

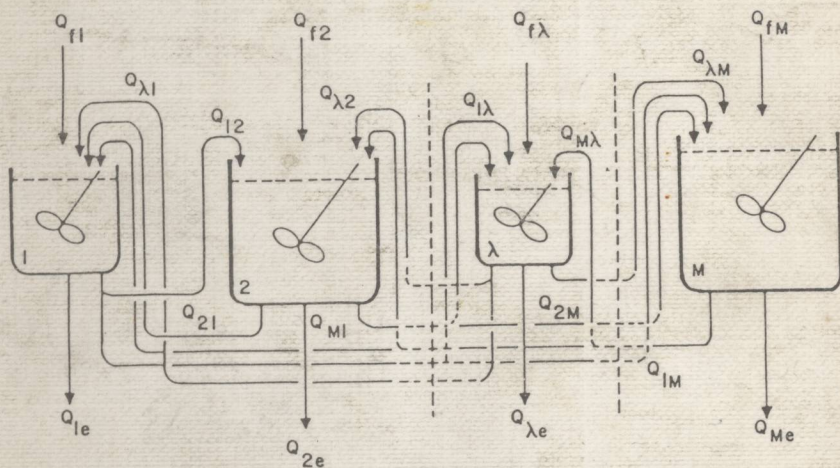
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CHEMICAL REACTION ENGINEERING

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the EFCE Working Party on Chemical Reaction Engineering,
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Symposium Co-Chairmen

Prof. G.S.G. Beveridge (*The University of Strathclyde*)

Prof. P.N. Rowe (*University College London*)

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PREFACE

ISCRE8 is the latest in a series of symposia on Chemical Reaction Engineering held every two years, alternating between the USA and Europe. ISCRE7 was held in Boston, USA, in October 1982 and ISCRE6 in Nice, France, in March 1980.

The conference aims to bring together experts in chemical reaction engineering from all over the world to provide a forum for discussion on developments in all aspects of the field, both academic and industrial.

ERRATUM

In paper 2.3 the text on page 687 should precede that on page 686.

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CONTENTS

Note: the Plenary Lectures are listed on page xiv

	<i>page</i>
Session 1: CATALYSIS & DE-ACTIVATION	
1.1 The Problem of Diffusional Transport in the Performance of Supported Liquid Phase Catalysts <i>E. Wicke and D. Hesse, (Inst. für Physikalische Chemie, Münster, W. Germany).</i>	1
1.2 Steady and Unsteady State Binary Gas Diffusion Measurements in Single Spherical Catalyst Pellets <i>P.E. Bower, S.P. Waldram (University College, London, U.K.) M.P. Dudukovic (Washington University, USA) and P.L. Mills, (Monsanto Corporation, USA).</i>	9
1.3 Performance of Diluted Catalysts <i>H.S. Weng, Y.F. Tzeng and Y. Chang (Cheng Kung University, China).</i>	17
1.4 Deactivation of a Supported Zeolitic Cracking Catalyst: A Pore Structural Approach <i>R. Mann, I.R. Moore (UMIST, UK) and F.Y.A. El-Kady (Egyptian Research Inst., Egypt).</i>	25
1.5 The Extension of Mobil's Kinetic Reforming Model to Include Catalyst Deactivation <i>P.H. Schipper, K.R. Graziani, B.C. Choi, and M.P. Ramage, (Mobil Research & Development Corporation, USA).</i>	33
 Session 2: FLUIDISED COMBUSTION	
2.1 Some Heat and Mass Transfer Considerations in the Design of Fluidised Bed Boilers <i>J. Moodie and M.A. Vickers (National Coal Board, UK).</i>	45
2.2 An Interpretation of Time-Resolved Oxygen Concentration Measurements in Coal-Burning Fluidised Beds <i>P.M. Walsh, C. Li, A. Dutta and J.M. Beer (MIT, USA).</i>	53
*2.3 A Study of In-Bed Oxygen Levels in a Fluidised Bed Combustor <i>B.M. Gibbs (University of Leeds, UK) and X.W.Ni (Chongqing University, China).</i>	683
2.4 The Effect of Pressure on the Kinetics and Extent of Sulphation of Calcareous Materials <i>J.S. Dennis and A.N. Hayhurst (University of Cambridge, UK).</i>	61
2.5 Kinetic Studies of the Fast Combustion of Coke Deposited on Cracking Catalysts <i>H.I. de Lasa and H. Schindler (University of Western Ontario, Canada)</i>	69

