IUPAC Subcommittee for Gas Kinetic Data Evaluation

International Union of Pure and Applied Chemistry (IUPAC)

Sub-committee members: R.A. Cox[1], G.D. Carver[1], R. Hynes[2], R. Atkinson[3], J.N. Crowley[4], R.F. Hampson[5], M.E. Jenkin[6], M. J. Rossi[7], and J. Troe[8]

1. Centre for Atmospheric Science, University of Cambridge, CB2 1EP, UK.
2. CSIRO Energy Technology, East Entrance, Riverside Corporate Park, Delhi Road, North Ryde, Sydney, 2113, PO Box 136, North Ryde, NSW 1670, Australia.
3. Air Pollution Research Center, University of California, Riverside, California 92521, USA
4. Max-Planck-Institut fur Chemie, Division of Atmospheric Chemistry, Postfach 3060, 55020 Mainz, Germany
5. U.S. Dept. of Commerce, National Institute of Standards and Technology, Bldg. 221, Rm A111, Gaithersburg, MD 20899, USA
6. Dept. of Environmental Science and Technology, Imperial College London, Silwood Park, Ascot, Berkshire SL5 7PY UK
7. Environment Naturel, Architectural et Construit, Pollution Atmospherique et Sol (LPAS/ENAC), EPFL, CH 1015 Lausanne, Switzerland
8. Institute of Physical Chemistry, University of Gottingen, Tammannstr. 6, D-37077, Gottingen, Germany

http://www.iupac-kinetic.ch.cam.ac.uk/

Background

The Sub-committee for Gas Kinetic Data Evaluation (I.4), which comes under IUPAC's Physical and Biophysical Chemistry Division, aims to enhance the accessibility and availability of evaluated kinetic data. The problem with data availability and consistency was noted in the 1970's, when it was recognised that a standardised data set was required for the modelling of atmospheric chemistry. Improvements to relevant physico-chemical data continue to be made and the need for reliable atmospheric chemistry modelling is as pressing as ever. Evaluation of gas kinetic data first started, under the auspices of IUPAC, in 1977. Recommendations were published in a series of nine peer reviewed articles in *J. Phys. Chem. Ref. Data*. Huge improvements have since been made, in the dissemination of the evaluated data, with the use of the Internet.

Website

The website, which has been operational since July 1998, currently has about 4000 accesses per week. The growth in Internet traffic can be seen in Figure 1. The number of regular users of the database is also growing: currently 336 people are subscribed to the mailing list, an increase of 10% on the previous year. From the homepage of the website, see Figure 2, it is possible to join the mailing list, access data sheets and download supplementary information. An example of a data sheet is shown in Figure 3.

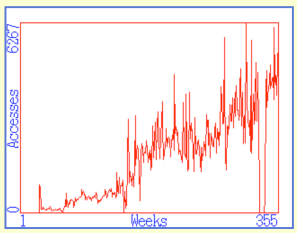

Figure 1. Graph to show the increase in web traffic to the IUPAC Gas Kinetics database over the last 6.5 years. Statistics were not counted for a period in 2004.

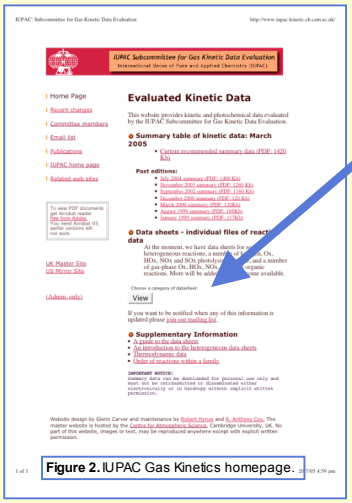

Figure 2. IUPAC Gas Kinetics homepage.

