FEBRUARY 1990

12th Int’l. CODATA Conference
Columbus, Ohio, 15-19 July 1990

INVITED PAPERS

KEYNOTE ADDRESS

FUTURE DIRECTIONS OF SCIENCE AND LARGE SCALE SCIENTIFIC COMPUTING
K.G. Wilson, Department of Physics, The Ohio State University, Columbus, Ohio

PREDICTION OF GLOBAL CHANGE
Session 1A - Chairman: S. Alexander

SOCETAL IMPERATIVES FOR GLOBAL CHANGE STUDIES
P. Thatcher, U.S.A.

DATA FOR PREDICTION OF GLOBAL CHANGE
Session 1B - Chairman: T. Malone

GLOBAL DATA SETS FOR THE IGBP: ACQUISITION, VALIDATION, DISTRIBUTION
I. Rasool, NASA, U.S.A.

A PROJECT OF A NATIONAL AUTOMATIZED SYSTEM FOR GEOINFORMATION ACQUISITION AND PROCESSING
A.S. Alekseev, D.L. Kouznetsov, and V.A. Sirotuyk, MNTK "GEOS", VNIIGeoinformsystem, Moscow 113105, U.S.S.R.

A NATIONAL GLOBAL CHANGE INFORMATION MANAGEMENT STRATEGY
F. Webster, U.S.A.  (Program continued on page 2)
GLOBAL CHANGE INFORMATION MANAGEMENT STRATEGIES
Session 1D - Chairman: J. Crease

THE GLOBAL CHANGE DISKETTE PROJECT
M. Chinnery, World Data Centre A, Boulder, Colorado, U.S.A.

COMMITTEE ON IGBP PILOT STUDY ON DATABASE INTERFACES
C. Bruce Wiersma, U.S.A.

DEVELOPMENT OF A GLOBAL SOILS AND TERRAIN DATABASE (SOTER)
M. Baumgardner, Purdue University, West Lafayette, Indiana, U.S.A.

GEOGRAPHICAL INFORMATION SYSTEMS
Session 1B - Chairman: R. Sinding Larsen

GEOGRAPHICAL INFORMATION SYSTEMS: MAPPING THE EXCLUSIVE ECONOMIC ZONE
J. Bieseker, U.S.A.

GLOBAL TRENDS IN MATERIALS DATA MANAGEMENT
Session 2B - Chairman: Professor D. Abir

GLOBAL TRENDS IN MATERIALS DATA MANAGEMENT: REGIONAL OVERVIEW
WESTERN EUROPE
Keith W. Reynard, Wilkinson Consultancy Services, Stable Cottage, Broad Lane, Newdigate, Surrey, U.K.

CURRENT ACTIVITY IN NORTH AMERICA ON NUMERICAL DATABASES ON MATERIALS PROPERTIES

MATERIALS AND FLUIDS DATA BANKS IN THE USSR AND COMECON COUNTRIES
A. Kozlov, VNITSMV, Moscow, U.S.S.R.

GLOBAL TRENDS IN MATERIALS DATA MANAGEMENT: REGIONAL OVERVIEW
PEOPLES' REPUBLIC OF CHINA
Xu Zhihong, Institute of Chemical Metallurgy, Beijing, China

GLOBAL TRENDS IN THE MANAGEMENT OF DATA ON MATERIALS

CHEMICAL DATA USED IN PROCESS CONTROL
Session 2C - Chairman: C.B. Alcock

PREDICTION OF THERMODYNAMIC PROPERTIES OF ORGANIC MIXTURES
Henry V. Kehiaian, Institut de Topologie et de Dynamique des Systèmes, Université Paris VII - CNRS, Paris, France

THERMODYNAMIC DATABASES: A SURVEY
R. Eckermann, DEHEMA, Federal Republic of Germany

CHEMICAL DATA USED IN PROCESS CONTROL: INDUSTRIAL NEEDS
M. Gaune-Escard, S.E.T.T., Université de Provence, Centre de St.-Jérôme, Marseille, France

ADVANCES IN SPATIAL DATA INTEGRATION
Session 2D - Chairman: Professor J.R.G. Townshend

INTEGRATION OF VECTOR AND RASTER DATA AND MODULES
David J. Abel and M.A. Wilson, Centre for Spatial Information Systems, CSIRO Division of Information Technology, Canberra, Australia
A SPATIAL DATABASE FOR AN IMAGE UNDERSTANDING SYSTEM
D.C. Mason, S.B.M. Bell, E. Pearson, Natural Environment Research Council Unit for Thematic Information Systems (NUTIS), Dept. of Geography, University of Reading, Whiteknights, Reading, U.K.
D. Brewster, C. Oddy, A.J. Rye, GEC Marconi Research Centre (MRC), Space and Defence Research Laboratory, West Hanningfield Road, Great Baddow, Chelmsford, Essex, U.K.

INNOVATIVE ACTIVITIES IN MATERIALS DATA HANDLING
Session 2E - Chairman: F. Kuznetsov

MODELING OF HYDRODYNAMICS, HEAT AND MASS TRANSFER PROCESSES ON THE BASIS OF UNSTEADY NAVIER-STOKES EQUATIONS. APPLICATIONS TO THE MATERIAL SCIENCES IN EARTH AND SPACE AND REQUIREMENTS FOR INITIAL DATA
V.I. Poleshaev, Institute for Problems in Mechanics, Academy of Sciences of the U.S.S.R., Prospect Vernadskogo 101, 117526 Moscow, U.S.S.R.

THE INFORMATION BASE SYSTEMS FOR MATERIALS RESEARCH
Yuzuru Fujiwara, University of Tsukuba, Institute of Electronics and Information Science, Tsukuba, 305 Japan

NEW APPROACHES TO DESIGN OF MATERIALS DATABASES
J. Rumble, NIST, Gaithersburg, Maryland, U.S.A.