2.6	The Combustion of Coke Particles in a Fluidised Bed – Some Aspects of Kinetic Data Collection <i>C.M.C.T. Pinho and J.R.F. Guedes de Carvalho (Instituto Nacional de Investigacao Cientifica, Portugal).</i>	77
2.7	A Stepwise Analysis of Processes Involved in the Sulfur Capture During Fluidised Bed Combustion of Coal <i>I.W. Noordergraaf, J.J. van Deemter, J. van Kooten and P.J. van den Berg (Delft University of Technology, The Netherlands).</i>	85
Session 3: DYNAMICS AND STABILITY		
3.1	Dynamic Characteristics of the Fluid Catalytic Cracking Process <i>C. McGreavy and P.C. Smith (University of Leeds, UK)</i>	93
3.2	Exotic Behaviour in the Continuous Flow, Stirred-Tank Reactor (CSTR) Experimental Studies of Oscillations and of Isola and Mushroom Patterns in Stationary States under Gaseous Conditions. <i>P. Gray, J.F. Griffiths, S.M. Hasko and J.R. Mullins (University of Leeds, UK).</i>	101
3.3	Thermodynamic Limitations on the Dynamic Behaviour of Heterogeneous Reacting Systems <i>I.G. Kevrekidis, R. Aris and L.D. Schmidt (University of Minnesota, USA).</i>	109
3.4	The Effect of Cyclic Operation on Heterogeneous Catalytic Reaction with Educt Inhibition <i>A. Renken, M.A. Truffer (Lausanne Federal Inst. of Technology, Switzerland) and M. Dettmer (Deutsch Texaco, West Germany).</i>	117
3.5	Dynamic Behaviour and Stability of Continuous Reactors for Bulk Polymerization <i>R. Thiele (Ingenieurhochschule, Kothen, East Germany).</i>	125
3.6	Transient and Oscillatory Phenomena in Catalytic Reactors <i>M.B. Cutlip (University of Connecticut, USA) C.N. Kenney, W. Morton, D. Mukesh and S.C. Capaskis (University of Cambridge, UK).</i>	135
3.7	Multiplicity in Adiabatic Fixed-Bed Reactors: Ignition of Reactors <i>Q.H. Zhang (East China Inst. of Textile Tech), M.H. Chen and W.K. Yuan (East China Inst. of Chemical Tech., China).</i>	143
3.8	An Oxidation-Reduction Model for Reaction Rate Oscillations in Fischer-Tropsch Synthesis over Iron Catalysts <i>L. Caldwell (Council for Scientific & Ind. Research, S. Africa).</i>	151