Drop down menu gives access to data sheets:

- Heterogeneous data sheets (non-reactive)
- Heterogeneous data sheets (reactive)
- Data sheets for photolysis of halogenated species
- Data sheets for gas phase Ox reactions
- Data sheets for photolysis of Ox species
- Data sheets for gas phase HOx reactions
- Data sheets for photolysis of HOx species
- Data sheets for gas phase NOx reactions
- Data sheets for photolysis of NOx species
- Data sheets for gas phase SOx reactions
- Data sheets for photolysis of SOx species
- Data sheets for gas-phase organic reactions:Ox + VOC
- Data sheets for gas-phase organic reactions:HOx + VOC
- Data sheets for gas-phase organic reactions:NO_3 + VOC
- Data sheets for gas-phase organic reactions:halogens + VOC
- Data sheets for gas-phase organic reactions: organic peroxy radicals
- Data sheets for gas-phase organic reactions: organic alkoxy species
- Data sheets for gas-phase organic reactions: organic radicals + oxygen
- Data sheets for inorganic FOx reactions
- Data sheets for organic FOx reactions
- Data sheets for inorganic ClOx reactions
- Data sheets for organic ClOx reactions
- Data sheets for inorganic BrOx reactions
- Data sheets for organic BrOx reactions
- Data sheets for inorganic IOx reactions
- Data sheets for organic IOx reactions
- Data sheets for the photolysis of organic species

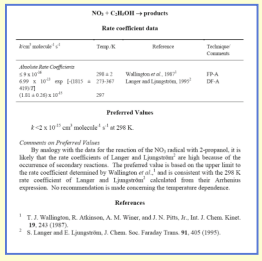

Figure 3. An example of a data sheet. This is not a typical example: it has been chosen for its brevity!

Scope

The Internet-based Gas Kinetic Data Evaluation consists of a summary table of reactions and preferred rate data, together with more detailed data sheets. Supplementary information is also included, which aims to assist individuals in their use of the data, and includes explanations of nomenclature and conventions etc. A list of relevant enthalpy data is also included. Heterogeneous data sheets are currently only a compilation and not a recommendation.

The data sheets are available in a series of categories which include:

- Gas phase and photolysis reactions of Ox, HO_x, NO_x and SO_x species.
- Gas-Phase and photolysis reactions of organic species (including reactions with HO_x, NO_3 and halogen radicals).
- Reactions of organic peroxy radicals, organic alkoxy radicals and other organic radicals with oxygen.
- Gas Phase and photolysis reactions of inorganic FO_x, ClO_x, BrO_x and IO_x species.
- Gas Phase and photolysis reactions of organic halogen species.
- Uptake coefficients for non-reactive and reactive heterogeneous processes.

In carrying out its work the Sub-committee also aims to stimulate and direct further laboratory-based research, as well as encouraging consistent usage of the existing data.

Figure 3: The figure shows research being carried out at the laboratories of LPAS, EPFL, Lausanne. One of the aims of the Gas Kinetics Subcommittee is to help stimulate and direct further research.

Current Projects

In order to produce a peer-reviewed, citable and permanent archive of the data evaluation, at the present time, the evaluated data are being published in the Journal of Atmospheric Physics and Chemistry http://www.copernicus.org/EGU/acp/. As the database covers a large number of reactions, the publication is being broken down into four sections. The first is now in Atmospheric Chemistry and Physics Discussions and the second is awaiting publication. Two further sections will be published in the near future. The website is also being regularly updated. Changes have been made to enable more rapid updating of the site and a mirror site has been set up at the IUPAC headquarters website in North Carolina. Updates to the data sheets have been made and a new summary table was published in March 2005. The remaining work for this year includes updating some of the halogen species datasheets and datasheets for the heterogeneous reactions.

Future Projects

The user community has informed members of the Sub-committee of their requirements to access the evaluated data directly by using model input code etc. It is also apparent that a more readily searchable database is required. A consultation exercise, in conjunction with the EU ACCENT programme, http://www.accent-network.org/, will be carried out, to determine the preferred database format(s). Please register with the IUPAC Gas Kinetics mailing list (see website) to take part in the questionnaire.

Acknowledgements

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