COMMITTEE ON DATA FOR SCIENCE AND TECHNOLOGY

66 **CODATA** / NEWSLETTER

FEBRUARY 1994

HIGHLIGHTS

The **Committee on Data for Science and Technology (CODATA)** was established in 1966 by the International Council of Scientific Unions.

Working on an interdisciplinary basis, CODATA seeks to improve the quality, reliability, processing, management, and accessibility of data of importance to science and technology.

14th International CODATA Conference
Chambéry, France — September 18-22

CODATA '94 was organized by CODATA France, on behalf of international CODATA, an interdisciplinary Scientific Committee on Data for Science and Technology of the International Council of Scientific Unions (ICSU).

CODATA '94 has two principal objectives: to update research and the choice of essential data in two, sometimes associated fields—that of *innovation* (search for new materials) and that of the *environment*. This latter leads to a search for data fundamental for carrying out vast geopolitical projects of a humanitarian nature, proposed by many international bodies and agencies.

These often ambitious objectives require a deeper knowledge of our universe, its sensitivity to natural phenomena, and the perturbation of the latter by our civilization's progress.

The need for basic data has become all-important for short and medium term actions because of the recent enhancement of modeling and simulation techniques for evolving systems. Modeling, a prediction tool, provides arguments for prevention and can justify plans for intervention.

In our information civilization, the absence of sufficient data, well-adapted to our needs and ambitions, often limits important plans for improvement on both regional and world-wide levels. Data and computer aided systemic theories have become inseparable; expert systems, knowledge systems, data banks, networks are all vectors of scientific and technical communication.

Due to extant strong limitations in handling complex systems CODATA contributes to progress in modeling methods and conceptual tools development, particularly those enhancing heuristic interpretation of processes favoring inductive and abductive contributions to innovative thought mechanisms. Constantly, CODATA '94 will deal with all of these various aspects and underlines the need to improve data representation in many fields. Computer science and information engineering thus constitute the third and important objective of CODATA '94

CODATA '94 is organized in three Symposia covering the following fields:

- .Symposium M - Materials and Structural Properties
- Symposium E - Environment, Biodiversity, and Toxicity
- Symposium I - Computer Aided Systems and Communication

The third symposium deals with the intellectual and material logistics of the two others as well as with questions of information engineering, the best answers to which still elude us. In a world rapidly tending towards an information civilization, many questions arise concerning the parallel progress made on the physical reality of "future electronic highways" where "data vehicular" traffic creates unsolved and highly complex problems of traffic and of property ownership.

Several topics were chosen to ensure the cohesion and the complementarity of the 34 sessions grouping some 180 lectures and talks. The criteria governing the choice of topics were:

- the current importance of the three Symposia and the urgency for defining these programs concretely,
- the interest of modeling and validation strategies centered imperatively on certain defined data.,
- the need to identify the increasingly diverse aspects of problems and tools in all fields of action and particularly with regard to uncertain data and exchange standards.
- the need to raise the awareness of researchers to the importance and to the urgency of major ICSU programs,
- the evaluation of strategies to create *significant data* extracted from huge masses of *raw data* (*e.g.*, satellite data).

CODATA '94 will facilitate meetings between experts, specialists, users, and young researchers. The topical or thematic sessions will present syntheses and results from specialized laboratories and institutions. Plenary lectures will tackle problems of society from a prospective angle. For the informatics systems, presentations will take place in sessions and in an exhibit, but also directly with the help of computers or of animated visual presentations (videos).

In several general sessions discussions will focus on obstacles encountered in the free movement of data, in technological transfer and in the development, after the year 2000, of computerized deployment of Scientific and Technical Information.

The conference will follow broadly the same pattern as previous conferences with

- about six general keynote lectures
- 300 technical papers
- the three symposia (M, E, I) organized in subsections (poster sessions will include short oral seminar-type discussions organized by the session coordinator in the poster rooms)
- a *late* poster session (for papers accepted without review by a referee).

The chart of the Conference on page 3 provides a bird's eye view of the presentations within each symposium.

PLENARY LECTURES

Dealing with the Data Deluge: Visualization and Data Management of Complex Data

Nahum Gershon, The MITE Corporation, McLean, VA 22102, USA

Human Dimension in Artificial Intelligence. Taste and Preference Systems: Art or Science?