Session 4: MULTIPHASE SYSTEMS

- 4.1 The Separation of Tritium from Heavy Water in Trickle Bed Reactors 159
D.R.P. Thatcher, K.T. Chuang, R.J. Quasttini and J.H. Rolston, (Atomic Energy of Canada Ltd, Canada)
- 4.2 Modelling and Design of a Trickle Bed Reactor 169
S. Scardà (Politecnico di Torino, Italy)
- 4.3 Modelling of a Gas-Solid Trickleflow Reactor for the Catalytic 177
Oxidation of Hydrogen Sulphide to Elemental Sulphur
A.B. Verver (Akzo Engineering) W.P.M. van Swaaij (Twente Univ., The Netherlands)
- 4.4 Holdup & Pressure Drop in Trickle Bed Reactors 185
J. Levec (Eduard Kardelj University, Yugoslavia) A.E. Saez and R.G. Carbonell (North Carolina State University, USA)
- 4.5 Determination of the Enhancement Factor for Gas Absorption in a 195
Shurry Reactor
O.J. Wimmers and J. Fortuin (University of Amsterdam, The Netherlands)
- 4.6 Modelling of a Batch Reactor for Hydrogenation of *o*-Nitroanisole 205
to *o*-Anisidine
R. V. Chaudhari, M.G. Parande, P.A. Ramachandran and P.H. Brahme, (National Chemical Laboratory, India)
- *4.7 Oxidation of Calcium Sulfite in Shurries 691
S.D. Reynolds and J.L. Hudson (University of Virginia, USA)
- 4.8 Selectivity in Gas-Liquid Reactors: Theoretical Modelling, 215
Original "Profiled" Analytical Solution and Confrontation with
Experiments on Chlorination of Paracresol in Bubble Column
T. Dardé (Koninklijke Shell, Netherlands) N. Midoux and J.C. Charpentier (CNRS-ENSIC, France)
- 4.9 Two Bubble Class Model for Mass Transfer in a Bubble Column with 223
Internals
S. Joseph, Y.T. Shah (University of Pittsburgh, USA) and N.L. Carr, (Gulf Research & Development Co., USA)
- 4.10 High Intensity Gas/Liquid Mass Transfer in the Bubbly Flow Region 231
During Co-Current Upflow through Static Mixers
A.W.M. Roes, A.J. Zeeman, and F.J.H. Bukkems (Shell, The Netherlands)

Session 5: NOVEL PROCESSES & TECHNIQUES

- 5.1 Computations of Flow Fields and Complex Reaction Yield in 239
Turbulent Reactors and Comparison with Experimental Data
J.C. Middleton, F. Pierce, and P.M. Lynch (ICI, UK)

5.2	Thermal Images of Catalyst Surfaces During Reaction <i>G.A. D'Netto, J.R. Brown, and R.A. Schmitz (University of Notre Dame, USA)</i>	247
5.3	Modelling of Reactors for Chemical Vapor Deposition of Microelectronic Materials <i>K.F. Jensen and K.F. Roegnigk (University of Minnesota, USA)</i>	255
5.4	The Application of Optical Measurements (CARS) to Chemical Reaction Engineering <i>W.A. England and D.A. Greenhalgh (AERE, UK)</i>	263
5.5	Chemical Reaction Engineering in Photovoltaic Cell Processing <i>T.W.F. Russell (University of Delaware, Newark, USA)</i>	271
5.6	The Refractory Tube Burner as an Ideal Stationary Chemical Reactor <i>S.W. Churchill (University of Pennsylvania, USA) and L.D. Pfefferle (Yale University, USA)</i>	279
5.7	The Design and Operation of a Laboratory Ketene Generator <i>P.H. Nielson and J. Villadsen (Danmarks Tekniske Højskole, Denmark)</i>	287

Session 6: INDUSTRIAL PROCESSES & SAFETY

6.1	Benzene Hydrogenation in the Annular Bed Reactor – Experimental Behavior and Simulation <i>M.E. Davis, N. Bungard, L.T. Watson (Virginia Poly. Inst., USA) M.D. Burnett, E. Hawkins (Hercules Inc., USA) and J. Yamanis (Corporate Technology Allied Corp., USA)</i>	295
6.2	The Three Phase Hydrodynamic Characteristics of the EDS Coal Liquefaction Reactors: their Development and use in Reactor Scale up <i>B.L. Turmy, M. Chang, C.A. Coulaloglou and P.R. Ponzi (Exxon Research & Engineering Co, USA)</i>	303
*6.3	Modelling of Methanol Synthesis in the Liquid Phase <i>D.M. Brown (Air Products Inc., USA)</i>	699
6.4	The Influence of Intraparticle Diffusional Limitations in Naphtha Hydrodesulfurization <i>I.A. van Parijs and G.F. Froment (Rijksuniversiteit Gent, Belgium)</i>	319
6.5	Production of Methane for Advanced Gas-Cooled Reactors by Reaction of Hydrogen and Carbon Dioxide over a Supported Ruthenium Catalyst <i>B.J. Gliddon, R.C. Hotchkiss and R.A. Roberts (CEGB, UK)</i>	329

