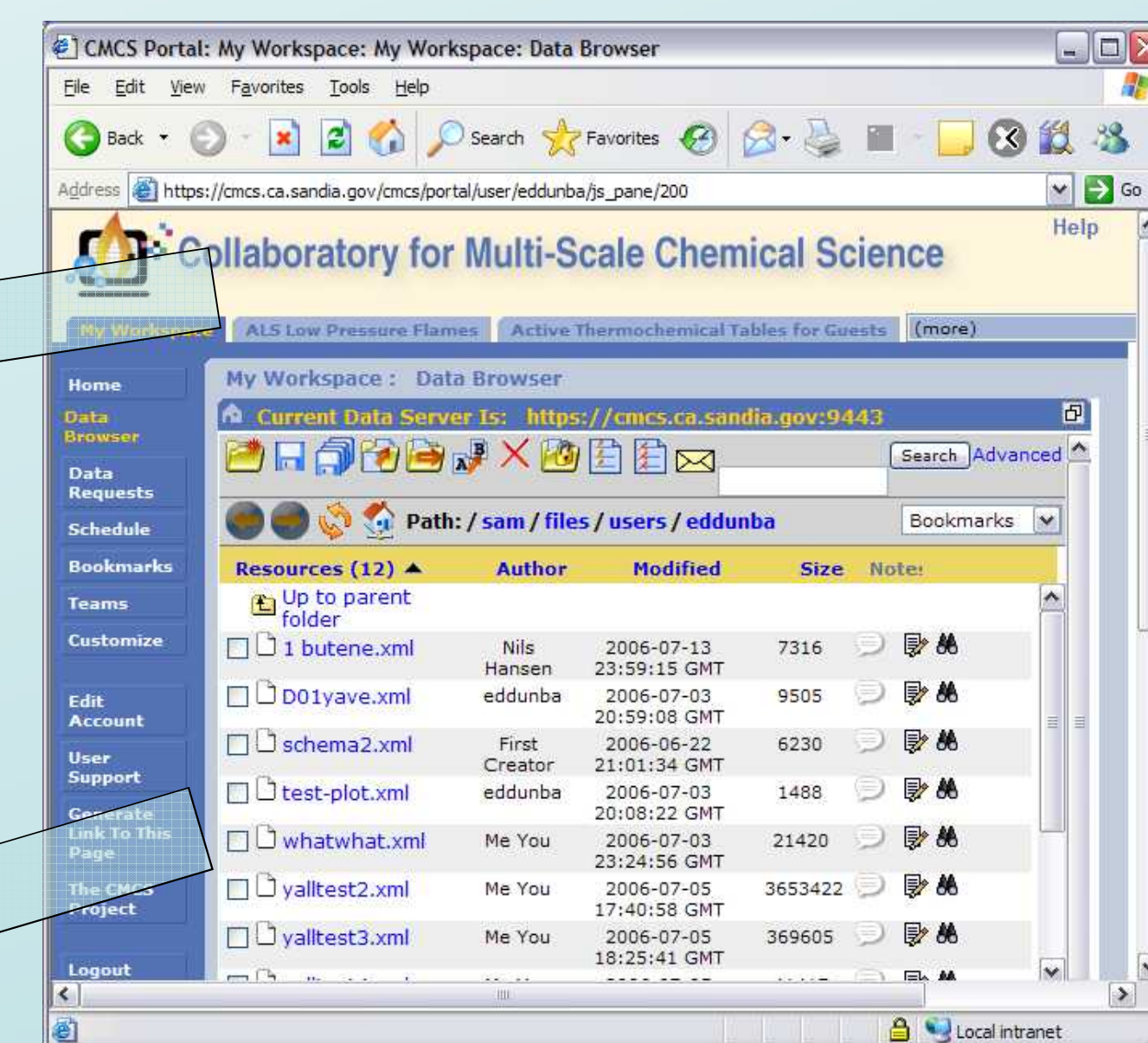
TNF Archive Pages
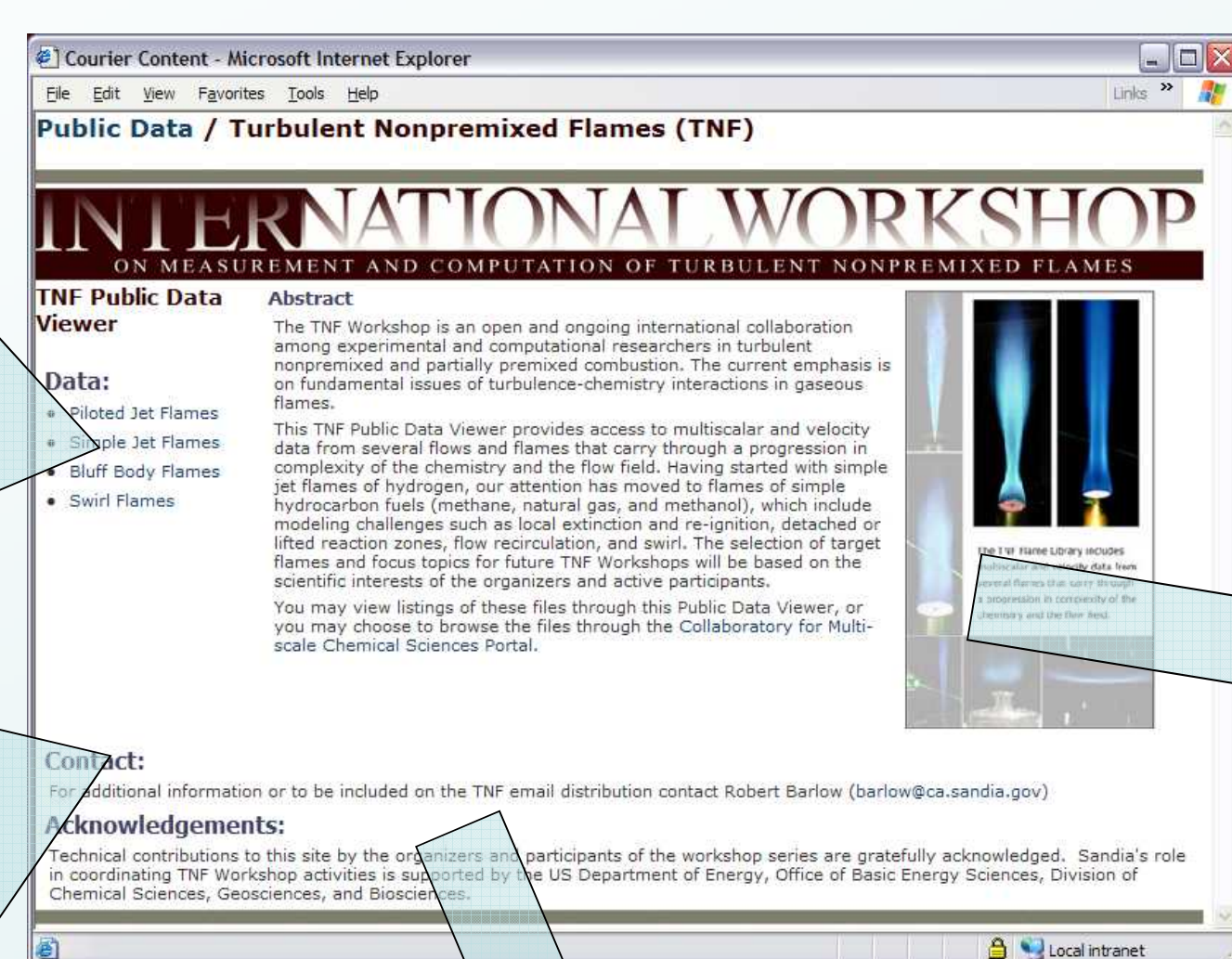
Downloadable Formats

Plain Text Data

XML Data

CMCS Portal
www.cmcs.org

Data Views
Plots
Tables