Finally, Dr. Zudkevitch encouraged all involved in the teaching of chemical engineering to stress in their presentations and contacts with students that the computer is not always right and owing to bad input, or programmed decision-making routine, it can quite often provide wrong results.

PROF. C.A. NIETO DE CASTRO (University of Lisbon) summarized the discussion by thanking all participants and encourage them to spread all the ideas presented among the academitians and industrialists, hoping that the industry can foresee the importance of thermophysical properties for the design and operation of chemical plants and that henceforth, can invest in the thermo-physical properties research to a level much bigger than the actual one. He finally stressed the importance of a good academic training of chemists and chemical engineers, namely in the area of computer aided design.

CHEMPOR '85

★ ★

4th INTERNATIONAL CHEMICAL ENGINEERING CONFERENCE

University of Coimbra
Coimbra — Portugal
April 15-19, 1985

CHEMPOR '85

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4ª CONFERÊNCIA INTERNACIONAL DE ENGENHARIA QUÍMICA

Universidade de Coimbra
Coimbra — Portugal
Abril 15-19, 1985

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CHAIRMEN OF SESSIONS

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Session | TP1 - Professor Joaquim J.B. Romero, Universidade do Minho
TP2 - Professor Jorge C.G. Calado, Universidade Técnica de Lisboa
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TP5 - Professor Carlos A. Nieto de Castro, Universidade de Lisboa
TP6 - Dr. Bernard LeNeindre, C.N.R.S. (Paris-Nord)
TP7 - Dr. William A. Wakeham, University of London

Workshop | TP8 - moderator: Professor Carlos A. Nieto de Castro

Session | EN1 - Dr. Theodore R. Bott, University of Birmingham
EN2 - Dr. Clemente P. Nunes, C.N. Petroquímica
EN3 - Professor Bengt Sundén, Chalmers University
EN4 - Mr. A. Norton de Matos, C.N. Petroquímica
EN5 - Professor J. Almiro A.M. e Castro, Universidade de Coimbra
EN6 - Professor Lélio Q. Lobo, Universidade de Coimbra

Panel | EN7 - moderator: Dr. Clemente P. Nunes

SCIENTIFIC PROGRAMME

BLOCK 1 - THERMOPHYSICAL PROPERTIES

Monday, 15th April

11.15 - 12.30 h   SESSION TP1: Plenary lecture

The need for new developments in Thermodynamics
Jorge C.G. Calado (Cornell, USA, and T. Lisboa, PORTUGAL)

14.30 - .15.45 h   SESSION TP2: Communications

01 *Computer Simulation and Theoretical Studies of Liquid Mixtures: Brute Force vs. Insight*
K.E. Gubbins (Cornell, USA)

02 *Prediction of VLE Data for Two-Component Mixtures from Heats of Mixing and the Complete Local Concentration Model*
N. Chiou and D. Yarbrough (Tennessee, USA)

03 *Prediction of VLE and LLE by the ASOG Method*
A. Arce, A. Blanco, J.M. Correa, M.R. Mendez and J. Tojo (Santiago and Vigo, SPAIN)

04 *Some Difficulties on the Application of the UNIFAC Model for the Prediction of LLE Compositions*
M.G. Bernardo Gil and L.J.S. Soares (Lisboa and Minho, PORTUGAL)

05 *VLE of Polar Mixtures: A New Generalized Correlation*
S. Persio Ravagnani and S.G. d'Ávila (Campinas, BRASIL)

16.15 - 18.00 h   SESSION TP3: Communications

06 *Binary Parameter Values for VLE Calculations*
Y. Adachi and B.C.-Y. Lu (Ottawa, CANADA)

07 *Thermodynamics of Liquid Mixtures - A Unified Approach for Predicting Isothermal VLE and Viscosity from Heat of Mixing*
T.R. Kubendran, M.R.V. Krishnan and G.S. Laddha (Anna/Madras, INDIA)

08 *Sensitivity of Separation Process Design to Phase Equilibria and Operation Parameters*
A.M. Sereno and S. Macchietto (Porto, PORTUGAL and London, UK)

09 *An Exercise on the Influence of the Uncertainty in the Calculation of VLE on the Costs and Performance of Distillation Columns*
M. Margarida L.F.L. Rebola, A.G.M. Ferreira and L.Q. Lobo (Coimbra, PORTUGAL)

10 *Thermal Properties of Binary Mixtures at Infinite Dilution*
P. Alessi, M. Fermeglia and I. Kikic (Trieste, ITALY)