FUTURE OF HANDBOOKS IN SCIENCE (PRINTED VS ELECTRONIC MEMORY)
Session 2F - Chairman: H. Behrens

THE ROLE OF PRINTED HANDBOOKS IN THE ELECTRONIC AGE
D.R. Lide, Jr., Editor, CRC Handbook of Chemistry and Physics

AN ELECTRONIC HANDBOOK: AN OXYMORON OR A USEFUL DATABASE?
Laszlo Domokos, Clemens Jochum, Sandy Lawson

GMELIN HANDBOOK OF INORGANIC CHEMISTRY - RELATION OF PLANNED ELECTRONIC AND PRINTED VERSIONS AND FUTURE POLICY
Ekkehard Fluck, Gmelin Institute for Inorganic Chemistry of the Max-Planck-Society, Varrentappstr. 40/42, D-6000 Frankfurt/M. 90, F.R.G.

COMPUTER-AIDED SPECTROSCOPY
Session 2G - Chairman: K. Rao

RECENT ADVANCES IN THE AUTOMATED STRUCTURE ELUCIDATION SYSTEM, CHEMICS
Shin-ichi Sasaki and Kimito Funatsu, Toyohashi University of Technology, Toyohashi 440, JAPAN

TOPOLOGY AND TOPOGRAPHY CONCEPTS IN CONFORMATION ELUCIDATION
J.P. Doucet, Institut de Topologie et de Dynamique des Systèmes, Associé au CNRS, Université Paris VII, 75005 Paris

DATA AND SOCIETY
Session 3A - Chairman: M.E. Courain

CODATA PERSPECTIVES FOR THE 1990's
D.R. Lide, Jr., President, CODATA, U.S.A.

HUMAN GENOME SEQUENCING: TECHNICAL, LEGAL, AND ETHICAL ISSUES
C. Cantor, Lawrence Berkeley Laboratory, U.S.A.

DATA AND NEW TECHNOLOGIES
Session 3B - Chairman: B. Janicki

NEW DRUG SEARCH STRATEGIES
Babu Venkataramhavan, Medical Research Division, American Cyanamid Company, Pearl River, New York, U.S.A.
MOLECULAR SHAPE REPRESENTATION AND CODES
A. Panayot, Institut de Topologie et de Dynamique des Systèmes, Associé au CNRS, Université Paris VII, Paris

TECHNOLOGY RECONCILIATION: THE ROLE OF PEOPLE
Session 3C - Chairman: R. Wigington

DATABASES: INDISPENSABLE TOOLS FOR RESEARCH AND DEVELOPMENT
Dieter Rehm, Institute für Organische Chemie, Johann Wolfgang Goethe-Universität, Frankfurt am Main, F.R.G.

THE ROLE OF TECHNOLOGY RECONCILIATIONS IN THE USE OF REMOTE SENSING DATA IN WEATHER FORECASTING
M. Courain, U.S.A.

TITLE TO BE ANNOUNCED
J. Tucker, U.S.A.

PLENARY LECTURE
Session 4A - Chairman: M. Krichevsky

COMMISSION ON THE TERMINOLOGY AND NOMENCLATURE OF BIOLOGY: GOALS AND ACTIVITIES
L. Blaine, Hybridoma Data Bank, American Type Culture Collection, Rockville, Maryland, U.S.A.

KNOWLEDGE TOOLS
Session 4B - Chairman: Professor J.E. Dubois

MATERIALS DATA SYSTEMS FOR MATERIALS DESIGN
Shuichi Iwata, Nuclear Engineering, University of Tokyo, Tokyo, Japan

CONSTRUCTING EXPLANATIONS OF DATA: THE ROLE OF EXPERT SYSTEMS IN DATA ANALYSIS
B. Chandrasekaran, Laboratory for AI Research, The Ohio State University, Columbus, Ohio, U.S.A.

PROLOG: RECENT PROGRESS AND KNOWLEDGE BASED SYSTEMS
H. Bestougeff, Université Paris VII, Paris, France

KEY ISSUES IN MATERIALS DATA
Session 4C - Chairman: Dr. Jack H. Westbrook

MATERIALS DATA INTERCHANGE USING TABULAR FORMATS
Philip M. Sargent, Cambridge University Engineering Dept., Cambridge, U.K.

STANDARDS FOR MATERIALS DATABASES: AN INTERNATIONAL CONCERN
H. Kröckel, Joint Research Centre of the CEC, Petten Establishment, Petten, The Netherlands

ISSUES IN NETWORKING MATERIALS DATABASES
J.G. Kaufman, MPD Network, Columbus, Ohio, U.S.A.

COLLABORATION AND LINKAGE AMONG BIOLOGICAL DATABASES
Session 4D - Chairman: A. Tsugita

COMPUTERIZED ANIMAL VIRUS INFORMATION AND ITS LINK WITH OTHER BIOLOGICAL DATA BANKS
A.S. Kolaskar, Officer-in-Charge, Bioinformatics, D.I.C., Zoology Department, University of Poona, Pune, India

SEQUENCE DATABANKS: TOWARDS A DE FACTO NETWORK
W.C. Barker and D.G. George, National Biomedical Research Foundation, Washington, D.C. 20007, U.S.A.

THE DEVELOPMENT OF DATABASES AND METHODS OF ANALYSIS OF MOLECULAR BIOLOGICAL INFORMATION IN THE SOVIET UNION
A.A. Alexandrov, Institute of Molecular Genetics, U.S.S.R. Academy of Sciences
ON NEURAL NETWORKS AND FRACTALS
Jordan V. Pollack, Laboratory for Artificial Intelligence Research, Dept. of Computer and Information Science, The Ohio State University, Columbus, Ohio, U.S.A.