6.6	The Scale-up of a Two-Phase Acid Catalyzed Transalkylation Reaction <i>S.H. Pan, C.B. Rosas, A. Epstein (Merck Sharp & Dohme, USA)</i> <i>H. Goldschmitz and J.C. Perlberger (Lonza, Switzerland)</i>	337
6.7	Prediction of Dynamic Change in CO₂ Gasification Rate of Coal Char with Increased Conversion <i>T. Adschiri, T. Kojima, T. Furusawa and D. Kunii (University of Tokyo, Japan)</i>	345
6.8	Selective Oxidation of Benzene to Maleic Anhydride at Commercially Relevant Conditions <i>R.K. Sharma (Rijksuniversiteit, Belgium) D.L. Cresswell (ICI, UK) and E.J. Newson (Swiss Aluminium, Switzerland)</i>	353
6.9	Design of an Emergency Venting System for a Batch Reaction Involving a Highly Reactive Chemical <i>R. Davies (Glaxochem Ltd, UK)</i>	361
6.10	Reactor Engineering for Inherent Safety <i>W. Regenass, U. Osterwalder and F. Brogli (Ciba-Geigy, Switzerland)</i>	369
 Session 7: FIXED BEDS		
7.1	An Irreducible Coupling: Heat and Mass Diffusion-Reaction in a Gas-Solid Reactor. An Experimental Approach <i>G. Crozat, N. Mazet, B. Spinner (Université de Perpignan) and G. Arnaud (Université de Poitiers, France)</i>	377
7.2	Interphase Heat Transfer and the Validity of Pseudo-Homogeneous Models of Packed Bed Reactors <i>J. Wei, R.R. Cwiklinski and J. Tomuro (MIT, USA)</i>	385
7.3	Optimal Operation of a Tube Cooled Ammonia Converter in the Face of Catalyst Bed Deactivation <i>D.R. Lewin and R. Lavie (Technion, Israel)</i>	393
7.4	Simulation of Non-Catalytic Reactors <i>M. Kawamura (National Chemical Lab. for Industry, Japan)</i> <i>G.S.G. Beveridge (University of Strathclyde, UK) and S. Toyama (Nagoya University, Japan)</i>	403
7.5	The Regeneration of Molybdenum Catalysts Kinetics and Fixed Bed Simulation <i>W.J. Hatcher and T.H. Burton (University of Alabama, USA)</i>	411
7.6	The Use of an Integral Reactor with Sidestream-Analysis for the Kinetic Investigation of Complex Reactions <i>H. Hofmann, G. Enig and W. Roder, (University of Erlangen-Nurnberg, West Germany)</i>	419

Session 8: POSTER SESSION

- *8.1 Kinetics of Anatase-Rutile Transformation and its Application to the computation of an Industrial TiO_2 Calciner 709
G. Marziano, G. Donati (Ist. Guido Donegani) and R. Pace (SIBIT/SpA, Italy)
- 8.2 Diffusion and Reaction of Chloride Ions in Porous Concrete 427
C.J. Pereira and L.L. Hegedus (W.R. Grace & Co., UK)
- 8.3 Residence Time Distributions in Laminar Flow through Reservoirs from Momentum and Mass Transport Equations 439
E. Brunier, G. Antonini, A. Zoulallan (University of Compiègne, France) and A. Rodrigues (University of Porto, Portugal)
- 8.4 The Effects of Optimal Temperature and Feed Addition Rate Profiles on Batch Reactions and Sequences of Batch Operations – The Development of a Catalogue of Attainable Regions 447
T. Hättopglu and D.W.T. Ripptn (ETH, Switzerland)
- 8.5 Diffusional Kinetics of Catalytic, Vapor-Phase Reversible Reactions with Decreasing Total Number of Moles 455
J.M. Berty, S. Lee, K. Sivagnanam (University of Akron, USA) and F. Szeferf (Veszprem College of Engineering, Hungary)
- 8.6 Reactor Design for Quench Catalytic Cracking of Crude Oil and Residua 463
J.R. Walls, J.K. Lee and A. Ovenston (Teesside Polytechnic, UK)
- 8.7 A Computer Model of a Atmospheric Fluidised Bed Combustor 471
M.J. Knight (BP International Ltd, UK)