11 *The Use of Infinite Dilution Activity Coefficients in Process Design*
J.C. Bastos, M.E. Soares and A.G. Medina (Porto, PORTUGAL)

12 *Computer Simulation of Aromatics Extraction*
A.M. Sereno and A.G. Medina (Porto, PORTUGAL)

Tuesday, 16th April

9.30 - 10.45 h   SESSION TP4: Communications

13 *Use of Isothermal Microcalorimetry for the Characterization of Thermal Power Occuring in Technically Important Materials and Products*
J. Suurkuusk and I. Wadsö (Lund, SWEDEN)

14 *Thermodynamics of Phase Transitions in Some Organic Polyols*
M. Conceição P. Lima and C.D. Maycock (Coimbra, PORTUGAL)

15 *Expansivities of Pure Organic Compounds at Moderate Temperatures*
J. Ortega, J.S. Matos, J. Trujillo, M.I. Paz-Andrade and E. Jimenez (Las Palmas and Santiago, SPAIN)

16 *Thermal Expansion Coefficients of Mixtures: Benzene + 1-Pentanol and + 2-Pentanol at Moderate Temperatures*
J. Ortega and M.I. Paz-Andrade (Las Palmas and Santiago, SPAIN)

17 *Excess Molar Volumes of Binary Mixtures: Ethyl Formate + Isomers of Hexanol at 298.15 K*
J. Ortega, J.S. Matos, M.I. Paz-Andrade and R. Bravo (Las Palmas and Santiago, SPAIN)

18 *Excess Molar Volumes of Binary Mixtures: Ethyl Acetate + Isomers of Hexanol at 298.15 K*
J. Ortega, J.S. Matos, M.I. Paz-Andrade, and R. Bravo (Las Palmas and Santiago, SPAIN)

11.15 – 12.30 h   SESSION TP5: <u>Communications</u>

19 *Partial Molar Volumes of Naphthalene Dilute in Supercritical*
    Fluid Solvents
    E.J.S. Gomes de Azevedo and J.M. Prausnitz (T. Lisboa, PORTU
    GAL and Berkeley, USA)

20 *Excess Molar Volumes of Mixtures of n-Butyl Acetate with an*
    n-Alkane
    E.F.G. Barbosa, J.C.G. Calado, E. Jimenez, I.M.S. Lampreia, L.
    Pias and M.I. Paz-Andrade (Lisboa, PORTUGAL and Santiago,
    SPAIN)

21 *VLE for Binary Systems Ethyl Formate with 1-Propanol and*
    2-Propanol at 760 mm Hg
    J.A. Peña, J. Ortega, M.I. Paz-Andrade and J. Fernandez (Las
    Palmas and Santiago, SPAIN)

22 *VLE of the System Benzene – Cyclohexane – 1, Propanol at 760 mm Hg*
    A. Arce, A. Blanco, J.M. Correa and J. Tojo (Santiago, SPAIN)

23 *Interfacial Tensions in Hydrocarbon + Perfluorocarbon Mixtures:*
    A Microcosm of Intermolecular Forces and Close-to-critical
    Endpoint Effects
    I.A. McLure and V.A.M. Soares (Sheffield, UK and Lisboa,
    PORTUGAL)

24 *A Microscopic Model for the Interfacial Properties of Mixtures*
    of Oil, Water and Non-Ionic Surfactants
    M.M. Telo da Gama and K.E. Gubbins (Cornell, USA)

14.30 – 15.45 h   SESSION TP6: <u>Communications</u>

25 *The Transport Properties of Gases with Multipole Moments*
    G.C. Maitland, R.D. Trengove and W.A. Wakeham (London, UK)

26 *On the Role of the External Effects in the Intermolecular*
    Parameters Determination from Experimental Thermophysical Data
    Galina P. Dudchick and G.G. Kuleshov (Minsk, USSR)

27 *Calculation of Transport Collision Integrals for Lennard-Jones*
    Gases
    E.V. Akhmatskaya and L.A. Pozhar (Kharkov, USSR)

28 *A General Relationship Between Dynamic Viscosity and Reduced*
    Temperature for Liquids in the Reduced Temperature Range 0.4 to
    0.8
    C. Baroncini, G. Latini and P. Pierpaoli (Ancona, ITALY)

29 *The Effect of Uncertainty in Diffusion Coefficients in the*
    Design of Packed Columns
    M.L.S. Matos Lopes, C.A. Nieto de Castro and W.A. Wakeham
    (Lisboa, PORTUGAL and London, UK)