Vincent Douzal, CEMAGREF (French Institute of Agricultural and Environmental Engineering Research), Paris-Anthony, France

Capturing the Global Hydrological Cycle

John C. Rodda, World Meteorological Organization (WMO-OMM), Geneva, Switzerland.

Materials Data for the ERA of AGILE Manufacturing

Kenneth Preiss, Ben Gurion University, Israel, and Agility Forum, Bethlehem, USA.

Selected (Representative) Papers

SYMPOSIUM I - Computer Aided Systems and Communication

"The future of data – The future of memory," *M. J. Kurtz, Harvard-Smithsonian Center for Astrophysics, Cambridge, U.S.A.*

"Computerization of knowledge concerning material databases," *Gustaf Ostberg, Risk Handling, Lund, Sweden.*

"Statistical cleaning of "polluted" data," *Rudy Tan, United Laboratories INC, Mandaluyong, Philippines.*

"Shape-data processing in the natural sciences and technology," *Paul G. Mezey, University of Saskatchewan, Saskatchewan, Canada.*

"Shape fractal modelization: simulation of growth and form of sponges and corals," *Jaap A. Kaandorp, University of Amsterdam, Amsterdam, The Netherlands.*

"Error and uncertainty in physical measurements," *E. Richard Cohen, Rockwell International Science Center, Thousand Oaks, U.S.A.*

"The use of STEP for the automotive industry," *N. Mohrmann, Daimler-Benz, Germany.*

"Emerging bioinformatics infrastructure in Russia," *T.S.A. Egorov, Acad. Sci. of USSR, Moscow, Russia.*

"Networking in Indian and Asian regions," *J.R. Arora, Dept. of Biotechnology, New Delhi India, or A. Tsugita.*

SYMPOSIUM M - Materials and Structural Properties

"Perspective on intelligent materials," *B. Yanagida, Japan.*

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Bird's Eye View of "Chambéry" Conference

Session Numbers	(M) Materials and Structural Properties	(E) Environment, Biodiversity, Toxicity	(I) Computer Aided Systems and Communication
1	Pure Compounds 1: new developments in state equations and their applications *Coordinator:* Jacques JOSE	Environmental issues: national and international policies *Coordinators:* Jean-Claude OPPENEAU and Phillippe BOURDEAU	Obstacles to open exchange of scientific data. *Coordinator:* Michael A. CHINNERY
2	Pure Compounds II: prediction and validation of physical and energy data by group correlation *Coordinator:* Maurice CHASTRETTE	Biogeochemical cycles: health perspectives, global change *Coordinator:* Pierre MASCLET	Distributed data and computer networks: the new information retrieval *Coordinator:* Fionn MURGAGH
3	Mixture Properties: Modeling and prediction *Coords:* Marie-Thérèse and Roger COHEN-ADAD	Water in ecosystems: role, disfunctions and pollution *Coordinator:* Christian LEVEQUE	Knowledge and data interplay *Coordinator:* C. ROCHE
4	Understanding the dynamics of complex biomolecular systems *Coordinator:* Richard LAVERY	Environment and toxicity: Methodology and concepts in ecotoxicology *Coordinator:* Gérard BLAKE	Future Knowledge based systesm: uncertainty management *Coordinator:* Nahum GERSHON
5	Complexity of polyphase structures-emulsions, gels, foams, micelles *Coordinator:* Danielle CLAUSSE	Genetic toxicology *Coordinator:* Paul H. M. LOHMAN	Cognition and recognition in design strategy: structures and/or materials *Coordinator:* Gustaf OSTBERG
6	Materials surfaces and interfaces: data for innovation *Coordinator:* Michel DELAMAR	Biodiversity survey data systems *Coordinator:* F. DI CASTRI	Standards and CAD aspects of industrial exchange *Coordinator:* Anne-Françoise CUTTING-DECELLE
7	Computer-Aided design of composite materials *Coordinators:* Claude BATHIAS and Nicole ALBEROLA	Regional environment changes: data on geodynamics, seismic risks, erosion *Coords:* Christian BECK and Georges MASCLES	Enhancing the value of online and CD-ROM information *Coordinator:* Clément PAOLI
8	*Thermodynamics in metallurgical processes* *Coordinators:* Claude BERNARD and Yves BIENVENU	Regional environmental changes: desertification of Mediterranean mountains & regions, modeling & monitoring *Coordinator:* Laurence BOURJOT	Recognition of rigid and "deformable" objects" *Coordinator:* Paul MEZEY
9	Soft chemistry products and powders properties *Coordinator:* Michel FIGLARZ	Biodiversity: taxonomic and information structures *Coordinator:* Micah KRICHEVSKY	Physical and molecular data: validation and prediction *Coordinator:* Gérard THIROT
10	Materials structure and behavior modeling *Coordinators:* Albert TRUYOL and François SIDOROFF	Master species inventories and biodiversity data systems *Coordinator:* F. A. BISBY	Physics and Chemistry in action *Coordinator:* Jean AUBARD
11	Data capture and monitoring: intelligent materials and new microsensors *Coord:* Paul CLECHET		Bioinformatics: infrastructure in the world today *Coords:* Harrie LALIEU (BIOREP) & A. TSUGITA
12			Merging biological databases with the bench scientist's computer *Coordinator:* Akira TSUGITA
13			Information requirements in developing countries: local needs and solutions *Coordinator:* Belhadri MESSABIH