Session 9: FLUIDISED BED REACTORS

- 9.1 How to Find the Suitable Kinetics for Modelling and Scale-up of Fluidised Bed Reactors in the Case of Complex Reaction Systems? 479
W. Bock, W. Sitzmann, G. Emig, and J. Werther (Technical University Hamburg, West Germany)
- 9.2 Catalytic Dehydration of Ethanol in a Fluidised Bed Reactor 487
P.L. Yue (University of Bath, UK) and R.H. Birk (The Dow Chemical Co., USA)
- 9.3 Solids Entrainment from Turbulent Fluidised Beds 495
H.J.A. Schuurmans (Shell Research, The Netherlands)
- 9.4 Sulfur Dioxide Removal in a Batch Fluidized Bed Reactor 509
M. Hartman, K. Svoboda and O. Trnka (Inst. Chemical Process Fundamentals, Czechoslovakia)
- 9.5 Scale-up of a Catalytic Fluid-Bed Reactor Involving Complex Kinetics 517
S. Dutta, S.C. Arnold, G.D. Suctu (C.E. Lummus, USA) and L. Verde, (Ahusuisse Italia, SpA, Milan, Italy)

Session 10: RESIDENCE TIME DISTRIBUTION

- 10.1 Comparison and Prediction of Reactor Performance for Packed Beds with Two Phase Flow: Downflow, Upflow and Countercurrent Flow
P.L. Mills (Monsanto Company, USA) E.G. Beaudry and M.P. Dudukovic, (Washington University, USA) 527
- 10.2 A Generalized Residence Time Distribution Model for a Chemical Reactor
D. Glasser (University of Witwatersrand, South Africa) and R. Jackson (Princeton University, USA) 535
- 10.3 Micromixing and Fast Reactions in a Centrifugal Pump
O. Bolzern and J.R. Bounre (ETH Zurich, Switzerland) 543
- 10.4 Comparisons of Partial Segregation Models for the Determination of Kinetic Constants in a High Pressure Polyethylene Reactor
J. Villiermaux (CNRS-ENSIC, France), M. Pons (CdF Chimie SA) and L. Blavier (Rhône-Poulenc Sante). 553
- 10.5 A Master Equation Formulation for Stochastic Modelling of Mixing and Chemical Reactions in Inter-Connected Continuous Stirred Tank Reactors
R.O. Fox and L.T. Fan (Kansas State University, USA) 561
- 10.6 New Results and Old Problems in Residence Time
E.B. Nauman (Rensselaer Polytechnic Inst., USA) 569
- 10.7 The Experimental Estimation of Axial Thermal Dispersion in Fixed Beds
D.J. Gunn (University College Swansea, UK) and D. Vortmeyer (Tech. Universitat, Munchen, West Germany) 583