BLOCK 2 - ENERGY CONSERVATION IN THE CHEMICAL AND ALLIED INDUSTRIES

9.30 - 10.45 h   SESSION EN1: Plenary lecture

Integrated Design of Processes and Service Systems.
Improving Energy, Capital and Flexibility
Bodo Linnhoff (Manchester, UK)

11.15 - 12.30 h   SESSION EN2: Communications

41   *The Relationship Between Energy Analysis and Operating Costs for*
Energy Conservation in Chemical Processes
C.D. Grant and A.N. Anozie (Strathclyde, UK and Ife, NIGE-
RIA)

42   *Improvements of the Energy System at an Oil Refinery by*
Optimization of the Heat Exchanger Network
B. Sundén, H. Thersthol and C. Wernersson (Chalmers and Shell/
Göteborg, SWEDEN)

43   *Energy Savings Through Improvements of a Heat Transfer System in*
a Petrochemical Plant - A Case Study
C.P. Nunes and J. Vasconcelos (CNP, PORTUGAL)

44   *Energy Recovery in Distillation Columns with Direct Vapour*
Recompression. Application to the Distillation of the Ethanol-
Water System
Teresa M.K. Ravagnani and J.A.F.R. Pereira (Campinas, BRASIL)

45   *Thermally Integrated Distillation Columns: A Comparison of*
Different Control Schemes
S. Bigini, A. Brambilla, G.F. Nencetti and C. Scali (Pisa,
ITALY)

14.30 - 16.00 h   SESSION EN3: Communications

46   *Extraction as an Energy-Saving Alternative to Rectification in*
the Recovery of Organic Compounds from Aqueous Solutions
R. Billet and M. Pajak (Ruhr/Bochum, WEST GERMANY)

47   *Um Programa Global de Economias de Energia e Utilidades no*
Complexo Petroquímico de Sines
C.P. Nunes and M.M. Palma (CNP, PORTUGAL)

48   *Thermodynamic Analysis of a Shale Oil Production Plant for Energy*
Conservation
R. Mundstock, L.C. Casavechia and K. Rajagopal (PETROBRAS and
Fed. Rio de Janeiro, BRASIL)

49   *Project of Energy Recovery from Flue Gases at Sociedade Nacional de Sabões*

A.R. Janeiro Borges, J.C. Galvão Teles and J. Braga (U.N. Lisboa, AM Lisboa and SNS, PORTUGAL)

50   *Temperature Profile-Basis for Heat Accounting*

M. Fehr (Uberlândia, BRASIL)

51   *Heat Recovery in Glass Fusion Furnaces - A Case Study*

A.A.B. Neves, M.N. Nina and J.F.P. Gomes (LNETI and T. Lisboa, PORTUGAL)

16.15 - 17.30 h   SESSION EN4:   Communications

52   *Intensification of Design and Operation of Continuous Treatment Processes*

R. Burley (Heriot-Watt, UK)

53   *A Quasi Steady State Model for Low Density Polyethylene Pipeline Reactors*

J.A. Howell and S. Feyo de Azevedo (Swansea, UK and Porto, PORTUGAL)

54   *The Effect of Temperature on the Rate of Photodegradation (weathering) of Polymer Films*

M.S. Carvalho, J.J.C. Cruz Pinto and J.F.A. Ferreira (Minho, PORTUGAL)

55   *Transfert de Chaleur en Lit Fluidisé*

K. Alia, F. Bentahar, M. Benali, H. Ait-Sahlia and C. Dahmane (H. Boumediene, ALGERIA)

56   *Simulation of Industrial Chemical Processes. I - Synthesis of Phthalic Anhydride from O-Xylene in a Fixed Bed Reactor*

J.C. Oliveira and A.E. Rodrigues (Porto, PORTUGAL)

Friday, 19th April

9.30 - 11.00 h   SESSION EN5:   Communications

57   *Influence of the Intermolecular Potential on the Calculated Detonation Characteristics of Explosives with Positive Oxygen Balance*

O. Heuzé, H.N. Presles and P. Bauer (Poitiers, FRANCE)

58   *Determination of the Composition of Gaseous Mixtures*

O. Heuzé, P. Bauer and H.N. Presles (Poitiers, FRANCE)

59   *Ignition of White Pine and Cork Dust*

L. Araújo and J. Campos (Coimbra, PORTUGAL)

60   *Combustion Characteristics of Wood and Cork Dust Suspensions*

L. Lemos and J. Campos (Coimbra, PORTUGAL)

61 *Obtenção de Gás de Poder Calorífico Médio a Partir da Madeira*
  Z.T. Makray and J.A.F.R. Pereira (Campinas, BRASIL)