NEW NUMERIC DATA RETRIEVAL SYSTEMS
Andreas Barth, Fachinformationszentrum Karlsruhe, D-7514 Eggenstein-Leopoldshafen 2

ADVANCES IN MOLECULAR ELECTRONICS AND BIOCOMPUTERS
Hiroyuki Sasabe, Frontier Research Program, RIKEN (The Institute of Physical & Chemical Research), 2-1, Hirosawa, Wako Saitama, Japan

OBJECT-ORIENTED KNOWLEDGE BASE SYSTEMS
F.J. Smith and S.R. Tripathy, Department of Computer Science, The Queen's University of Belfast, Belfast, Northern Ireland

EXPLORATORY MOLECULAR SUBSTRUCTURE MANIPULATION USING KNOWLEDGE BASED SYSTEMS
Session 4F - Chairman: S. Heller

ESTHETICS AND SYMMETRY: A SOURCE OF INSPIRATION FOR MOLECULAR RESEARCH AND DISCOVERIES
J.E. Dubois, ITODYST, Paris, France

SUBSTRUCTURE SEARCH STRATEGIES IN BIOLOGY: TRENDS AND PERSPECTIVES
David G. George and Winona C. Barker, Protein Identification Resource, National Biomedical Research Foundation, Georgetown University Medical Center, Washington, D.C., USA

KNOWLEDGE PATTERN RECOGNITION: APPLICATION TO LANDSAT AND SPOT/STEREO DIGITAL DATA ON CHINA
2. Laboratoire d'Image ENST, Paris, France

STN NETWORK STRATEGIES FOR DISCOVERY ASSISTANCE
Nick Farmer, Chemical Abstracts Service, Columbus, Ohio, U.S.A.

POTENTIAL FOR IMPROVEMENTS AND NEW USES OF CRYSTALLOGRAPHIC DATABASES
Session 4G - Chairman: G.H. Wood

THE PROTEIN DATA BANK
Thomas F. Koetzle, Enrique E. Abola, Frances C. Bernstein, Judith A. Callaway, Pamela A. Esposito, Arthur Forman, John P. Rose, and Jenny C. Weng, Chemistry Department, Brookhaven National Laboratory, Upton, New York, U.S.A.

INTEGRATED ACCESS TO SEQUENCE AND STRUCTURAL DATA
Arthur M. Lesk, EMBL, Heidelberg, F.R.G. and MRC Laboratory of Molecular Biology, Cambridge, U.K.

TITLE TO BE ANNOUNCED
Shoshana Wodak, Free University of Brussels, Brussels, Belgium

(Program continued on page 8)
A new temperature scale, the International Temperature Scale of 1990 (ITS-90), was officially adopted by the Comité International des Poids et Mesures (CIPM), meeting 26-28 September 1989 at the Bureau International des Poids et Mesures (BIPM). The ITS-90 was recommended to the CIPM for its adoption following the completion of the final details of the new scale by the Comité Consultatif de Thermométrie (CCT), meeting 12-14 September 1989 at the BIPM in its 17th Session. The ITS-90 became the official international temperature scale on 1 January 1990. The ITS-90 supersedes the present scales, the International Practical Temperature Scale of 1968 (IPTS-68) and the 1976 Provisional 0.5 K to 30 K Temperature Scale (EPT-76).

The ITS-90 extends upward from 0.65 K, and temperatures on this scale are in much better agreement with thermodynamic values than are those on the IPTS-68 and the EPT-76. The new scale has subranges and alternative definitions in certain ranges that greatly facilitate its use. Furthermore, its continuity, precision and reproducibility throughout is ranges are much improved over that of the present scales. The replacement of the thermocouple with the platinum resistance thermometer at temperatures below 961.78 °C resulted in the biggest improvement in reproducibility.

The ITS-90 is divided into four primary ranges:

1. Between 0.65 K and 3.2 K, the ITS-90 is defined by the vapor pressure-temperature relation of $^3$He, and between 1.25 K and 2.1768 K (the $\lambda$ point) and between 2.1768 K and 5.0 K by the vapor pressure-temperature relations of $^4$He. $T_{90}$ is defined by the vapor pressure equations of the form:

$$T_{90}/K = A_0 + \sum_{i=1}^{9} A_i \left[ \frac{\ln(p/Pa)}{B} - C \right],$$

The values of the coefficients $A_i$, and of the constants $A_0$, $B$ and $C$ of the equations are given in the reference cited.

2. Between 3.0 K and 24.5561 K, the ITS-90 is defined in terms of a $^3$He or $^4$He constant volume gas thermometer (CVGT). The thermometer is calibrated at three temperatures—at the triple point of neon (24.5561 K), at the triple point of equilibrium hydrogen (13.8033 K), and at a temperature between 3.0 K and 5.0 K, the value of which is determined by using either $^3$He or $^4$He vapor pressure thermometry.

3. Between 13.8033 K (-259.3467 °C) and 1234.93 K (961.78 °C), the ITS-90 is defined in terms of the specified fixed points given below, by resistance ratios of platinum resistance thermometers obtained by calibration at specified sets of the fixed points, and by reference functions and deviation functions of resistance ratios which relate to $T_{90}$ between the fixed points.

(4) Above 1234.93 K, the ITS-90 is defined in terms of Planck’s radiation law, using the freezing-point temperature of either silver, gold or copper as the reference temperature.

Full details of the calibration procedures and reference functions for various subranges are given in:

### Defining Fixed Points of the ITS-90

<table>
<thead>
<tr>
<th>Material</th>
<th>Equilibrium State</th>
<th>Temperature ($T_{90}$ K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>VP</td>
<td>3 to 5</td>
</tr>
<tr>
<td>e-H$_2$</td>
<td>TP</td>
<td>13.8033</td>
</tr>
<tr>
<td>e-H$_2$ (or He)</td>
<td>VP (or CVGT)</td>
<td>~17</td>
</tr>
<tr>
<td>e-H$_2$ (or He)</td>
<td>VP (or CVGT)</td>
<td>~20.3</td>
</tr>
<tr>
<td>Ne$^*$</td>
<td>TP</td>
<td>24.5561</td>
</tr>
<tr>
<td>O$_2$</td>
<td>TP</td>
<td>54.3584</td>
</tr>
<tr>
<td>Ar$^*$</td>
<td>TP</td>
<td>83.8058</td>
</tr>
<tr>
<td>Hg$^*$</td>
<td>TP</td>
<td>234.3156</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>TP</td>
<td>273.16</td>
</tr>
<tr>
<td>Ga$^*$</td>
<td>MP</td>
<td>302.9146</td>
</tr>
<tr>
<td>In$^*$</td>
<td>FP</td>
<td>429.7485</td>
</tr>
<tr>
<td>Sn$^*$</td>
<td>FP</td>
<td>505.078</td>
</tr>
<tr>
<td>Zn$^*$</td>
<td>FP</td>
<td>692.677</td>
</tr>
<tr>
<td>Al$^*$</td>
<td>FP</td>
<td>933.473</td>
</tr>
<tr>
<td>Ag$^*$</td>
<td>FP</td>
<td>1234.93</td>
</tr>
<tr>
<td>Au$^*$</td>
<td>FP</td>
<td>1337.33</td>
</tr>
<tr>
<td>Cu$^*$</td>
<td>FP</td>
<td>1357.77</td>
</tr>
</tbody>
</table>

