Reaction kinetics data in the ReSpecTh information system

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Introduction

Increased fuel flexibility and carbon efficiency of energy production are important aims of recent combustion research. Improved science-based understanding of these processes requires modern, preferably active chemical information systems containing carefully validated data of traceable origin. Such information systems exist in the field of reaction kinetics, but most of them focus on direct experiments only (*i.e.* experiments for the determination of rate coefficients of elementary reactions) or their main interest is not combustion, but atmospheric chemistry.

ReSpecTh is an information system containing **re**action kinetics, high-resolution molecular **spe**ctroscopy, and **th**ermochemistry data. ReSpecTh is a dynamic website written in PHP with client-side jQuery services. Most data are stored in MySQL databases. One of the unique features of ReSpecTh is the joint and extended utilization of all available experimental and computational information. The reaction kinetics data and computer codes are all related to combustion simulations.

The ReSpecTh website was set up at the dedicated address http://respecth.hu/. The datasets and computer codes are available after a login authentication.

Experimental data

The experimental reaction kinetics data are currently all related to the combustion of hydrogen. In the near future, this collection will be extended to include the combustion of syngas, hydrocarbons, and alcohols. The data include 223 indirect combustion experimental datasets related to ignition delays, measured in shock tubes and rapid compression machines (RCMs), as well as laminar burning velocities and concentration profiles, measured in various types of reactors. A dataset contains those datapoints that were consecutively measured using the same apparatus at similar conditions except for one condition that was systematically varied. 56 direct measurements of rate coefficients of 10 H/O elementary reactions are also included in the database. The hydrogen combustion related data have been used for testing several recently published reaction mechanisms [1] and for the creation of a new optimized reaction mechanism [2].

The database of indirect experiments is searchable according to the type of the experiment (*e.g.* RCM, shock tube, jet stirred reactor), the experimental conditions (initial pressure and temperature), and the type of the fuel and bath gas. The direct experiments can be searched according to the stoichiometry of the elementary reaction.

All reaction kinetics data are stored according to the ReSpecTh Kinetics Data Format Specification (RKDFS). RKDFS is directly based on the PrIMe experimental data format [3] and most of the specification is directly derived from the XML elements and attributes defined within PrIMe. However, in the PrIMe format some experimental setups are not

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defined unambiguously. The RKDFS format extended the PrIMe format with new elements, therefore it is uniquely interpretable by computer codes. This data format is described in a document and consists of a set of specifications, aiming to provide an unambiguous definition of the storage of combustion experimental data and rate coefficient measurements. RKDFS defines an XML data format to provide flexible data representation and allow for easy extension of the format specification.

Utility codes

The ReSpecTh site contains a utility code (called Rep) for the creation of RKDFS-format datafiles from the users own measurements or published experimental data. Also, Rep automatically creates input files for the SENKIN, PRS, and PREMIX simulation codes of the CHEMKIN-II [4] package from an RKDFS-format indirect experimental datafile. This way the experimental data can be easily simulated using any CHEMKIN-format reaction mechanism. Since the source code of the Rep program is provided, it can be easily modified to use with any other combustion simulation code. The aim of providing an accurate data format specification, and utility codes for the creation and interpretation of datafiles is that we want to support the long-term and laboratory-independent storage of experimental data and make mechanism testing faster.

A series of utility programs developed in Budapest [5] and relevant to the analysis of reaction kinetics models are also available on the ReSpecTh site. The names of these codes are KINALC, MECHMOD, KINAL, FluxViewer, SEM, *u-Limits*, UBAC, JPDAP, SAMAP and ReactionKinetics.

Combustion mechanisms

A collection of hydrogen and syngas combustion mechanisms was also made available on the ReSpecTh site. These mechanisms were investigated in the recent publications of Olm *et al.* on hydrogen combustion [1] (20 mechanisms) and syngas combustion [6] (16 mechanisms). The ELTE-2015 optimized hydrogen combustion mechanism [2] and the Leeds Methane Oxidation Mechanism are also available. The ReSpecTh site contains the mechanisms in Chemkin format, together with the corresponding transport files and references to the origin of the mechanisms.

References

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