MARGARET E. COURAIN   1928-1994

Margaret E. Courain, Ph.D., retired Deputy Assistant Administrator of the National Environmental Satellites, Data and Information Service, National Oceanic and Atmospheric Administration (NOAA), died of cancer at her South Orange, NJ home on January 13, 1994.

Margaret was known best to CODATA for her masterful program management of the Columbus 1990 International CODATA Conference.

Dr. Courain was a pioneer in information management. During a 32-year career at Merck & Co., Inc., she developed the Research Information Systems Department of Merck Research Laboratories and provided management development and education programs for the Corporation. In 1981 Dr. Courain joined NOAA, where she directed the consolidation of four major national databases and retired in 187.

She was the author of 23 publications in management, scientific data systems design and management, and environmental data management. She was associated with numerous information organizations, including as a member of the U.S. National Committee. She also served on the Board of Directors of the Drug Information Association, and as a founding member of the New York Chapter of the American Society for Information Science.

While at NOAA, she was Representative to the National Data Advisory Board of the National Research Council, National Academy of Sciences, Co-chair of Data Management subcommittee of the NOAA/USGS Interagency Coordination committee, and a member of the Commission on climatology of the World Meteorological Organization.

Dr. Courain was an elected Fellow to the American Institute of Chemists, and a member of the Board of Advisors, Rutgers Women in Science and Mathematics.

She was a graduate of Bayonne High School, received a B.S. in Chemistry from Douglass College, an M.S. in Library Service from Columbia University, and in 1991, a Ph.D. from the school of Communication, Information, and Library Studies, Rutgers University. Born in Bayonne, N.J. in 1928, Dr. Courain's principal residence since 1959 was in South Orange, N.J.

CODATA Conference Selected Papers

"Modeling the dynamics and the thermodynamics of biological macromolecules and their interactions," *Peter Kollman, Dept. of Pharmacy, University of California, San Francisco, U.S.A.*

"The application of thermodynamics to the development of processes and materials," *Philip Spencer, R.W.T.H., Aachen, Germany.*

"CAD/CM: State of the art and prospective," *Z. Y. Hashin, University of Tel-Aviv, Tel-Aviv, Israel.*

"Thermodynamic guide lines for the design of cermets processed by liquid phase sintering," *C. Allibert, INGP-CERMEP, Grenoble, France, with H. Pastor.*

"Thermodynamic mimicry," *Joel F. Liebman, University of Maryland, U.S.A.*

"Heat capacity and sound velocity data for the improvement of compositional modeling of condensate gas thermodynamic properties," *E. Behar, Institute Français du Pétrole, Rueil-Malmaison, France.*

"Thermodynamic models for the monitoring of deoxidation treatments and the control of inclusions in steel," *H. Gaye, IRSID, Maizières les Metz, France, with C. Gatellier and I. Lehmann.*

SYMPOSIUM E - Environment, Biodiversity, Toxicity

"Large databases and networks in Earth and Space sciences," *James R. Thieman, Goddard Space Flight Center NASA, Greenbelt, U.S.A.*