*a e-H$_2$ indicates equilibrium hydrogen, that is, hydrogen with the equilibrium distribution of its ortho and para states. Normal hydrogen at room temperature contains 25% para hydrogen and 75% ortho hydrogen.

*b VP indicates vapor pressure point; CVGT indicates constant volume gas thermometer point; TP indicates triple point (equilibrium temperature at which the solid, liquid and vapor phases coexist); FP indicates freezing point and MP indicates melting point (the equilibrium temperatures at which the solid and liquid phases coexist under a pressure of 101 325 Pa, one standard atmosphere). The isotopic composition is that naturally occurring.

* Previously, these were secondary fixed points.
**Japanese National Committee**

The Japanese National Committee for CODATA—a research liaison committee of the Science Council of Japan—has recently been reconstituted. The revised composition comprises:

**Chairman**
Prof. Kazuo TAKAYANAGI (Institute of Space & Astronautical Science)

**Honorary Member**
Prof. Masao KOTANI

**National Delegate to CODATA**
Prof. Akira TSUGITA (Science University of Tokyo)

**Vice Chairman**
Prof. Makoto KIZAWA (Kanagawa Institute of Technology)

**Secretary**
Dr. Hideaki SUGAWARA (Institute of Physical and Chemical Research)

**Members**

Dr. Sukehiro GOTO (National Institute for Environmental Studies)
Prof. Atsunobu ICHIKAWA (Tokyo Institute of Technology)
Prof. Shuichi IWATA (University of Tokyo)
Mr. Toshiko KANDA (Japan Information Center for Science and Technology)
Dr. Tadashi MAKITA (Research Institute for Production Development)
Dr. Satoshi NISHIJIMA (National Research Institute for Metals)
Prof. Masahisa SUGIURA (Tokai University)
Prof. Mitsuo TASUMI (University of Tokyo)
Prof. Yukio YONEDA (Tokai University)

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**CODATA Calendar**

**1990**

**March**
1-3 CODATA East-Asian Data Sources Task Group. Kyoto, Japan
16-19 CODATA Biological Macromolecules Task Group. Menton, France
21-22 CODATA Referral Database Task Group. Paris, France
22-24 CODATA Executive Committee Meeting. Paris, France
26-28 CODATA Chemical Thermodynamic Tables Task Group. Paris, France

**June**
15 CODATA Fundamental Constants Task Group. Ottawa, Canada

**July**
15 CODATA Hybridoma Data Bank Task Group. Columbus, OH, U.S.A.
15 CODATA Microbial Strain Data Network Task Group. Columbus, OH, U.S.A.
15-19 12th International CODATA Conference, "Data for Discovery," Columbus, Ohio, U.S.A.
20-21 17th CODATA General Assembly, Columbus, Ohio, U.S.A.

*(Notice also the Calendar in MDN, page 14)*

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**Statistical and Scientific Database Management**

The 5th International Conference on SSDBM, April 3-5, 1990, Charlotte, North Carolina, USA, continues the series started nine years ago in California (1981 and 1983), then in Europe (Luxembourg, 1986, and Rome, 1988). Its purpose is to bring together database researchers, users, and system builders, working in this specific area of activity, to discuss the particular issues of interest, to propose new solutions to the problems of the area, to extend the themes of the previous conferences, both from the theoretical and from the application point of view, and to foster the cross-fertilization of ideas in the following areas: semantic modeling, statistical expert systems, graphical interfaces, distributed databases, query optimization, database security, object oriented databases, temporal data, and implementational issues on statistical/scientific databases.

For additional information, contact: Zbigniew Michalewicz, University of North Carolina, Department of Computer Science, Charlotte, N.C., 28223; tel: 704-547-4873; e-mail (Internet): zbyszek@unccvax.uncc.edu; FAX: 704-547-2352.

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**CODATA Personalities in the News**

Dr. Brian W. Petley of the CODATA Fundamental Constants Task Group was awarded the Sir George Thomson Gold Medal by the Institute of Measurement and Control late in 1989, for his contributions to measurement science which have resulted in fundamental improvements to the understanding of the nature of the physical world. Dr. Petley works in the Division of Quantum Metrology of the National Physical Laboratory, Teddington, U.K.

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*Courtesy NPL News*
CONTRIBUTED PAPERS

Theme #1: GLOBAL CHANGE

ORAL PRESENTATION

SPACE ALTIMETRY DATA MANAGEMENT FOR OCEAN-CLIMATE BEHAVIOR PREDICTIONS
P. Vincent, J.F. Minster and the "PAVIE" group, CNES/GRGS/UM39, Toulouse, France

THE NASA MASTER DIRECTORY AND THE INTEROPERABLE EARTH AND SPACE SCIENCE DATA INFORMATION SYSTEM
James E. Thieman, NASA/GSFC, Greenbelt, Maryland, U.S.A.

ECO-ENVIRONMENT CHANGE MONITORING IN CHINA
Wang Chang-yao, Institute of Remote Sensing Application, Academia Sinica, China, National Remote Sensing Center, Beijing, China

OPTIMAL PLANNING OF A GLOBAL SYSTEM FOR ECOLOGICAL OBSERVATIONS
K.Y. Kondratyev and O.M. Pokrovsky, U.S.S.R.