62 *Energy Recovery in the Pyrolysis and Gasification of Wood Wastes*
  for Local Energy Production
  S.S. Alves and J.L. Figueiredo (T. Lisboa and Porto, PORTUGAL)

11.15 - 13.00 h **SESSION EN6:** <u>Communications</u>

63 *The Use of Hot Wire Techniques in Fouling Tests. A Word of*
  Awareness
  J.D. Pinheiro, L.F. Melo and R.T. Oliveira (Minho, PORTUGAL)

64 *Fouling in Heat Exchangers: A Study of the Mechanisms of*
  Formation of Kaolin Deposits
  L.F. Melo and J.D. Pinheiro (Minho, PORTUGAL)

65 *Biofouling in Tubes - Some Trends and Perspectives*
  J.D. Pinheiro, L.M.F. Melo and M.M.S. Pinheiro (Minho, PORTU-GAL)

66 *An Improved Method to Estimate Kinetic Thermal Properties in*
  the Design of Heat Exchangers
  V.G. Dovi, B. Canepa, P. Costa and L. Maga (Genova, ITALY)

67 *Parametric Pumping: An Energetically Efficient Separation*
  Process
  C. Costa and A.E. Rodrigues (Porto, PORTUGAL)

68 *Analysis of Transient Thermal Measurements on Fibrous Insulations*
  Obtained with an Unguarded Flat Tester
  D.W. Yarbrough, D.L. McElroy, T.W. Tong and J.K. Wood III
  (Oak Ridge, Tennessee and Kentucky, USA)

69 *Improving Thermal Insulation Performance in the Process Industries*
  R.P. Tye (DYNATECH, USA)

15.00 - 17.00 h **SESSION EN7:** <u>Panel session</u>

  Energy Conservation in the Chemical and Allied Industries

THE NEED FOR NEW DEVELOPMENTS IN THERMODYNAMICS

Jorge C.G. Calado

Department of Chemical Engineering, Instituto Superior Técnico,
1096 Lisboa, PORTUGAL

and

School of Chemical Engineering, Cornell University, Ithaca,
N.Y. 14853, U.S.A.

A brief, historical survey of the development of experimental thermodynamics, with special focus on equilibrium properties, is presented. The present situation where a growing need for data coexists with a precarious diminution of a capacity to measure the thermophysical properties of fluids and their mixtures, in Europe and in the U.S., is analyzed. Part of the problem seems to be an "out-of-fashion" attitude, hence the necessity of new developments which might stimulate the intellectual curiosity of the younger generation of potential thermodynamicists.

A tripartite approach, which combines concerted efforts in theory, experiment and computer simulation has already been proposed. Strong emphasis should be given to the molecular approach and visualizability of models and theories. This is particularly crucial to the "forest" of equations-of-state, since more than 4 500 types and variations have been proposed in the last twenty years ! The discriminating factor should be their sound molecular basis, derived from a better understanding of the behaviour of matter at the microscopic level. Model substances should be chosen to test different equations and theories. Special attention is given to the second generation of the van der Waals -type equations, namely those of Deiters, BACK and Kohler, and how they fare with a simple substance like tetrafluoromethane.

The link between these equations-of -state and perturbation theory is stressed. Some successful examples of how these theories deal with polarity or shape are presented.

Different properties respond to different parts of characteristics of the intermolecular potential, and a deeper knowledge of this kind of influence can lead to the construction of better effective fluid potentials.

The emphasis on visualization, still possible in molecular thermodynamics, is also observed in the concept of local composition. The suitability of the square-well model potential to this concept is analyzed. The statistical basis for the combination rules (one of the major vulnerabilities of any statistical theory) is analyzed, and some new promising developments are discussed. Finally, continuum thermodynamics shows how predictions can be made even for the most complex of systems where neither the number of components nor their nature is known.

Time, complexity and cost which have plagued most of the sophisticated treatments so far, will be conquered by the new supercomputers already being developed. It is estimated that within ten years we will have large scale computing systems with a thousand times the power

of the present large scale systems, such as the
CRAY-1 or IBM-3081.   The first industrial
revolution gave birth to thermodynamics;   the
third industrial revolution will make it
exciting once again.

INTEGRATED DESIGN OF PROCESSES AND SERVICE SYSTEMS
IMPROVING ENERGY, CAPITAL AND FLEXIBILITY

Bodo Linnhoff

U.M.I.S.T., U.K.