"Global change data at regional scale in the Himalaya of Nepal and Tibet," *Gottfried Gabert, CODATA Germany, Isernhagen, Germany, with Claude Bardinet.*

"Information and geoinformation models of the great ore deposits of Russia," *Nicolai Laverov, IGEM RAS, Moscow, Russia, with Alexandre Vesselovsky.*

"Expert systems for geotechnical data quality assessment," *J. L. Favre, Laboratoire MSS, Ecole Centrale, Paris, France, with Reda M. Bakeer and Lyes Matmatic.*

"Desertification of Mediterranean mountains and regions: state of art," *Michael Dubost, ICALPE, Corte, Corse, France.*

"Change detection in a region of southern Algeria using multidata multisource satellite images," *Y. Smara, Laboratoire de Traitement d'Images, Alger, Algeria, with A. Belhadj-Aissa and M. Mahrour.*

"Risk assessment state of the art in ecotoxicology," *Peter Callow, Sheffield, U.K.*

"Genetic toxicology in evaluating carcinogenetic hazards and risks," *Douglas McGregor, CIRC, Lyon, France.*

"'Use of the European Pollen databank to retrace the evolution of the Mediterranean surface vegetation during the last few centuries," *Jean-Louis de Beaulieu, IMEP, Marseille, France.*

"Land cover changes detection in the Mediterranean area by remotely sensed data - the maritime Syria," *Jean-François Khreim, CEFE, Montpellier, France.*

CODATA Books

(a) New Data Challenges in Our Information Age. Proceeding of the International CODATA Conference in Beijing, China, 1992, edited by Phyllis Sloane Glaeser, Michael T. I. Millward, and Keith W. Reynard.

Books

Le Veille Technologique. L'information scientifique, technique et industrielle, edited by Hélène Desvals and Henri Dou. (b)

Vapor-Liquid Equilibrium Data Collection. Aldehydes (Supplement 1), by J. Gmehling, U. Onken, and J. R. Rarey. (c)

Vapor-Liquid Equilibrium Data Collection. Ketones (Supplement 1), by J. Gmehling, U. Onken, and J. R. Rarey. (d)

Electrolyte Data Collection. Part 1: Conductivities, Transference Numbrs, Limiting Ionic Conductivities, by J. Barthel and R. Neueder. (e)

Databases

Romulus 2— Inter-Library Loan — CD-ROM System.(f)

DIPPR® Pure Component Data Compiltion. Version 7. (g, h)

ECDIN, a new database from the Commission of the European Community's Joint Research Centre. (h, i)

QSAR, predicts chemical properties, environmental fate and persistence, and the risk of hazardous exposure. (h)

PPDS2, phase equilibria and thermodynamic properties. (h, j)

DETHERM®, the online version of the DECHEMA Chemistry Data Series. (h, k)

TRC Vapor Pressure. (h, l)

EQS Chemical Equilibrium Software, software that performs multiphase equilirium calculations. (h)

POLARPROPS. (h, m)

(a) In press.

(b) 1992. 436+xii pp. Dunod, Paris. ISBN: 2-10-00246-5.

(c) 1993. 280 pp. Chemistry Data Series, Vol. 1, Part 3a. DECHEMA, Frankfurt am Main. ISBN: 3-921 567-93-9. DM 293,00.

(d) 1993. 750 pp. Chemistry Data Series, Vol. 1, Part 3b. DECHEMA, Frankfurt am Main. ISBN: 3-926 959-44-4. DM 494,00.

(e) 1992. 414 pp. Chemistry Data Series, Vol. XII, Part 1. DECHEMA, Frankfurt am Main. ISBN: 0940-9645.

(f) A detailed brochure on Romulus 2 is available by calling 1-800-668-1222 or fax (613) 952-9112. The cost of the 2nd. version is $650 for single site use, and $975 for network use, within Canada. (Prices outside Canada are available on request.) Romulus is a product of the Canada Institute for Scientific and Technical Information (part of the National Research Council of Canada) and The National Library of Canada.

(g) Contains data for 26 constant and 13 temperature-dependent properties for 1351 commercially important substances, critically evaluated by the Design Institute for Physical Property Data of the AIChE.

1994

March	
17	CODATA Officer's Meeting. Paris, France
18-19	CODATA Executive Committee Meeting. Paris, France

July	
2	CODATA Task Group on Fundamental Constants. Boulder, Colorado, USA

September	
15-17	CODATA Task Group on Biological Macromolecules. Chambéry, France
16-17	CODATA Long-Term Planning Meeting. Chambéry, France
17-18	CODATA Task Group on Materials Database Management. Chambéry, France
18-22	International CODATA Conference. Chambéry, France
23-24	CODATA General Assembly. Chambéry, France

1996

------	International CODATA Conference. Tsukuba, Japan
------	CODATA General Assembly. Tsukuba, Japan

ILL Enhanced by Romulus 2

The second version of Romulus, the CD-ROM system for inter-library loans (ILL), has been completely updated and includes many of the new features that Romulus users requested. ILL has never been faster, easier or more economical. Designed as a multifunctional tool for finding periodical titles and ordering documents, Romulus has achieved recognition for its keyword search capabilities (using Boolean logic) and as a tool for evaluating collections.

Romulus can create document orders and send them to CISTI and the National Library of Canada through an Internet connection— the least expensive method. The new version is compatible with all CD-ROM networking platforms. ROMCOM, the Romulus communications software, allows one to print orders as well as incoming requests and messages.

Romulus combines three different union lists of serials held in Canadian libraries (social sciences and humanities, science and technology, and newspapers), the CISTI serials list, and the *Directory of Interlibrary Loan*.

Over half of the 200,000 records were updated in the new version, and the holdings of 60 new libraries have been added.

European Days of Thermodynamics

The Center for Non-Linear Phenomena and Complex Systems, Institutes Internationaux de Physique et de Chimie Solvay and the European Center for Advanced Studies in Thermodynamics held a meeting at the Université Libre in Brussels on 13-15 December 1993. This "Third European Days of Thermodynamics" was chaired by Messieurs P. Glansdorff and I. Prigogine. Approximately 100 teachers, researchers, and members of the industry attended this international conference. This year's subject, "Inhomogeneous Phases and Pattern Formation" was broken down into six sessions: Inhomogeneous Equilibrium Systems, Constrained Systems, Polymers and Interfaces, Supramolecular Fluids, Nucleation and Non-equilibrium Patterns, and Pattern Growth. Several instability phenomena were highlighted both in equilibrium and non-equilibrium systems.

This meeting was held with support from the Commission of the European Communities, the Fonds National de la Recherche Scientifique (Belgium), Gaz de France, and the Centre National de la Recherche Scientifique (France).

The 26 scientific lectures will be published in *Physica*, 1995. For further details on the publication, please contact M. Lefevre (Université Libre de Bruxelles, Brussels) or A. Truyol (CERET, Paris).

--A. Truyol

(h) For further information: Technical Database Services, Inc., 135 West 50th Street, New York, NY 10020-1201; Tel: (212) 245-0044; Fax: (212) 247-0587.

(i) Provides a wealth of information about the 120,000 substances on the EINECS (European Inventory of Existing Chemical Substances) list. In one search, the user can retrieve over 30 data files which have been organized into 9 categories: chemical registry numbers and synonyms; legislation and guidelines from around the globe; occupational safety and health, including labelling requirements in 8 languages; hazards during transport and storage; methods for detecting chemicals; chronic and acute toxicity (LD50s, LC50s, EC50s, etc.); concentration and fate in the environment; physical and chemical properties; and use in commerce. Sources for experimental and regulatory data are referenced.

(j) Developed by the national Engineering Laboratories (UK) to provide phase equilibrium and thermodynamic properties for pure chemicals and mixtures of up to 50 components.

(k) DETHERM has reference experimental data for phase equilibria, thermodynamic, transport, PVT and interfacial properties for over 11,000 pure components and their mixtures.

(l) From the Thermodynamics Research Center at Texas A&M University, this program has a fully referenced database of critically evaluated experimental data, and can also calculate vapor pressures and boiling points.

(m) Calculates physical properties and phase equilibria for polar and non-polar fluids.

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CODATA, 51 bd. de Montmorency, 75016 Paris