OPERATIONAL DATA MANAGEMENT AT ECMWF
J.K. Gibson, Head, Meteorological Applications Section, ECMWF

POSTER PRESENTATION

INFORMATION SYSTEM ON LAND RESOURCES OF THE WUWEI REGION AND LAND USE PLANNING
Cao Ligeng, National Land Planning Office of Planning, Committee of Gansu Provincial People's Government, Lanzhou, Gansu, China

ESTABLISHMENT AND APPLICATION OF A RESOURCES AND ENVIRONMENT SCIENTIFIC DATABASE
San Jiulin, Commission for Integrated Survey of Natural Resources, Chinese, Academy of Science, Beijing, China

NEW TECHNOLOGIES OF ECOLOGICAL MONITORING OF OIL AND GAS FIELDS
G.I. Belchansky, A.P. Pichugin and N.E. Zhuravel, Moscow, U.S.S.R.

PROBLEMS AND EXPERIENCES IN NUCLEAR DATA EVALUATION, PROCESSING AND INTEGRAL TESTING IN DEVELOPING COUNTRIES
S. Ganesan, Nuclear Data Section, Indira Gandhi Center for Atomic Research, Tamil Nadu, India

CASE STUDIES ON GLOBAL ENVIRONMENTAL DATA SOURCES SELECTED FROM THE NEDRES COMPUTER DATA DIRECTORY
Gerald S. Barton, NOAA, National Oceanographic Data Center, Washington, D.C., U.S.A.

LONG-TERM TRENDS OF CHANGE OF THE IONOSPHERE PARAMETERS

DATABASES AND KNOWLEDGE TOOLS IN GEOMAGNETISM: GEOMAGNETIC INFORMATICS AND GLOBAL CHANGE
V.O. Papitashvili, IZMIRAN, Troitsk, Moscow Region, U.S.S.R.
N.E. Papitashvili, WDC-B2, Soviet Geophysical Committee, Moscow, U.S.S.R.

METEOR DATA FOR ASTRONOMY AND GEOPHYSICS: OBSERVATION, INTERPRETATION, MODELING AND SIMULATION
V.A. Nechitailenko, Soviet Geophysical Committee, Moscow, U.S.S.R.
R.G. Roper, Georgia Institute of Technology, Atlanta, Georgia, U.S.A.
Yu I. Voloshchuk, Institute of Radioelectronics, Kharkov, U.S.S.R.
Theme #2 - SPATIAL DATABASES

ORAL PRESENTATION

USE OF GIS IN THE BIOSPHERE RESERVES: PERSPECTIVE, POTENTIAL PROBLEMS AND GUIDELINES FOR SYSTEM DEVELOPMENT
Han Qunli, Beijing, China

DECISION SUPPORT SYSTEM FOR ECOLOGICAL STRATEGY OF TIANJIN CITY'S DEVELOPMENT
Yang Bangjie, Department of Systems Ecology, Chinese Academy of Sciences, Beijing, China

MODELISOL: A DATABASE FOR PREDICTING THE BEHAVIOR OF SOILS
Prof. Favre, Ecole Centrale de Paris, Laboratoire M.S.S.M., Chatenay-Mal, France

THE USE OF OPTIMAL ESTIMATION FOR GROSS ERROR DETECTION IN DATABASES OF SPATIALLY CORRELATED DATA
C.C. Tscherning, Geophysical Institute, University of Copenhagen, Copenhagen N., Denmark

POSTER PRESENTATION

GENERATION OF A SPATIAL DATABASE OF CLIMATIC VARIABLES IN A DEVELOPING REGION
S.D. Lynch, R.E. Schulze, Department of Agricultural Engineering, University of Natal, Pietermaritzburg, Republic of South Africa
M.C. Dent, Computing Center for Water Research, University of Natal, Pietermaritzburg 3200, Republic of South Africa

Theme #3 - MATERIAL DATA SYSTEMS

ORAL PRESENTATION

ONLINE REAL TIME DATA SAMPLING SYSTEM AT EXPERIMENTAL FACILITIES FOR ELEVATED TEMPERATURE STRUCTURAL MATERIALS
H. Kawasaki, K. Aoto and Y. Wada, Materials Development Section, Systems and Components Development Division, Oarai Engineering Center, Power Reactor and Nuclear Fuel Development Corporation

APPLYING INFORMATION ENGINEERING AND COMPUTER AIDED SYSTEMS ENGINEERING (CASE) TO MATERIALS PROPERTIES MANAGEMENT
John J. Herbert, Jr., Maxima Corporation, Oak Ridge, Tennessee

MATERIALS DATABASES IN TERTIARY EDUCATION
Mr. D. Phelan, Chisholm Institute of Technology, Caulfield East, Victoria, Australia

LASER PROCESSING TECHNIQUES IN MATERIAL SCIENCE
Jin Kang, Institute of Physics, Chinese Academy of Sciences, Beijing, China

HOW TO INTRODUCE COMPUTERIZED MATERIALS INFORMATION: A SMALL COUNTRY'S POINT OF VIEW
Aki E. Valkonen, Academy of Finland, VTT Technical Research Centre of Finland, Espoo, Finland

ACTIVITIES IN THE DEVELOPMENT OF THE NEW KINETIC DATABASE KINDAS
H.A. Friedrichs and U. Seidl, Lehrstuhl für Theoretische Hüttentechnik and Metallurgie der Kerbrennstoffe, RWTH Aachen, Aachen, F.R.G.

POSTER PRESENTATION

MATERIALS DATA NETWORKS FOR DEVELOPMENT OF ADVANCED NUCLEAR MATERIALS
Shuichi Iwata, Nuclear Engineering, University of Tokyo, Tokyo, Japan; Mitsuuru Fujita, NRIM; Hajime Nakajima, JAERI; Hideki Kanou, PNC; Toshihide Takeshita, Tecnova; Shunichi Kikuchi, JICST; and Tsukasa Sakai, JAIS
TOOLS FOR MATERIALS DATA SYSTEMS
T. Ashino, K. Furuya, T. Ishikawa, T. Okuyama and S. Iwata, Nuclear Engineering, University of Tokyo, Tokyo, Japan

MATERIALS DATA SYSTEMS FOR NUCLEAR FUELS
Shuichi Iwata, Hirofumi Yamada and Toshihiro Ashino, Nuclear Engineering, University of Tokyo, Tokyo, Japan

MATERIALS DATA SYSTEM FOR SUPERCONDUCTING MATERIALS
Shuichi Iwata, Kiwame Tokai, Toshihiro Ashino, Nuclear Engineering, University of Tokyo, Tokyo, Japan
Kenichi Hoshimoto, Yuji Asada, National Research Institute for Metals, Tokyo, Japan

ESTIMATION OF PHYSICAL PROPERTY DATA WITH DETHERM
David F. Itten, DEHEMA, Frankfurt, F.R.G.