SYNOPSIS

Over the last five years or so, the concept of the "Network Pinch" has become quite well-known in the chemical industry as instrumental in energy savings in the design of integrated heat exchanger networks. Several international companies reported improvements using the concept such as

- 50% plus energy cost reductions
- up to 25% capital cost reductions
- playback times in retrofit projects of up to 1 month (average: six months)

see for instance ref.(1) and ref.(2)

The lecture will present an overview of the original concept. Further, the lecture will show how the concept has now been extended to help tockling the task of design of entire chemical processes and production sites. From reactor conversions, separator and recycle arrangements right "inside" a process through to furnaces, steam levels and turbines in the site services, a generalizing design procedure emerges which enables the engineer to correctly quantify and implement integration changes.

Last, the lecture will discuss new concepts which help the engineer to deal with capital cost minimisation and the task of finding flexible integrated structures (summer/winter, throughput, feedstock, etc.). It is now possible to save energy, reduce capital cost and enhance flexibility simultaneously.

Ref. 1. Linnhoff, B. and Turner, J.A. "Heat--recovery networks: new insights yield big savings", Chemical Engineering, pp 56-70, Nov. 2 (1981).

Ref. 2. Linnhoff, B. and Vredeveld, D.R., "Retrofit projects through process synthesis", Paper Nº 5f, AIChE Diamond Jubilee Meeting, Washington, 30 Oct. - 4 Nov., (1983).

INTEGRATED DESIGN OF PROCESSES AND SERVICE SYSTEMS
IMPROVING ENERGY, CAPITAL AND FLEXIBILITY

Bodo Linnhoff

U.M.I.S.T., U.K.

SYNOPSIS

Over the last five years or so, the concept of the "Network Pinch" has become quite well-known in the chemical industry as instrumental in energy savings in the design of integrated heat exchanger networks. Several international companies reported improvements using the concept such as

- 30% plus energy cost reductions
- up to 25% capital cost reductions
- payback times in retrofit projects of up to 1 month (average: six months)

see for-instance ref.(1) and ref.(2)

The lecture will present an overview of the original concept. Further, the lecture will show how the concept has now been extended to help tackling the task of design of entire chemical processes and production sites. From reactor conversions, separator and recycle arrangements right "inside" a process through to furnaces, steam levels and turbines in the site services, a generalizing design procedure emerges which enables the engineer to correctly quantify and implement integration changes.

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Ref. 2. Linnhoff, B. and Vredeveld, D.R. "Retrofit projects through process synthesis," Paper No 51, AIChE Diamond Jubilee Meeting, Washington, 30 Oct. - 4 Nov., (1983).

Report of the WORKSHOP ON THERMOPHYSICAL PROPERTIES
THEIR IMPACT ON TECHNOLOGICAL INOVATION

Prepared by C.A. Nieto de Castro and W.A. Wakeham

INTRODUCTION

The report summarizes the discussion held on 17th April 1985 concerning the impact of Thermophysical Properties on Technological Inovation. By prior arrangement the subject had been divided into three complementary topics, namely: The contribution of the theory of Thermophysical Properties for the Chemical Industry; Experimental data, prediction correlation - mutual interaction, with emphasis on special fluids; Thermophysical Properties in the Chemical Industry - their relevance, accuracy and effects on equipment design. The structure of the workshop was such that invited speakers contributed short presentations on each subject which was followed by a period of discussion and further short communications on the subjects.

The present summary of the proceedings of the workshop is an attempt to represent the general content of the invited contribution and the subsequent discussion. As such it is not intended to be fully comprehensive or to include all details. The authors have tried to include the comments of all contributions and any ommissions are their responsability.

THE FORMAL PRESENTATIONS

PROF. K.C. CHAO (Purdue University) addressed the topic of the contribution of the theory of Thermophysical Properties for the Chemical Industry. He concentrated his presentation on the description of the equilibrium properties of pure fluids and binary mixtures by means of equations of state. In particular he employed an equation of state, derived from statistical mechanics of chain molecules which was appropriate for large and small molecules. It was applied to nonpolar and slightly polar molecules. Many examples were given of the sucess of this equation of state procedure. For applications on smaller computer installations a simplified cubic chain of rotators equation of state was described which although not quite as accurate, was nevertheless quite useful.

DR. R. BURLEY (Hariot-Watt University) spoke of the need for thermophysical properties in important industrial problems which he had encountered which involved fluids under unusual and sometimes extreme conditions. The first example concerned the coating of solid films with a liquid in a process involving drawing the film through the surface of a liquid. Dr. Burley emphasized the high shear stresses in such a process the fact that surface properties and properties in their fluid layers under such conditions were rarely known. These facts made the modelling of the process extremely difficult. The second example quoted by Dr. Burley involved