Session 11: HYDROMETALLURGY

- 11.1 A Kinetic Study of the Oxidation of Complex Nickeliferous Sulfide Ore in a Aqueous Ferric Sulfate
C.Q. Zheng and R.G. Bautista (Iowa State University, USA) 593
- 11.2 Mathematical Modelling of Leaching of Vanadium from High Calcium Contents Steel Slag by Sodium Carbonate and Bicarbonate Solutions
Z. Chen, Z. Zhu, S. Yang and C. Chen (Inst. of Chemical Metallurgy, China) 603
- 11.3 Chemical Reactor Analysis of Hydrometallurgical Solvent Extraction: Fe(II)/Sulfate-Kelex 100/Xylene System
P.M. Bapat, C.A. Savastano, C.K. Lee and L.L. Tavlarides, (Syracuse University, USA) 611
- 11.4 Modelling of the Absorption of Gold on Activated Carbon in a Periodic Counter-Current Cascade of Continuous Stirred Tank Reactors
J.S.J. van Deventer (University of Stellenbosch, South Africa) 619
- 11.5 Hydrometallurgical Extraction of Zinc Using Sulphur Dioxide
P.B. Linkson and D.M. Larsen (University of Sydney, Australia) 627
- 11.6 Kinetics of Acid Leaching of Zinc Oxide
A.J. Monhemius and G. Katunga (Imperial College, UK) 635

Session 12: POLYMERIZATION AND BIOCHEMICAL ENGINEERING

- 12.1 Individual Rate Constants of the Polymerization of Ethylene Under High Pressures 643
P. Ch. Lim and G. Luft (Technische Hochschule, Darmstadt, West Germany)
- 12.2 Polymerization of Vinyl Monomers in Tubular Reactors 651
J.W. Hamer and W.H. Ray (University of Wisconsin, USA)
- 12.3 Polymerization in Bubble Columns, Problems of Mass and Heat Transfer at High Solid Contents 659
K.H. Reichert and R. Michael (Technische Universität, Berlin, West Germany)
- 12.4 Electroenzyme Reactors: Some General Concepts and Their Application to Analysis, High Grade Chemical Preparation and Cofactor Regeneration 667
M. Comtat, A. Bergel and J. Mahenc (Université de Paul Sabatier, France)
- 12.5 Microprocessor Based Systems for Fermentation Study and Control 675
M.N. Pons, J. Brdet and J.M. Engasser (CNRS-ENSIC, France)
- * Late papers, marked by an asterisk, are out of page sequence.

PLENARY LECTURES

- P.1 Gas-Liquid-Solid Reaction Engineering 717
Y.T. Shah (University of Pittsburg) and D. Smith (Pittsburg Energy Technology Center, USA).
- P.2 Computers and Modern Analysis on Reactor Design 733
F.J. Krambeck (Mobil Research & Development Corporation, USA).
- P.3 Selective Removal of Gases by Chemical Solvents 755
G. Astarita (University of Naples, Italy) and Wei-Chung Yu (Cabot Corporation, Boyertown, USA)
- P.4 Crystallization as Chemical Reaction Engineering 767
J. Garside and N.S. Tavare (UMIST, Manchester UK).
- P.5 Chemical Reaction Engineering of Polymer Processing: Reaction Injection Moulding. 783
M.F. Edwards (University of Bradford, UK).
- P.6 Micromixing Revisited 797
J.R. Bourne (ETH Zurich, Switzerland)

RECOMMENDED NOMENCLATURE AND SYMBOLS

815

THE PROBLEM OF DIFFUSIONAL TRANSPORT IN THE PERFORMANCE OF SUPPORTED LIQUID PHASE CATALYSTS

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In SLP catalysts the liquid loading q of the porous carrier material occupies part of the pore space and thereby diminishes the permeability of the pore system. A study of the diffusion as a function of gas pressure yields detailed information on the distribution of the liquid within the porous framework. This is demonstrated by means of two types of support, with mono- and bi-disperse pore structures. The blocking effect can be described by a simple model equation that yields the effectiveness factor of the catalyst solution and explains the maximum of the reaction rate usually observed at $q \approx 0.5$.