THERM: THERMODYNAMIC PROPERTY ESTIMATION FOR GAS PHASE RADICALS AND MOLECULES
Edward R. Ritter and J.W. Bozzelli, New Jersey Institute of Technology, Newark, New Jersey, U.S.A.

POST-PROCESSING SYSTEMS OF A MATERIAL DATABASE TO ESTABLISH ELEVATED TEMPERATURE STRUCTURAL MATERIALS STRENGTH STANDARDS FOR LMFB
Y. Wado and K. Aoto, Systems and Components Development Division, Materials Development Section, Oarai-Engineering Center, Power Reactor and Nuclear Fuel Development Corporation

SMAT: A STRUCTURAL MATERIAL DATA PROCESSING SYSTEM FOR LMFB COMPONENTS
K. Aoto and Y. Wado, Systems and Components Development Division, Materials Development Section, Oarai-Engineering Center, Power Reactor and Nuclear Fuel Development Corporation

DATABASE SYSTEM DESIGN FOR THE PROPERTIES OF RARE EARTHS
Li Guoquan, Xu Lu and Wang Shuyun, Changchun Institute of Applied Chemistry, Academia Sinica, Changchun, China

VAPOR PRESSURE AND ACENTRIC FACTOR OF ORGANIC COMPOUNDS
PART 3: HYDROCARBONS
Ma Peisheng and Xu Ming, Tianjin University, Tianjin, China

CRITICAL ASSESSMENT OF SOLUBILITY PARAMETER AND ITS CLASSIFICATION
Ma Peisheng, Tianjin University, Tianjin, China

DETERMINING THE QUALITY LEVEL OF ANALYZED MATERIALS PROPERTIES DATA
Martin F. Marchbanks, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

Theme #4: EXPERT SYSTEMS AND OTHER KNOWLEDGE TOOLS

ORAL PRESENTATION

AN INTERACTIVE SEARCH AND ESTIMATION SYSTEM IN $^{13}$C AND $^1$H NMR DATABASES
Osamu Yamamoto, Kikuko Hayamizu and Masaru Yanagisawa, National Chemical Laboratory for Industry, Tsukuba Research Center, Ibaraki, Japan

EXPERT SYSTEM FOR EVALUATING PHYSICO-CHEMICAL PROPERTY DATA

SYMBOLISM OF INORGANIC STRUCTURE TYPES
E.E. Hellner, R. Schwarz, Institute for Mineralogy, Philipps University, D-3550 Marburg, F.R.G.
W.B. Pearson, Depts. of Physics and of Chemistry, University of Waterloo, Waterloo, Ontario, Canada

KNOWLEDGE BASED ORGANIC COMPOUND PROPERTY DATA SYSTEM
Xu Zhihong, Dong Qian, Lia Xiaoxia, Yan Xinjian, Guo Li, Institute of Chemical Metallurgy, Academia Sinica, Beijing, China

QUALITATIVE APPROACHES FOR NUMERICAL REASONING
POSTER PRESENTATION

STRUCTURAL DATA ACQUISITION OF NOMENCLATURE AND STRUCTURE DATABASE IN THE CHEMICAL INFORMATION SYSTEM
Nianhua Xiao, Senliang Li, The Center of Scientific Databases, Academia Sinica, China

ELDAR, A HYBRID KNOWLEDGE BASE SYSTEM FOR THE CALCULATION OF ELECTROLYTE SOLUTION PROPERTIES
J. Barthel and H. Popp, Institute for Physical and Theoretical Chemistry, University of Regensburg, F.R.G.

AN EFFECTIVE MODEL FITTING TO LINEAR SYSTEM BY HOLOTRANSFORMATION-EQUIVALENT NORMAL EQUATION METHOD
Edip Büyükkoca, Yildiz University, Sisli-Istanbul, Turkey

DEVELOPMENT OF A SCIENCE’S INTEGRATED INFORMATION SYSTEM
E. Kostolansky, Information Center of Slovak Academy of Sciences, Bratislava, Czechoslovakia

IMPLEMENTATION OF IPES AND ITS APPLICATIONS
Xu Zhihong and Huang Guosheng, Institute of Chemical Metallurgy, Academia Sinica Beijing, Beijing, China

PARTICLE PHYSICS DATA SYSTEMATIZATION PROJECT - COMPAS

POWER PLANTS WORKING SUBSTANCE CHARACTERISTICS IN A KNOWLEDGE BASE SYSTEM
V.E. Alcemasov, A.F. Dregalin, R.N. Nazyrova, U.S.S.R.

A GENERALIZED SOFTWARE SYSTEM ON AUTOMATION OF GROUP CONTRIBUTION METHODS
Dong Qian, Yan Xinjian and Xu Zhihong, Institute of Chemical Metallurgy, Chinese Academy of Sciences, Beijing, China

ORGANIC COMPOUND STRUCTURE MATCHING WITH DISTANCE MATRIX
Yan Xinjian, Xu Zhihong, and Dong Qian, Institute of Chemical Metallurgy, Academia Sinica, Beijing, China

Theme #5: TRENDS IN INTEGRATION OF INFORMATION ACROSS BIOLOGY

ORAL PRESENTATION

ANIMAL VIRUS INFORMATION SYSTEM - AN INDIAN ATTEMPT
P.S. Naik, Urmila Kulkarni and A.S. Kolaskar, Bioinformatics, DIC, University of Poona, Pune, India

DATA STANDARDS IN THE US EPA

AUTOMATIC EVALUATION OF DIAGNOSTIC CAPABILITY OF AMINO ACID FUNCTIONAL PATTERNS
Temple F. Smith, Roderic Guigo and Ann Johansson, Molecular Biology Computer Research Resource, Dana-Farber Cancer Institute, Boston, Massachusetts, U.S.A.

BIOREP - PERMANENT INVENTORY OF BIOTECHNOLOGY RESEARCH IN EUROPE
M.L.H. Lalieu, Library and Information Centre of the Royal Netherlands Academy of Arts and Sciences (KNAW), Amsterdam, The Netherlands

AN ALGORITHM FOR MULTIPLE ALIGNMENT OF PROTEIN SEQUENCES
Kiejung Park, Korean Collection for Type Cultures, Genetic Engineering Center, Korea Institute of Science and Technology, Seoul, Korea
Chankyu Park, Department of Biological Science and Engineering, Korea Advanced Institute of Science and Technology, Seoul, Korea
LANGUAL

POSTER PRESENTATION

THE CARCINOGENICITY INFORMATION DATABASE OF ENVIRONMENTAL SUBSTANCES (CIDES) AND THE ASSESSMENT OF POSSIBLE HUMAN RISK

DATA ACQUISITION OF THE CHINESE MEDICINAL PLANT DATABASE
Senliang Li, Center of Scientific Databases, Academia Sinica, Beijing, China

THE TRADITIONAL CHINESE MEDICINE DATABASE FOR PREVENTION AND CURE OF CANCER
Senliang Li, Center of Scientific Databases, Academia Sinica, Beijing, China

Theme #6 - IMPACT OF NEW TECHNOLOGY ON DATA HANDLING

ORAL PRESENTATION

TOWARD A WIRED WORLD: HOW NEW NEURAL NETWORK TECHNOLOGIES AFFECT S&T DATA ORGANIZATION AND USE
Prof. B. Ray Horn, Management and Information Systems, School of Business and Management, U.S. International University-Europe (USIU-E), Bushey, Herts., U.K.
Dr. David Ellis, Michigan State University, East Lansing, Michigan, U.S.A.
Dr. Rosser A. Rudolph, Dept. of Laboratory Medicine, Mercy Hospital, Yorktown, Indiana, U.S.A.
Jaime G. Nunez-Cruz, Ball State University, Muncie, Indiana, U.S.A.

IMPACT OF NEW TECHNOLOGY
C. Jaschek, Centre de Données Stellaires, Observatoire Astronomique, Strasbourg, France

DIPPR IN ITS ELEVENTH YEAR
T.B. Selover, Shaker Heights, Ohio, U.S.A.

CREATION AND DEVELOPMENT OF THE SCIENTIFIC DATABASE SYSTEM IN THE CHINESE ACADEMY OF SCIENCES (CAS)
Luo Baichang, Scientific Databases, Chinese Academy of Sciences, Beijing, China

DEVELOPMENT OF CD-ROM BASED SEA ICE DATA SETS: PRELIMINARY LESSONS
Ronald L.S. Weaver and Roger G. Barry, National Snow and Ice Data Center, Cires, University of Colorado, Boulder, Colorado, U.S.A.

POSTER PRESENTATION

DATABASE ACCESS THROUGH THE NATIONAL COMPUTER INTERNETWORK
Clifford A. Lynch, Division of Library Automation, University of California, Oakland, California, U.S.A.

LIBRARIES AND SCIENTIFIC DATA
Katherine Chiang, Computer Files Librarian, Mann Library, Cornell University, Ithaca, New York, U.S.A.

TDS/NUMERICA: NUMERICA DATA IN CHEMISTRY AND ENGINEERING

A NEW CONCEPT FOR USER-FRIENDLY INTERROGATION AND NETWORKING OF DATABASES
P. Vannson, F. Franck and H. Over, Institute of Advanced Materials, CEC, Joint Research Centre, Petten, The Netherlands
G. Fattori, Ispra, Italy
Post Scriptum

From the Program Committee:

The poster session indicating country activities in the Global Change Program on the first day of the Conference will feature an oral wrapping-up and summation by Thomas Malone. It is presumed that this will take place on July 15th, 1530-1700, at a site to be designated in the final program.

Finally, for the benefit of those who have lately come to CODATA and have a need to know—and for those with experience just wishing to reminisce—an illustrated "history piece" on CODATA progress and achievement through the years is to be presented at the closing session by Edgar Westrum.

Forthcoming CODATA Work on Materials Data Management

A CODATA Bulletin (No. 22-1) to be available this spring summarizes the presentations made at the two-day September 1989 Novosibirsk Symposium of the CODATA Task Group on Materials Database Management. The consequently important hundred plus page text covers global collaboration, standards and accessing materials databases (Barrett, Kaufman); regional collaboration—CEC, COMECON, VAMAS—(Swindells, Kozlov, and Reynard); as well as representative national activities—including those of France, Japan, U.K., and U.S.S.R.—(Vinard, Nishijimi, Jackson, Bogomolij, and others).

Although the volume will be sent routinely to CODATA Bulletin subscribers, the publishers anticipate a considerable sale of separate copies.

The Task Group held its 6th Meeting on 28th November, 1989, at Lake Buena Vista, Florida, prior to the Second ASTM International Symposium on Computerization of Materials Property Data. Members from six CODATA nations were present. Ongoing projects were reviewed; these included the Newsletter, progress in the production by other groups in CODATA and ICSTI of directories of materials data sources and numeric databases, and the project on evaluating the benefits of materials databases. Feedback is being collected on CODATA Bulletin 69, Guide to Material Property Database Management. This was edited by J. G. Kaufman to whom comments should be sent so that they may be reviewed to determine whether a need exists for an updated version of the guide.

Papers presented at the Task Group’s Symposium held in Novosibirsk in September 1989 (see Newsletter No. 8) are to be published as a CODATA Bulletin early in 1990. A wide range of materials database sources was revealed at the Symposium. Accordingly, the Task Group recommended that CODATA co-sponsor an international workshop to study the rapidly changing technical, political, and economic aspects of the trans-border flow of materials property data on a global scale. At its most recent meeting, the Task Group reviewed the plans for this workshop which is scheduled to take place in the spring of 1991. Professor Alexander Kozlov is chairman of the programme subcommittee. A further new items of business is a proposal to establish a standard for the description of materials property databases. A draft paper clarifying the issues involved is being prepared by Dr. Norman Swindells for discussion by the Task Group. The next meeting will take place on 14th and 15th July 1990 in Columbus, OH, immediately preceding the 12th International CODATA Conference.

**NETWORKS**

The CEC’s *Materials Database Demonstrator Programme* was concluded at a major workshop held at the Petten Research Centre in the Netherlands from 6th to 8th December 1989. The Workshop was attended by over 70 users and providers of materials data and representatives in and outside the EC, including the USA and Japan. The purposes of the workshop were to review the lessons learned in the Demonstrator Programme, to consider these in the light of developments elsewhere and to define the scope for follow-up actions. The participants reached a consensus on the need for continuing joint action by the CED, national governments, and industries of the Member Countries in the areas of: promotion of computerized materials information and its application, standardization of information products, integration of information products, sources of data, user support agencies, and international collaboration. The Workshop proceedings will be published early in 1990.

**DATABASES**

An updated version of the *MPR Structural Materials Selector* has been released. Designed to run on IBM PC, XT, or compatible machines, the package includes property data for other 750 powder metallurgy materials. FURTHER INFORMATION: MPR Publishing Services Ltd., Old Bank Buildings, Bellstone, Shrewsbury, England, SY1 1HU.

The National Association of Corrosion Engineers (NACE) and the US National Institute of Standards and Technology (NIST) have released *CHEM.COR I and CHEM.COR I PLUS*, expert systems that provide reliable corrosion engineering advice to assist the user in the shipping, handling, and storage of concentrated sulphuric acid (70-100%) and oleum (100% sulphuric acid plus free sulphur trioxide). Minimum system requirements include IBM PC-XT compatibility. FURTHER INFORMATION: T. S. Lee, NACE, P. O. Box 218340, Houston, TX 77218, USA.

(continued on page 15)
VAMAS Technical Working Area 14: *The Technical Basis for a Unified Classification System for Advanced Ceramics* was established in September 1988 with the aims of: 1. identifying and assessing the issues inherent in developing a classification system for advanced ceramics; 2. establishing a building-block structure for international use; and 3. developing mechanisms and institutional links for system implementation. Participation by interested persons is encouraged. A classification workshop will be held at the Petten Research Centre in June 1990 (see Calendar listing). FURTHER INFORMATION: Samuel Schneider, NIST, Gaithersburg, MD 20899, USA.

ASTM has published STP10170 *Computerization and Networking of Materials Data Bases*, a comprehensive review of international developments in materials databases. 31 peer-reviewed papers cover the following aspects: standards for materials databases, national and international activities, emerging issues, impact of materials databases, materials database projects, and cooperative data programs in the United States. Glazman, J. S. and Rumble, J.R., eds. *Computerization and Networking of Materials Data Bases*, 360 pp, $66; $52.80 to ASTM members; available from ASTM, 1916 Race Street, Philadelphia, PA 19103, USA.

*Tietokoneperustelit Materiaalitietojärjestelmät (Computerized Materials Information Systems)* is the report of a presudy designed to enhance decision making in Finland in the area of computerized materials information systems by providing the necessary background information along with an analysis of the options available. The presudy involved interviews and system demonstrations in seven Western countries, participation in international workshops, acquisition, and analysis of several small materials information systems, theoretical conceptual analyses, and a national seminar. The report was compiled by Aki Valkonen and is published in Finnish with an English summary. It is available from KY-Palvelu Oy Kirjakauppa, Runeberginkatu 14-16 B, 00100 Helsinki, Finland.

13-14 March 1990, Le Bourget, FRANCE
Symposium on COMPOSITE MATERIALS: PRODUCTION, UTILIZATION AND DATA BANKS. Organized by CODATA France and Agence Francaise pour le Maitrise de l'Energie. CONTACT: Mr. Bernard Marx, MENJS, 3 Boulevard Pasteur, 75015 Paris, France. Tel: +33 1 40656097.

21-22 June 1990, Petten, THE NETHERLANDS
CERAMICS CLASSIFICATION Workshop. CONTACT: Mr. S. Schneider, NIST, Gaithersburg, MD 20899, USA. Tel: +1 (301) 975 5657. Fax: +1 (301) 926 8349.

15-19 July 1990, Columbus, OH, USA
12th International CODATA Conference DATA FOR DISCOVERY. CONTACT: CODATA, ’90, P. O. Box 23, Amlin, OH 43002, USA.

November 1990, Petten, THE NETHERLANDS
CEC/CODATA Workshop on MATERIALS DATA FOR COMPUTER AIDED ENGINEERING. CONTACT: Mr. H. Kröckel, CEC-JRC Petten, P. O. Box 2, 1755 ZG, Petten, The Netherlands.
CODATA Guides for Data Publication Revisited

The last issue (21-4) of the CODATA Bulletin for 1989 compiled most of the CODATA Guides for Data Publication to bring these to the attention of a new generation of scientists. Although neither time nor funding for convening updating working groups was available, such an endeavor might prove profitable in making the world more hospitable for data over the next several years. CODATA Guides for Data Publication, viii + 107 pages, Hemisphere Publishing Corporation, ISSN 0366-757x, CODBA4 21(4), 1-107 (1989) US$33.00.

Switzerland--The newest CODATA Member

The Swiss Academy of Engineering Sciences (SATW) has made overtures to CODATA for membership and has been unanimously accepted to CODATA as a Country member. Dr. Peter Schönholzer is the Acting Chairman of the Swiss National Committee for CODATA. Mail contact may be made through Secretariat SATW, Swiss Academy of Engineering Sciences, c/o Mrs. S. Müller, Postfach, CH-8034 Zurich, Switzerland.

Codata, 51 bd. de Montmorency, 75016 Paris