INTRODUCTION

Two methods are currently being studied for the heterogenization of homogeneously catalyzed reactions: "supported solid phase catalysts", SSPC, or "supported liquid phase catalysts", SLPC. In SSP catalysts the catalytically active transition metal complex is chemically bound by reactive groups to the internal surface of an inert porous support, whereas SLP catalysts are prepared by impregnating a porous support with the catalyst solution using a solvent with low vapor pressure. In these SLP catalysts blocking of pore space by the catalyst solution deserves special attention [1]. This effect lengthens the transport ways of pore diffusion, and diminishes the exchange area between the open pore space and the catalyst solution. The yield in such catalyst systems is determined by two opposing effects: with ascending grade q of filling up the pore system with catalyst solution the amount of catalyst in the support increases; simultaneously, however, this causes a decrease of gas-liquid exchange area. Thus a maximum should be observed in the course of reaction rate with the loading q of the support. Indeed this has been found by earlier workers in the field [2-4]. Fig. 1 presents an example obtained by L. Heinrich [5] in our group.

For understanding the blocking effect in detail it is necessary to determine not only the pore diffusion resistance but also the mean value of the pore radii open for gas diffusion, and their change with increasing loading of the support framework. In order to get these informations the pressure dependence of the gas diffusion resistance has to be measured down to about 10^{-2} bar. Most suitable for such investigations is the method of counter-current

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diffusion in a diffusion-reaction-cell [6] where use is made of the o-H₂/p-H₂ conversion. Measurements with this method are presented that have been made on two model pore systems impregnated with squalan [7]. The data obtained from an investigation like this on the blocking of the pore system can then be used to predict the optimal value of the support loading q of a given SLP catalyst.

PRESSURE DEPENDENCE OF GAS DIFFUSION THROUGH
IMPREGNATED POR SYSTEMS

The ortho-para hydrogen method, principle and evaluation

The porous sample with the shape of a flat disk of thickness d and cross sectional area A separates in the measuring cell (DRC in Fig. 2) the reaction chamber R from the mixing chamber M. The reaction chamber contains a highly active platinum catalyst that establishes the equilibrium ratio o-H₂/p-H₂ = 3/1 very quickly at room temperature. A constant flow Q of hydrogen, with about equal amounts of the two species is fed into the mixing chamber by means of a piston device AC. Part of the p-H₂ that enters the mixing chamber with the molar fraction x_E (see Fig. 2) diffuses through the porous wall (molar flux j_D) and is transformed in the reaction chamber to o-H₂ down to the equilibrium mole fraction x_{eq}. The rest of the p-H₂ leaves the mixing chamber with the exhaust (molar fraction x_A). Under steady state conditions the following p-H₂ balance for the mixing chamber holds:

$$Q \cdot c(x_E - x_A) = A \cdot j_D \quad (1)$$

where c is the overall molar gas concentration. With

$$j_D = D_{\text{eff}} \cdot c \cdot \frac{x_A - x_{\text{eq}}}{d} \quad (2)$$

it follows from equation (1) that

$$D_{\text{eff}} = \frac{d \cdot Q}{A} \cdot \frac{x_E - x_A}{x_A - x_{\text{eq}}} \quad (3)$$

This equation yields the coefficient D_{eff} of the countercurrent o-H₂/p-H₂ diffusion through the porous sample from the geometrical data of the sample, the flow velocity, and the molar fractions of the p-H₂. These were determined by means of a thermal conductivity cell (TCC in Fig. 2) at the temperature of liquid nitrogen. A series of measurements at normal temperature and different total pressures p yields the wanted function D_{eff} = D_{eff}(p). For a successful application of the method it is necessary that in the pressure range of the measurements the diffusion resistance is determined by gas-gas as well as by gas-wall collisions. With pore radii of the order 1 to 10 μm this happens with pressures in the range 10⁻² ≤ p ≤ 1 bar, as they were applied here. In this so-called transition range the overall diffusion resistance is to be taken as the sum of the resistances of normal gas diffusion and of Knudsen flow (Bosanquet-formula, see for instance [8]):

$$1/D_{\text{eff}} = 1/D_{\text{eff}}^G + 1/D_{\text{eff}}^K \quad (4)$$

The resistance of normal gas diffusion can be expressed by: