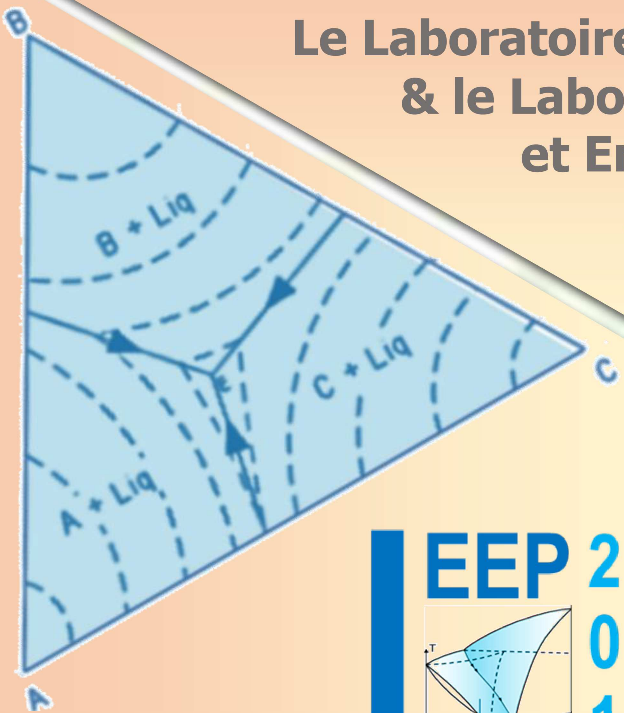
Université Ibn Zohr

Faculté des Sciences Agadir

Le Laboratoire Génie des Procédés (LGP)
& le Laboratoire Thermodynamique
et Energétique (LTE)

Organisent



JEEP 2019
AGADIR

La 44^{e} édition du Congrès International Journées d'Étude des Équilibres entre Phases

20 – 22 mars 2019
à la Faculté de Médecine
et de Pharmacie d'Agadir

Site : jeep2019.sciencesconf.org

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44th Conference on Phase Equilibria
44es Journées d’Étude des Équilibres entre Phases

JEEP 2019 AGADIR

Agadir 20-22 Mars 2019

*L’**U**niversité **I**bn **Z**ohr*
*La **F**aculté des **S**ciences d’**A**gadir*
*Le **L**aboratoire **G**énie des **P**rocédés*
*Le **L**aboratoire Thermodynamique et **E**nergétique*

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La 44ème édition du congrès international

Journées d’**E**tude des **E**quilibres entre **P**hases (JEEP)

« Les équilibres entre phases au service du développement industriel »

The 44th Conference on Phase Equilibria

Sientific Program

and

Book of Abstracts

XLIV JEEP

Conference on Phase Equilibria

20-22 March 2019

Agadir

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Preface

Je remercie infiniment le professeur Bellajrou de l'honneur qu'il me fait en me demandant d'écrire cette préface et parce que j'ai vécu l'origine des JEEP, Je me permettrai de rappeler dans quelles conditions a été créé ce rendez-vous des scientifiques travaillant sur les diagrammes de phases.

- A l'extrême origine est un laboratoire de la Faculté des sciences à Alger où, nous dirions maintenant, trois maîtres assistants, Mme Carbonel, M. Cohen-Adad et M. Potier, travaillaient sous la direction d'un professeur, M. Rollet. La spécialité de ce laboratoire était l'étude des diagrammes de phases.

- Entre temps, ces 3 maitres-assistants deviendront professeurs et chacun à la tête d'une équipe développera le domaine des diagrammes de phase.

- 1962, l'Algérie devient indépendante, M. Rollet et ses équipes rentrent en France mais sont dispersés entre Paris, Marseille, Montpellier et Lyon. Chacun a la chance de garder son équipe et en même temps de prendre de nouveaux élèves. Voulant rester en contact, chacun décide qu'il serait bon de créer un bloc et de se retrouver tous les deux ans pour discuter de l'évolution de leurs travaux : les JEEP étaient créées.

- Très vite des laboratoires français et étrangers intéressés par le thème se sont associés et les réunions se sont tenues non seulement en France, mais en Allemagne, en Espagne, en Hongrie etc.. : les JEEP étaient devenues internationales au point qu'un organisme international, l'IUPAC (International Union of Pure and Applied Chemistry) créa un groupe chargé de recenser les diagrammes de phase connus et de les éditer par famille.

Quel est l'intérêt de l'étude des diagrammes d'équilibre entre phases ? Là je me permettrai de reprendre ce que disait le Professeur Roger Cohen-Adad à ses élèves et Miloud El Hadek et Raddoine Bellajrou doivent s'en souvenir :

« Le diagramme d'équilibre entre phases exprime de façon concrète, en fonction des variables pression, température et composition, le nombre et la nature des phases qui peuvent être observées. Il renseigne sur leur stœchiométrie et précise leur domaine d'existence à l'état stable et instable.

Etablir ou étudier un diagramme de phase est donc d'un intérêt primordial dans de nombreux domaines de la chimie, de la physique, de la géologie, de la métallurgie ou de la science des matériaux

Cette étude n'est que très rarement une fin en soi parce que c'est un préalable indispensable à d'autres études qui dans ces conditions pourront être abordées de façon rationnelle.

C'est ainsi que, dans l'industrie chimique, les problèmes de synthèse, de séparation, d'extraction ou de distillation peuvent être optimisés par des études de cheminement dans les diagrammes.

Les diagrammes de phases permettent de simuler un procédé industriel, de définir des bilans matières et énergie reposant sur des données expérimentales sures, de définir les températures et compositions correspondant au rendement maximal, de définir les temps de séjour dans les différents réacteurs et les débits…

Dans la pratique où l'état d'équilibre est rarement observé, le diagramme d'équilibre est la référence indispensable si l'on veut comprendre et interpréter les phénomènes observés : une cinétique réactionnelle lente, des phénomènes de diffusion pourront être étudiés, le diagramme d'équilibre servant de système de référence. »

Dans les études académiques, il est indispensable de donner, aux diagrammes d'équilibre entre phases, leur place car les exemples d'application ne manquent pas :

- la récupération de Na_2SO_4 et de K_2SO_4 à partir de saumures des chotts et sebkhats du Sud Tunisien - Thèse de Lotfi Zayani ;

- Contribution à l'étude et à la modélisation des systèmes salins, application aux polyphosphates de métaux alcalins et de lanthanides et aux saumures – Thèse de Dalila ben Hassen-Chehimie ;

- Matériaux supraconducteurs à température critique élevée

  $Tl_{1-x}(Pb/Bi)_x(Sr_{1-y}Ba_y)_2Ca_2cu_3O_z$ et $Tl_{1-x}Pb_x(Sr_{1-y}Ba_y)_2Ca_2cu_3O_z$

Elaboration et caractérisation de phases de pureté contrôlée – Thèse de Kheirreddine Lebbou

- Lors de la préparation des carburants Ariane IV, les réactions conduisaient à une solution à 2% de 1,1,dimethylhydrazine et le diagramme d'équilibre diméthylhydrazine-H_20 montrait que par distillation, il était impossible d'aboutir à une solution à 99%, taux demandé par les industriels. L'addition d'un 3ème élément (NaOH) et l'étude du diagramme diméthylhydrazine-NaOH-H2O à permis d'augmenter la concentration en 1,1,diméthylhydrazine jusqu'à 99,3%.

- Représentation du système quinaire Sm-Co-Z-Cu-Fe dans le cadre d'une optimisation des aimants permanents 2/17 utilisés dans les sous-marins – Thèse de A. Lefèvre. Il suffira alors d'associer représentation du système/mesures magnétiques en fonction de la concentration pour définir la composition optimale.

- Mise au point d'une méthode conductimétrique pour établir le diagramme d'équilibre liquide-solide K^+,Na^+,$Fe^{3+/}Cl^-$ - H_2O entre 15 et 30°C - A. Atbir, M. El Hadek

Marie Thérèse Cohen-Adad

JEEP history

Edition	Année	Ville	Noms des organisateurs
1st	**1975**	**Marseille**	**L. CARBONNEL**
2nd	1976	Lyon	R. COHEN-ADAD
3rd	1977	Montpellier	A. POTIER
4th	1978	Grenoble	I. ANSARA
5th	1979	Chatenay-Malabry	B. LEGENDRE
6th	1980	Nancy	J. HERTZ
7th	1981	Genève	J.L. JORDA
8th	1982	Orsay	M. GHELFENSTEIN
9 th	1983	Barcelona	M.T. CLAVAGUERA-MORA
10 th	**1984**	**Tours**	**R. CEOLIN**
11 th	1985	Marseille	M. GAMBINO, G. HATEM
12 th	1986	Bordeaux	Y. HAGET
13 th	1987	Lyon	J.J. COUNIOUX, M.T. COHEN-ADAD
14 th	1988	Montpellier	G. MASHERPA, J.C. TEDENAC
15 th	1989	Grenoble	I. ANSARA, C. COLINET
16 th	1990	Marseille	J. PASTOR, J. KALOUSTIAN
17 th	1991	Utrecht	H. OONK
18 th	1992	Chatenay-Malabry	B. LEGENDRE
19 th	1993	Barcelona	M.A. CUEVAS-DIARTE, J.L. TAMARIT, E. ESTOP
20 th	**1994**	**Bordeaux**	**Y. HAGET, A. MARBOEUF**
21 th	1995	Rouen	R. BOUAZIZ, G. COQUEREL, M.N. PETIT
22 th	1996	Toulon	J. MUSSO, P. SATRE, A. SEBAOUN
23 th	1997	Hammamet	M.M. ABDELKAFI, N. ARIGUIB, N. GUERFEL
24 th	1998	Nancy	J.C. GACHON ET AL.
25 th	1999	Annecy	J.L. JORDA ET AL.
26 th	2000	Marseille	C. BERGMAN, G. HATEM
27 th	2001	Montpellier	J.C. TEDENAC ET AL.
28 th	2002	Agadir	M. EL HADEK ET AL.
29 th	2003	Lyon	J.C. VIALA ET AL.
30 th	**2004**	**St Avold**	**M. COCHEZ, M. FERRIOL**
31 th	2005	Barcelona	T. CALVET, JL. TAMARIT
32 th	2006	Rouen	G. COQUEREL, M.N. PETIT, Y. CARTIGNY
33 th	2007	Villeurbanne	M. PERONNET, C. GOUTAUDIER
34 th	2008	Marrakech	M. NADIFIYINE, M. BENCHANAA
35 th	2009	Annecy	M. LOMELLO
36 th	2010	Montpellier	R.M. AYRAL, F. ROUESSAC, J.C. TEDENAC
37 th	2011	St Avold	M. AILLERIE, M. COCHEZ, M. FERRIOL
38 th	2012	Rouen	G. COQUEREL, Y. CARTIGNY, M. PETIT, N. COUVRAT
39 th	2013	Nancy	N. DAVID, J.N. JAUBERT, R. PRIVAT
40 th	**2014**	**Lyon**	**C. GOUTAUDIER ET AL.**
41 th	2015	Coimba	M.ERMILINDA, SEUSEBIO, J.CANOTILHO
42 th	2016	Paris	I.B. RIETVELD, B.NICOLAI, N. MATHE, B. DO
43 th	2017	Barcelona	J.LI TAMARIT
44 th	2019	Agadir	M. EL HADEK, R. BELLAJROU, F. CHIBANE

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F. CHIBANE
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S. MANÇOUR-BILLAH	Laboratoire de Génie des Procédés, Université Ibn Zohr
A. MARROUCHE	Lab. de Génie des Procédés, Université Ibn Zohr

Mardi 19 mars 2019 à 10h00
Ecole Nationale des Sciences Appliquées (ENSA)

Le second principe de la thermodynamique enfin démystifié

Jean-Noël JAUBERT
Professeur des universités
Resp.équipe "Thermodynamique et Énergie"
École Nationale Supérieure des Industries Chimiques
Laboratoire Réactions et Génie des Procédés
54001 Nancy Cedex 9 – France

Mardi 19 mars 2019 à 16h00
Faculté des Sciences d'Agadir

Relationship of Thermodynamic Data with Periodic Law

Pr. V. Vassielev
Lomonosov Moscow State University, Chemistry Department, 119991 Moscow, Russia

Mercredi 20 mars 2019 à 10h00
Complexe Universitaire d'Ait Melloul

Combustion of green energetic materials applied for space propulsion

Pr. Keiichi Hori

Institute of Space and Astronautical Science (ISAS),
Japan Aerospace Exploration Agency, *Chōfu, Tokyo, Japan*
University of Tokyo

Mercredi 20 mars 2019 à 16h00
Faculté de Médecine et de Pharmacie

Synthetic methods for studying crystallization phenomena in high order systems

Pr. Christelle GOUTAUDIER
Université Claude Bernard Lyon 1
Laboratoire des Multimatériaux et Interfaces,
UMR CNRS 5615 Villeurbanne, France

Case Study of Phase Diagrams in Materials Science

Dr Professor Brahim ELOUADI
Laboratoire des Sciences de l'Ingénieur pour
l'Environnement. La Rochelle Cédex 01, France

Jeudi 21 mars 2019 à 10h00
Faculté de Médecine et de Pharmacie

Pharmaceutical Phase Equilibria A sword of Damocles or a tool prone to misunderstanding

Pr. Ivo B. RIETVELD
Laboratoire Sciences et Méthodes Séparatives, University of Rouen
Faculty of Pharmaceutical and Biological Sciences University Paris

Jeudi 21 mars 2019 à 14h30
Faculté de Médecine et de Pharmacie

Sol - Gel Smart Materials: Characterization and Application

Inas Kamal Battisha
Solid State Physics department
National Research Centre (NRC)
33 El Behooth St., Dokki, Giza, Egypt,

Scientific program

Wednesday / Mercredi 20/03/2019

14h00 - 15h00 **Reception and registration of participants**

15h00 – 18h00 **Course for master's students and PhD students**

- **Synthetic methods for studying crystallization phenomena in high order systems**
  Pr. Christelle GOUTAUDIER
  Laboratoire des Multimatériaux et Interfaces, Université de Lyon, France.
- **Case Study of Phase Diagrams in Materials Science**
  Pr. Brahim ELOUADI
  Laboratoire des Sciences de l'Ingénieur pour l'Environnement La Rochelle Cédex 01, France

Thursday / Jeudi 21/03/2019

08h00 - 09h30 **Reception and registration of participants**

09h30 - 10h00 **Official Opening Ceremony**

10h00 - 11h00 **Inaugural conference**

Pharmaceutical Phase Equilibria A sword of Damocles or a tool prone to misunderstanding

Pr. Ivo B. RIETVELD

Laboratoire Sciences et Méthodes Séparatives, University of Rouen
Faculty of Pharmaceutical and Biological Sciences University Paris Descartes

11h00 - 11h30 **Welcome coffee break**

11h30 – 12h45 **Oral communications : Session 1**

OC-01 **Preparation of ultrapure Phenanthrene by crystallization: use of phase diagrams and molecular structures to reinforce discrimination in the solid state**

Yohann CARTIGNY

Laboratoire de Sciences et Méthodes Séparatives, Université de Rouen Normandie, France

OC-03 **The phase behavior of pyrazinamide**

Kangli Li

Laboratoire de Sciences et Méthodes Séparatives, Université de Rouen Normandie, France

OC-05 **The surprising case of spironolactone polymorphism: enantiotropy in a system with a large difference in melting points**

Ivo B. RIETVELD

Laboratoire *Sciences* et Méthodes Séparatives, University of Rouen

Faculty of Pharmaceutical and Biological Sciences University Paris Descartes

13h00 – 14h30 **Lunch**

14h30 – 15h00 **Conference**

Pr. Inas Kamal BATTISHA

Solid State Physics department, Physics Research Division, National Research Centre (NRC), 33 El Behooth St., Dokki, Giza, Egypt

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15h00– 16h30 **Oral communications : Session 2**

OC-06 **Distribution of Co^{2+} and Ni^{2+} cations between the aqueous phase mono- and triclinic solid solutions of their hexahydrated nitrates within the range 258.15 - 313.15K**

Christelle GOUTAUDIER.

Université de Lyon, Laboratoire des Multimatériaux et Interfaces, 69622Villeurbanne, France.

OC-07 **Cryoscopic studies of aqueous solutions of phosphoric acid, sulphuric acid and nitric acid: Thermodynamic study of the equilibrium between liquid/solid phases**

Mouna GUESSOUS

LEE, Thermodynamics Surface and Catalysis Team, Faculty of Sciences, El Jadida Morocco

OC-08 **Thermodynamic study of phosphorus pentoxide-water binary system : The stability and solubility of phosphoric acid hydrates**

Z. BAKHER

Laboratoire de Physico-chimie des Procédés et des Matériaux, FST Settat, Maroc

OC-09 **Excess thermodynamic properties of the binary mixtures MethylCarbitol + 1-Hexene, Methylcyclohexane and Cyclohexane as fuel representative**

Mohamed LIFI

Science Engineer Laboratory for Energy, Chouaïb Doukkali University, El Jadida, Morocco

Department of Electromechanical Engineering, Universidad de Burgos, Spain

OC-10 **Thermodynamic behaviour of some 3d, 4d and 5d aluminides: The case of Al-V, Al-Ru and Al-Re systems**

Rkia TAMIM

Laboratoire de Thermodynamiques et énergétique, FSA, Université Ibn Zohr, Agadir

OC-11 **Liquid extraction of toluene from heptane using mixed solvents containing dimethyl sulfoxide and methanol at 298.15K: Experiments and modeling**

Fadoua FARGHI

Laboratoire de Physico-chimie des Procédés et des Matériaux, FST Settat, Maroc

16h30 – 17h00 **Coffee break, Stands, Poster session 1**

17h00 – 18h30 **Oral communications : Session 3**

OC-12 **Thermodynamic evaluation of Germanium-Lutetium binary system**

Khadija ACHGAR

Laboratory of Thermodynamics and Energy, Faculty of Sciences, University Ibn Zohr, Agadir

OC-13 **New mathematical expressions for the generalized Soave α-functions classically used in the Redlich-Kwong and Peng-Robinson equations of state.**

Jean-Noël JAUBERT

Université de Lorraine, ENSIC, Laboratoire Réactions et Génie des Procédés, Nancy, France

OC-14 **How the parameterization of equations of state influence their How the parameterization of equations of state influence their performances?**

Jean-Noël JAUBERT

Université de Lorraine, ENSIC, Laboratoire Réactions et Génie des Procédés, Nancy, France

OC-15 **Modeling of the ternary system $NaCl$-Na_2SO_4-H_2O**

Said MANÇOUR-BILLAH

LGP Laboratory, Faculty of Sciences, Ibn Zohr University, Agadir Morocco

OC-16 **Modelling the thermodynamics of fluids with Peng–Robinson + residual Helmholtz energy-based mixing rules**

Silvia LASALA

Université de Lorraine, ENSIC, Laboratoire Réactions et Génie des Procédés, Nancy, France

OC-17 **Discussion on the optimum form of the attractive term of translated cubic equations of state**

Andrés PINA-MARTINEZ

Université de Lorraine, ENSIC, Laboratoire Réactions et Génie des Procédés, Nancy, France

OC-18 **Sol - Gel Smart Materials: Characterization and Application**

Pr. Inas Kamal BATTISHA

Solid State *Physics department, Physics Research, El Behooth St., Dokki, Giza, Egypt*

Friday / Vendredi 22/03/2019

8h30 – 10h30 **Oral communications : Session 4**

OC-20 **Consequences of the Ni-enrichment in Co-based alloys designed to be TiC- or TaC-reinforced on their H.T. microstructures**

Patrice BERTHOLD

Institut Jean Lamour (UMR CNRS 7198), Campus ARTEM, 54011 NANCY Cedex, France

OC-21 **Pinning mechanism and Pinning Force variation in $YBa_2Cu_3O_7$-d**

Brahim LMOUDEN

Laboratory of Superconductors Materials at High Critical Temperature, Ibn Zohr University

OC-22 **Carachterization and identification of the products formed from Moroccan phosphogypsum**

B. BOUARGANE

LGP, Chemical Department, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco

OC-23 **Co-precipitation synthesis of $CePO_4$ nanostructures: Correlation between the calcination temperature and structural properties**

Abdessalam BOUDOUCH

LME, Université Ibn Zohr, faculté des sciences, Agadir, Maroc

OC-24 **Experimental study of CO_2 solubility on NaCl and $CaCl_2$ solutions from 333.15 K to 453.15 K and pressures up to 400 bar**

Lara Cruz José Luiz

Laboratoire de Thermique, Energetique et Procédés Univ Pau & Pays Adour, France

10h00-10h30 **Coffee break, Stands, Poster session 2**

10h30– 12h30 **Oral communications : Session 5**

OC-25 **Sea water desalination and remineralization steps in the south of Morocco**

Mohamed Gali BIYOUNE

LGP, Chemical Department, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco

OC-26 **Experimental and predictive study of the effect of seawater composition on liquid-solid equilibrium: Application of cryoscopy on marine water in El Jadida Bay: Atlantic Ocean, Morocco**

Fatima Zahra KARMIL

Water and Environment Laboratory. Chouaib Doukkali University El Jadida.

OC-27 **The inhibitory effect of a phosphate product on the sanitary waters of the tourist area of Agadir**

Abdallah HADFI

LGP, Chemical Department, Faculty of Sciences, Ibn Zohr University, Agadir, Morocco

OC-28 **Optimization and modeling of degradation of orang G by sulfate radicals using a response surface methodology (RSM) based on the central composite design**

Abdellah AIT EL FAKIR

Materials and Environment Laboratory, Ibn Zohr University, Agadir, Morocco

OC-29 **Study of the interaction between water and the red stigmas of saffron Crocuse Sativus L., : Kinetic of the Drying Process by traditional method**

Abderrahman. AAJMI

Laboratory of process engineering Faculty of Science university ibn zohr Agadir, Morocco

OC-31 **Thermal and structural analysis of cellulose phase from Moroccan cactus cladodes and its applications as reinforcing agent in PET composites**

Anass AIT BENHAMOU

Laboratoire REMATOP, FSS, Université CADI AYYAD Marrakech, Maroc.

OC-32 **Modelling and optimization of ultrasound-assisted competitive and simultaneous adsorption of toxic dyes onto activated carbonaceous anaerobically digested**

Zakaria ANFAR

Materials and Environment Laboratory, Ibn Zohr University, Agadir, Morocco

12h30 – 13h **Closing session and next JEEP**

Poster list

POSTER	TITE	AUTHOR
P 03	Measured densities and derived thermodynamic properties of waste cooking oil biodiesel from 298.15 K to 393.15 K and pressures up to 140MPa	AIT BELALE RACHID
P 05	Determination of the limits of ternary phases based on the compounds of the binary system Ni-Ti at high temperature	CHRIFI ALAOUI FATIMA ZAHRA
P 06	Numerical study of the evaporation of a thin film dripping along the active walls of a vertical channel	EL BAAMRANI HAYAT
P 08	New thermodynamic assessment of the Gallium - Aluminum binary system	KARDELLASS SAID
P 10	CALPHAD Description of The Manganese-Antimony Binary System	IDDAOUDI ABDELLAH
P 12	Thermodynamic evaluation of the Gallium - Lutetium binary system	AIT BOUKIDEUR MUSTAPHA
P 13	Disquac prediction of solid-liquid phase equilibria diagrams for systems PHA with octacosane.	DJELLOULI FAYROUZ
P 14	Thermodynamic assessment of The Ytterbium-Gold with the Kaptay equation for the excess Gibbs energy of the liquid phase	OTMANI SAMIRA
P 16	Calphad-Type Assessment of the Al-Ti-Au Ternary System	IDBENALI MOHAMED
P 17	Study of the interaction between water and the red stigmas of saffron Crocuse Sativus L., : kinetics of process of drying under microwave irradiation	AAJMI ABDERRAHMAN
P 18	Biodiesel density: experimental measurements of ternary blends of ether, alcohol and hydrocarbon	ABALA ILHAM
P 19	Study of clogging of the transport pipes of treated wastewater and sprinklers of Agadir Golf Ocean	MOHAREB S.
P 20	the interest of the phase diagrams in the Study of Structural hardening mechanisms of alloys Pb-Te , Pb-Te-Sn , Pb -Te -Ag For battery grids	AGUIZIR ABDELLAH
P 21	Thermodynamic assessment of the Scandium-Gold binary system	MOUSTAINE DRIS
P 22	Development and validation of a method for determination of antibiotic metronidazole using modified carbon past electrod by silver	ZOUBIR JALLAL

P 23	Survey of thermal performances of a solar system used for the heating of agricultural greenhouse and the improvement of tomato production in Morocco	BAZGAOU ABDERRAHIM
P 25	Transforming Moroccan phosphogypsum into potassium sulfate and precipitated calcium carbonate (PCC)	BOUARGANE BRAHIM
P 26	Hydro-chemical characterization with a statistical approach of groundwater quality in EL MERK region, south-eastern Algeria	KOUADRI SABER
P 27	Concentration and distribution of fluoride in Touggourt region (Algeria)	KADRI ABDELAZIZ
P 28	Di-hydrofolate reductase inhibitors: can 2,4-diaminopyrimidine be a model for co-crystal screening	BAPTISTA JOÃO
P 29	Investigation on solid forms of iguratimod: co-crystals and polymorphs	CANOTILHO JOÃO
P 30	Integration of photovoltaic energy and food production systems for the Mediterranean countries	EZZAERI KABIRA
P 31	On the Dimorphism and the Pressure-Temperature State Diagram of Gestodene, a Steroidal Progestogen Contraceptive	RIETVELD IVO and ALLOUCHI HASSAN
P 32	Interactive software for modelling of binary or ternary salt - water phase diagrams	MANÇOURBILLAH SAID
P 33	The new description of the Bi-Cu-I ternary phase diagram	BAHARI ZAHRA
P 34	Compatibility study between acebutolol and excipients	BEN YAHIA ARIJ
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Oral Communications

OC1

Preparation of ultrapure Phenanthrene by crystallization: use of phase diagrams and molecular structures to reinforce discrimination in the solid state

Antoine BUREL, Nicolas COUVRAT, Yohann CARTIGNY, Séverine TISSE, Pascal CARDINAEL, Gérard COQUEREL

Ultrapure materials (*e. g.*, substances exhibiting molar purity values larger than 99.9%) are required for various applications or major importance: (i) the development of active pharmaceutical ingredients; (ii) the elaboration of certified reference materials; (iii) the production of solar- or electronic-grade substances for high technicality purposes; etc. However, technical difficulties may make reaching such purity complex, the most common purification methods exhibiting limited efficiency.

The present study focuses on Phenanthrene ($C_{14}H_{10}$) purification by crystallization using several methods: solvent-assisted recrystallization, co-crystallization and zone refining. On the one hand, separate application of these three methods did not permit to eliminate impurities from the target compound by one shot. On the other hand, they exhibited different – and complementary – purifying effects that paved the way to their combination in a rightly selected order. To provide data required for the optimization of these crystallization processes, phase diagrams between crystallized solid phases of Phenanthrene and impurities of the molecule were studied from calorimetric (DSC) and structural (XRPD) measurements.

Purity measurements by gas chromatography after application of these purification processes indicated that co-crystallization of Phenanthrene with 3,5-dinitrobenzoic acid was able at reducing below detection thresholds (ca. 0,0001 mole %) the contents of impurities exhibiting non-planar chemical structures, which was not permitted by the other crystallization methods. Nevertheless, no complete elimination of planar impurities could be achieved.

To bypass this limitation, an original procedure was developed: phenanthrene was treated using some selected chemicals to operate a selective chemical modification of planar impurities. Treated product was then purified by co-crystallization, thus eliminating the major part of modified impurities. Remaining traces were then removed by zone refining, which permitted to prepare a few grams of 99.999 mole % Phenanthrene starting from 98 % commercial product.

The aims of this presentation are: (i) to show that reaching ultrapurity is possible for organic species, (ii) to demonstrate the necessity of combining purification methods to reach challenging purity specifications, (iii) to show the relevance of phase diagrams to select and optimize crystallization methods, (iv) to discuss the role of crystal and molecular structures in terms of solid-state discrimination during crystallization.

OC3

The phase behavior of pyrazinamide

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Keywords: Pyrazinamide, pressure-temperature phase diagram, phase behavior, X-ray diffraction, calorimetry

Pyrazinamide is an active pharmaceutical ingredient used against the mycobacterium tuberculosis. At least four polymorphs (α, β, δ and γ) have been reported in the literature[1]. Many literature papers focus on polymorph control, polymorphic transitions and the relative stabilities of pyrazinamide polymorphs[1-4]. Nonetheless, uncertainty remains about most of the transition temperatures between the different polymorphs. In this paper, the phase behavior of pyrazinamide has been reinvestigated and a pressure-temperature (P-T) phase diagram has been constructed using experimental data and information obtained from the literature[3].The triple point temperature and melting enthalpy of polymorph γ have been obtained by differential scanning calorimetry (DSC). It will be shown that the melting enthalpy is affected by the sublimation of pyrazinamide. Single crystals of polymorphαhave been prepared and its melting point and enthalpy have been measured by DSC. The transition temperatures of α to γ and δ to γ have been investigated as a function of the heating rate. The transition temperature of α to γ has been found to be 20 ℃lower than the temperature reported in the literature. Transitions β to γ and β to δ have been investigated by DSC and X-ray diffraction (XRD). High-pressure differential thermal analysis (HP-DTA) was applied to measure several transition temperatures as a function of pressure. The specific volume of the four polymorphs as a function of temperature has been determined by XRD.

In the resulting pressure-temperature phase diagram, it can be seen that α form only possesses a stable domain around room temperature and at ambient pressure. Under pressure, either the δ form at low temperature or the γ form at high temperature is stable.

References

[1] R. A. E. Castro, T. M. R. Maria, A. O. L. Évora, J. C. Feiteira, M. R. Silva, A. M. Beja, J. Canotilho and M. E. S. Eusebio,Cryst. Growth Des. **10**, 274 (2010).
[2] M. W. Hermanto, A. Yeoh, B. Soh, P. S. Chow and R. B.Tan, Org. Process Res. Dev.**19**, 1987 (2015).
[3] S. Cherukuvada, R. Thakuria, A. Nangia, Cryst. Growth Des. **10**, 3931 (2010).
[4] M. M.Smets, G.Baaklini, A. Tijink, L.Sweers, C. H. Vossen, C. Brandel, H. Meekes, H. M. Cuppen, G.Coquerel, Cryst. Growth Des.**18**, 1109 (2018).

The surprising case of spironolactone polymorphism: enantiotropy in a system with a large difference in melting points

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In the case that crystalline polymorphs of active pharmaceutical ingredients have considerably different properties, the study of their stability ranking becomes important, because they risk being prone to changes in the formulation and bioavailability due to a sudden polymorph transformation. In the case of spironolactone, an aldosterone agonist used as a diuretic, the melting points of the two polymorphs are more than 70 degrees apart, which is very rare as can be seen in the graph representing a major part of molecular (pharmaceutical) polymorphs observed in the last 50 years.

Form I, which has a melting point of 408 K compared to the melting point of form II of 480 K, possesses the highest density, making it likely the more stable form under pressure. Although in most cases, form I has never been observed to transform into form II before melting, serendipitously, a sample was found that exhibited the solid-solid transition, which led to an experimental measure of the enthalpy difference between the two solid forms.

Using the topological approach and the available experimental data, it can be shown that form I possesses a stable domain under pressure not unlike the system of paracetamol. It is however unlikely that form I will ever appear spontaneously from a batch of form II due the necessary pressure of 760 MPa to reach the triple point I-II-L, where the stable domain of form I commences [1].

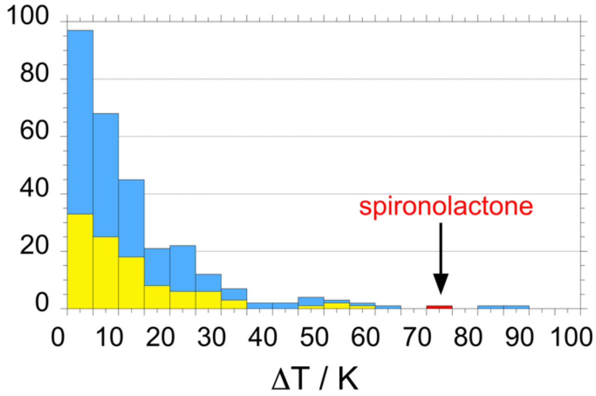

Figure 1. Differences in the melting points between the highest melting polymorph and other observed polymorphs for over 200 pairs

References
[1] I.B. Rietveld, M. Barrio, P. Lloveras, R. Céolin and J.-Ll. Tamarit, Int. J. Pharm. Sci. **552**, 193 (2018).

OC6

Distribution of Co^{2+} and Ni^{2+} cations between the aqueous phase and mono- and triclinic solid solutions of their hexahydrated nitrates within the range 258.15 – 313.15 K

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The isothermal studies of the H_2O-$Co(NO_3)_2$-$Ni(NO_3)_2$ ternary system [1-2] highlighted that hexahydrated nickel and cobalt nitrates form two widespread substitutional solid solutions, $Co_{(1-\sigma)}Ni_{\sigma}(NO_3)_2.6H_2O$ and $Ni_{(1-\omega)}Co_{\omega}(NO_3)_2.6H_2O$. Respectively they were formed by the substitution of Co^{2+} cations by Ni^{2+} cations in the monoclinic structure of the cobalt nitrate hexahydrate and the substitution of Ni^{2+} by Co^{2+} in the triclinic structure of the nickel nitrate hexahydrate. The analyses of the tie-lines enabled a thermodynamic modelling of the solid-liquid equilibria within a temperature range from 258.15 K to 313.15 K. The cationic partition curves between the liquid and the solid phases could be calculated and the results were compared to the experimental data as shown in figure below [3].

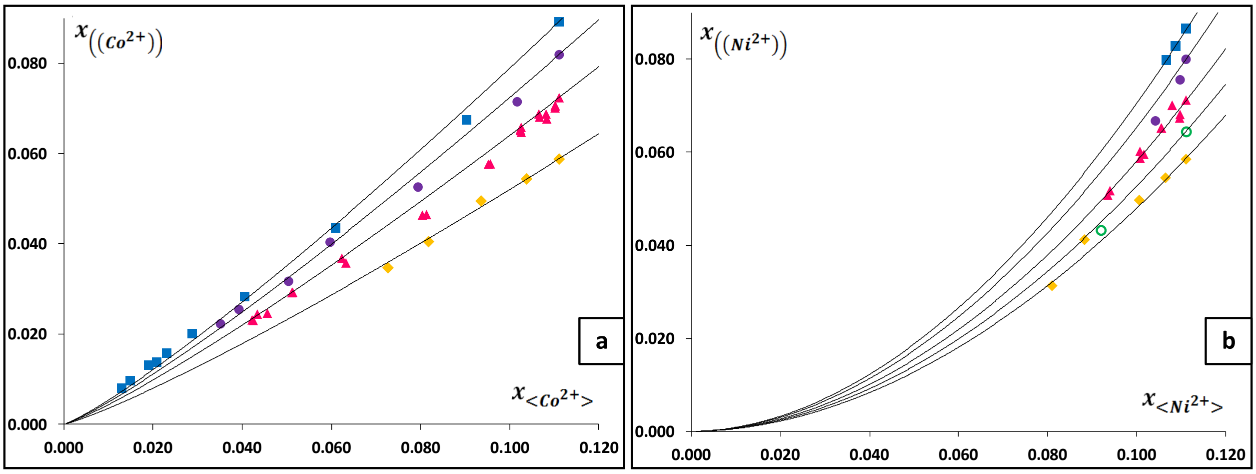

Figure 1: Distribution of cobalt ions of the monoclinic structure (a) or nickel ions of the triclinic structure (b) in the liquid and solid phases at several temperatures (♦: 258.15 K; ○: 273.15 K ; ▲: 287.15 K; ●: 303.15 K; ■: 313.15 K). $x_{<M^{2+}>}$ is the mole fraction of M^{2+} in the solid phase and $x_{((M^{2+}))}$ is the mole fraction of M^{2+} in the liquid phase.

References

[1] B. El Goundali, A. Teyssier, M. Kaddami, J.J. Counioux and C. Goutaudier, J. Chem. Thermodyn. **101**, 343-350 (2016).
[2] A. Teyssier, B. El Goundali, M. Kaddami, J.J. Counioux and C. Goutaudier, J. Chem. Eng. Data **62**, 1028-1035 (2017).
[3] A. Teyssier, J.J. Counioux, M. Kaddami and C. Goutaudier, J. Chem. Thermodyn. **118**, 274-282 (2018).

OC7

Cryoscopic studies of aqueous solutions of phosphoric acid, sulphuric acid and nitric acid: Thermodynamic study of the equilibrium between liquid/solid phases

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Abstarct

Wastewater generated by the mineral acid and fertilizer industry has a very low pH and contains high levels of nutrients such as phosphorus, sulfur and nitrate [1].The treatment of these industrial waters requires the determination of its physical and thermodynamic properties (the water activity coefficient, the osmotic coefficient, the boiling temperature, the melting temperature, the osmotic pressure...). The aim of this work is to study the physical and thermodynamic properties of the liquid-solid equilibrium of phosphoric acid, sulfuric acid and nitric acid solutions. Experimental determination of the freezing temperatures of aqueous solutions of three ionic synthetic binary solutions: H_2O/H_3PO_4, H_2O/H_2SO_4 and H_2O/HNO_3 was carried out in the concentration range from 0,15 to 4,76 mol·kg−1 by cryoscopy method. The obtained experimental values and those taken from the literature, were used to obtain the osmotic and activity coefficients in the studied system by the use of the numerical integration of the Gibbs-Duhem equation. The study was then extended to complex systems: $H_2O/H_3PO_4/H_2SO_4$ and $H_2O/H_3PO_4/HNO_3$.The performance of this technique has been validated for the phase diagram of the three binary system for the range of concentration studied. The obtained results could be more important for the study of desalination of wastewater by crystallization [2].

Keywords: Phosphoric acid; Sulfuric acid; Nitric acid; Solid-liquid equilibrium, Water activity; Osmotic coefficient.

References

[1] Chapter 20 Waste Water from the Inorganic Chemicals Industry. Studies in Environmental Science.V5, Pages 261-271, 1979.
[2] A. Rich, M.Siniti and al, 5, 45-52 (2015).

OC8

Thermodynamic study of phosphorus pentoxide-water binary system : The stability and solubility of phosphoric acid hydrates.

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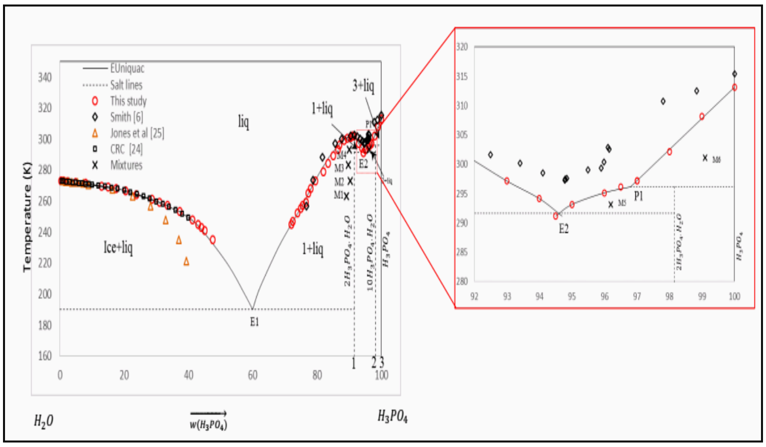
Abstract:

Phosphoric acid has a very important role in different industrial fields (fertilizers production for example) this is whythe purification of phosphoric acid has been the subject of several academic investigations. In this study, new experimental data for the binary system of H_2O–P_2O_5 are presented using the conductimetric method, this synthetic method was successfully and effectively used to define the branches of stable solubility of several complex systems.In this work, two hydrates $2H_3PO_4.H_2O$ (semi-hydrate) and $10H_3PO_4.H_2O$ (deci-hydrate) were identified and characterized by X ray diffraction and volumetric titration with discussion of their stability zone. Thermodynamic modeling of solid-liquid equilibrium in the binary system of P_2O_5–H_2O is also presented based on this experimental solubility data using a modified electrolytic Uniquac model (Extended Universal Quasichimical model).



Keywords: Deci-hydrate; Semi-hydrate; Phosphoric acid crystal; Conductimetric method; Extended Universal Quasichimical model.

OC9

Excess thermodynamic properties of the binary mixtures MethylCarbitol + 1-Hexene, Methylcyclohexane and Cyclohexane as fuel representative

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Abstract :

The need to reduce the environmental impact of fuel combustion has encouraged many studies to examine the effects on the addition of different oxygenates to fuel mixtures. The addition of oxygenated organic compounds (fuel reformulation) could help to improve engine combustion, leading also to a reduction in pollutant emissions (CO, NOx, unburned hydrocarbons…), and increasing its efficiency.

Diethylene Glycol Methyl Ether belongs to the family of glycol ethers. Commercially, it's known as MethylCarbitol. Some of their utilizations is as additives in jet fuels, diesel fuels, marine fuels and fuel oils for the antimicrobial control of fungi and bacteria present in hydrocarbon fuel systems. It's also used for anti-icing control, as brake fluid component and as solvent used in paints, printing inks, resins and waxes.

This work presents a study on excess enthalpies of mixtures MethylCarbitol + 1-Hexene, MethylCarbitol + Methylcyclohexane, and MethylCarbitol + Cyclohexane at 298.15 K and 313.15 K. Excess enthalpies have been measured with a quasi-isothermal flow calorimeter. The experimental data have been fitted using a Redlich-Kister equation and NRTL and UNIQUAC models. The values of the standard deviation indicate the agreement between the experimental results and these calculated from the equations.

OC10

Thermodynamic behavior of some 3d, 4d and 5d aluminides: The case of Al-V, Al-Ru and Al-Re systems

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Abstract

For high-temperature materials, as Ni-based and Fe-based super-alloys, intermetallic compounds containing aluminum and transition metals (Ni, Ti, Zr, Hf, V, Nb, Ta) have drawn a considerable attention as a candidate material qualified for high-temperature applications in aggressive environment. Because of its unusual high melting point, high strength, in addition to the oxidation and corrosion resistance properties and good thermodynamically stable [1, 2], Al-V, Al-Ru and Al-Re based compounds are promising high-temperature materials. Importantly, the high-temperature applications of these materials are also markedly influenced by the structural stability and thermodynamic properties. Therefore, phase equilibria and thermodynamic quantities must be obtained.

It should be noted that the Al-TM (TM=V, Ru and Re) phase diagram has not been fully characterized because of the experimental difficulties. The mean raison is the very large difference between the melting points of the starting elements: 660 °C for Al, and 3186 °C for Re. However, there is a lack of the systematical calculations of phase stability, elastic properties and electronic structure for these ten compounds.

The aim of this work is to compile all the available experimental information, to confirm their consistency and to create an optimized set of thermodynamic data by means of the CALPHAD (CALculation of PHAse Diagram) approach. In this context and based on the recent experimental information concerning the Al-rich part of the Al-Zr and Al-Re phase diagrams [5, 6], we have assessed the Al-Zr and the Al-Re systems through the CALPHAD technique. The Redlich–Kister polynomials as well as the exponential temperature dependence model of Kaptay were used to describe the excess Gibbs energy of all occurring phases.

In this work we presents a systematic study of the evolution of the thermodynamic properties of the 3d, 4d and 5d TM-aluminide intermetallics, depending on the location of the TM element in its relative series.

References

[1] Sauthoff G. Intermetallic compounds. In: Westbrook JH, Fleisher RL, editors. Wiley: New York, NY **1**, 991(1994).
[2] Cahn RW. Combining metals and sciences: ways of investigating intermetallics. Intermetallics **6**, 563–6 (1998).

OC11

Liquid extraction of toluene from heptane using mixed solvents containing dimethyl sulfoxide and methanol at 298.15K: Experiments and modeling

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Separation of aromatic hydrocarbons (benzene, toluene, xylene…) from naphtha streams using liquid-liquid extraction is one of the most challenging processes of chemical industries.These aromatics are separated and used in differentindustrial sectors (paints, textile, pharmaceutical ...).

Such extraction processis based essentiallyon the liquid-liquid equilibrium involved, given their very important role in the conception and optimization of industrial units.

The aim of the present work is to study the effect of adding different mass quantities of methanol to dimethyl sulfoxide, in order to extract toluene from heptane. Experimental liquid−liquid equilibrium data for four quaternary systems of heptane + toluene + dimethyl sulfoxide + 0.2-0.4-0.6 or 0.8 mass fractionof methanol were determined at T = 298.15 K under atmospheric pressure. The degree of reliability of the experimental LLE data was examined using Othmer-Tobias and Hand methods. Furthermore, selectivity and distribution coefficient were calculated to evaluate the efficacity of dimethyl sulfoxide + mass fraction of methanol as mixed solvent. NRTL (nonrandom Two-Liquid) activity coefficient model was used to correlate experimental results. Correlated results are in good agreement with experimental data.

OC12

Thermodynamic evaluation of Germanium-Lutetium binary system

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Rare Earth Elements (REEs) with germanium have been increasingly used in a wide range of advanced materials including permanent magnets, hydrogen storage materials, renewable energy technologies (i.e. wind turbines and small hydropower stations), and luminescent materials. To satisfy the ever-increasing demands of these materials, it is necessary to determine the phase diagram and thermodynamic properties of the chemical compounds and phases which are carriers of such properties.

In this sense the Ge-Lu binary system has been optimized by means of the CALPHAD approach [1] based on experiment information of phase equilibria [3] and thermodynamic proprieties from the published literature data [4]. The Ge-Lu system contains seven phases based on six intermetallic compounds: $Ge_{1.8}Lu$, Ge_3Lu_2, Ge_5Lu_4, $Ge_{10}Lu_{11}$, Ge_4Lu_5, and Ge_3Lu_5, which were all treated as stoichiometric compounds. The liquid phase was examined using two different descriptions: as substitutional solution phase, in which the excess term of the Gibbs energy was formulated with the linear temperature dependence of Redlich-Kister polynomial [5] and compared with the recent exponential temperature dependence of Kaptay model [6-8]. The process of modeling allows us to calculate the phase equilibria and thermodynamic properties of the liquid phase and intermetallic compounds for the first time. The results obtained are in good agreement with the phase diagram data and experimental thermodynamic values available in the literature.

References

[1] L. Kaufman, H. Bernstein, Computer Calculation of Phase Diagrams, (1970).
[2] B. Sundman, B. Jansson, J.O Andersson, CALPHAD, **9,** 153-190 (1985).
[3] Eremenko, V.N., Meleshevich, K.A., Buyanov, Yu.I., Petyukh, 76, (1987).
[4] S.V. Meschel, O.J. Kleppa, Journal of Alloys and Compounds 245 (1996).
[5] O. Redlich, A. Kister, Ind. Eng. Chem., 40 (1948).
[6] G. Kaptay, Calphad, **28–2,** 115–24, (2004).
[7] G. Kaptay, Calphad. **32–2,** 338–52 (2008).
[8] G. Kaptay. Mat SciEng A. **495**, 19–26, (2008).

OC13

New mathematical expressions for the generalized Soave α-functions classically used in the Redlich-Kwong and Peng-Robinson equations of state.

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All commercially available process simulation packages (ProSim, Pro/II, Aspen, UniSim …) include the Soave-Redlich-Kwong [1] and Peng-Robinson [2] equations of sate (EoS) among their thermodynamic models. Such EoS are usually used in their translated form [3-5] in order to improve their abilities to predict liquid densities. More than 40 years after their publication, updated versions of the generalized Soave α-function $\left(\alpha(T_r,\omega)=\left[1+m(\omega)\left(1-T_r^{0.5}\right)\right]^2\right)$ suitable for the Redlich-Kwong (RK) and Peng-Robinson (PR) equations of state (EoS) are proposed in this work. The new mathematical expressions of $m_{RK}(\omega)$ and $m_{PR}(\omega)$ have been determined by correlating the optimal m values, fitted on vapor pressures (P^{sat}) and/or enthalpies of vaporization ($\Delta_{vap}H$) and/or saturated-liquid heat capacities ($c_{P,liq}^{sat}$) against the acentric factor ω. The correlations determined in this study can be considered as broad-based and sound since they were established for 1721 pure compounds belonging to many different chemical families (hydrocarbons, halogenated, oxygenated, sulfur, nitrogen compounds …) for which experimental data were available. Significant improvements on the reproduction of vapor pressures were obtained for the PR EoS with respect to the original version. The updated SRK EoS achieved similar average deviations for the three properties of interest (P^{sat}, $\Delta_{vap}H$ and $c_{P,liq}^{sat}$), in comparison with the original SRK equation. A substantial improvement is however noticeable for heavy molecules with an acentric factor larger than 0.9.

References

[1] G. Soave, Chem. Eng. Sci. **27**, 1197–1203 (1972).
[2] D. Peng, D. Robinson, Ind. Eng. Chem. Fundam. **15**, 59–64(1976).
[3] J.-N. Jaubert, R. Privat, Y. Le Guennec, L. Coniglio, Fluid Phase Equilibria. **419**, 88–95 (2016).
[4] R. Privat, J.-N. Jaubert, Y. Le Guennec, Fluid Phase Equilibria. **427**, 414–420 (2016).
[5] Y. Le Guennec, R. Privat, J.-N. Jaubert, Fluid Phase Equilibria. **429**, 301–312 (2016).

OC14

How the parameterization of equations of state influence their performances?

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Attempts to improve the original formulation of cubic equations of state (CEoS) steaming from Van der Waals theory often led to introduce new temperature-dependent or constant parameters. These parameters can be either component-specific (e.g., volume translation parameters, parameters involved in the Twu 1991 or Mathias-Copeman alpha functions) or universal (e.g., constant parameters involved in the Soave or Twu 1995 alpha functions). The search for mathematical expressions for temperature-dependent parameters is essentially empirical: a flexible-enough mathematical expression is proposed to improve the representation of one or two physical properties by the EoS. Similarly, the estimation of constant parameters is generally carried out following a blind optimization procedure. At many occasions, it has been however observed that a blind parameterization of CEoS can lead to propose non-optimal parameters (and thus to underestimate the model capacities) or to predict unphysical thermodynamic behavior. Similar issues arise when it is desired to extend pure-component CEoS to mixture CEoS: the search for optimal mixing rules and their consistent parameterization is essential to reach the maximum capacity of a model. Indeed, recent works on CEoS mixing rules have clearly shown that some limitations identified for this class of models can be moderated, if not overcome, at the price of a re-parameterization of the model.

The same conclusions could be drawn for EoS issued from the Statistical Associating Fluid Theory (SAFT). This class of models which receives a considerable interest from the academic community, but is still not well setup in the industry, offers as main advantages:

- The capacity to account explicitly for association phenomenon,
- the possibility to get a coherent description of matter from the knowledge of molecular interactions and their – more or less empirical – quantification.

Beyond fashionable effects, this statistical theory is primarily popular because it makes it possible to build a bridge between atomic and macroscopic scales.

Similarly to CEoS, many versions of SAFT EoS exist that incorporate numerous temperature-dependent or constant, component-specific or universal parameters. A proper parameterization of these models is a necessary step before going further to the analysis of their strengths and limitations or to a comparative analysis between SAFT and cubic models, as well. In this study, some guidelines and rules are proposed to perform such a parameterization for both SAFT-type or Cubic-type EoS.

updated on March 24, 2019

OC15

Modeling of the ternary system NaCl-Na_2SO_4-H_2O

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Summary

The ternary system NaCl-Na_2SO_4-H_2O is part of the quinary system Na +, Mg^{2+}/Cl^-, SO_4^{2-}// H_2O representative of seawater brines. Six solid phases are observed in this system: ice solubility surface, anhydrous NaCl, Na_2SO_4 and NaCl.2H_2O hydrates, $Na_2SO_4 \cdot 10H_2O$ in addition to the metastable $Na_2SO_4 \cdot 7H_2O$ phase.

We have modeled the ternary system solubility surfaces apart from the metastable $Na_2SO_4 \cdot 7H_2O$ phase due to a lack of data and the $NaCl \cdot 2H_2O$ hydrate for which the surface of solubility is very small and the available experimental points are few.

A graphic selection is made, based on the different isotherms, to remove outliers.

For example, the coefficients of the system are given in molar fractions by:

$$A_{ij} = (1 - \sum_k y_k)\left(a_{ij} + \sum_k \sum_n y_k^n \left(a_{ijk}^{(n)} + \sum_l \sum_{n'} y_l^{n'} \left(a_{ijkl}^{(n)(n')} + \sum_{n''} y_m^{n''} \, a_{ijklm}^{(n)(n')(n'')} \right) \right) \right)$$

The smoothing equation is then: $\frac{A}{T} + B\ln(T) + C + DT = (1 - y_N)\left(U_{MC6} + y_N \, U_{MC6N}^{(1)}\right)$

The calculation of the parameters A, B, C ... by the least squares method is followed by a critical evaluation of the data. The isotherms of the different solubility surfaces are then calculated at different temperatures and graphically represented in Jänecké coordinates. A perspective projection of the calculated polythermic diagram is given with the experimental isotherms.

OC16

Modelling the thermodynamics of fluids with Peng–Robinson + residual Helmholtz energy-based mixing rules

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The thermodynamic modelling of multicomponent mixtures is mostly based on the knowledge of the phase behaviour of binary mixtures. Improving the modelling of the vapour-liquid equilibrium properties of two-component systems is thus a pivotal point for the accurate representation of the thermodynamics of fluids. This is one of the major thermodynamic obstacles that scientists struggle to overcome, since these binary mixtures typically consist of highly non-ideal systems characterised by extremely important critical pressures.

One of the most accurate models currently under development combines the Peng-Robinson cubic equation of state with an advanced class of mixing rules based on local composition activity coefficient models, the so-called "EoS/$a^{E,\gamma}$" mixing rules.

With the aim to further improve the accuracy of these models, we worked towards the theoretical development of this class of mixing rules and we showed [1, 2] that:

- the most thermodynamically consistent theoretical development of this class of mixing rules should not include the combinatorial part of the selected activity coefficient model but only the residual one, thus leading to the definition of "EoS/$a_{res}^{E,\gamma}$" mixing rules;
- there exists a strong correlation between the degree of non-ideality of the modelled binary systems and the mathematical complexity of the temperature-dependent models describing the binary interaction parameters to be used in these mixing rules;
- the combination of "EoS/$a_{res}^{E,\gamma}$" mixing rules with the Peng-Robinson equation of state highly increases the modelling accuracy of the original model, leading to a substantial improved representation of the phase behaviour of highly non-ideal fluids.

In the light of these results, which we will preliminarily present, we will introduce the strategy that we are following in order to develop a predictive form of the "Peng-Robinson + EoS/$a_{res}^{E,\gamma}$ mixing rules", with the support of an in-house database which classifies binary systems on the basis of specific features of their phase behaviour.

References

[1] S. Lasala, P. Chiesa, R. Privat, J.-N. Jaubert, Fluid Phase Equilibria **428**, 18-31 (2016).
[2] S. Lasala, P. Chiesa, R. Privat, J.-N. Jaubert, Ind. Eng. Chem. Res. **56**, 2259-2276 (2017)

OC17

Discussion on the optimum form of the attractive term of translated cubic equations of state

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The volume function, included in the attractive term of cubic equations of state (CEoS), controls the accuracy of calculations of volume properties. This function contains two parameters u and w that define the form of the equation of state. In this study, the influence of values of the parameters u and w in the accuracy of the prediction of volumetric properties is analyzed for untranslated and translated CEoS. It is found that optimum parameters u and w are located in a restricted zone for untranslated EoS. For translated EoS, in turn, there exists a large zone, define by a second-order polynomial, where equivalent optimum values of u and w are located. Moreover, it is shown that parameters u and w should be set as universal constants when a volume-translation parameter is included in the volume function [1-4]. Finally, the pertinence of different choices of u and w in volume functions of well-known CEoS is evaluated [5-8].

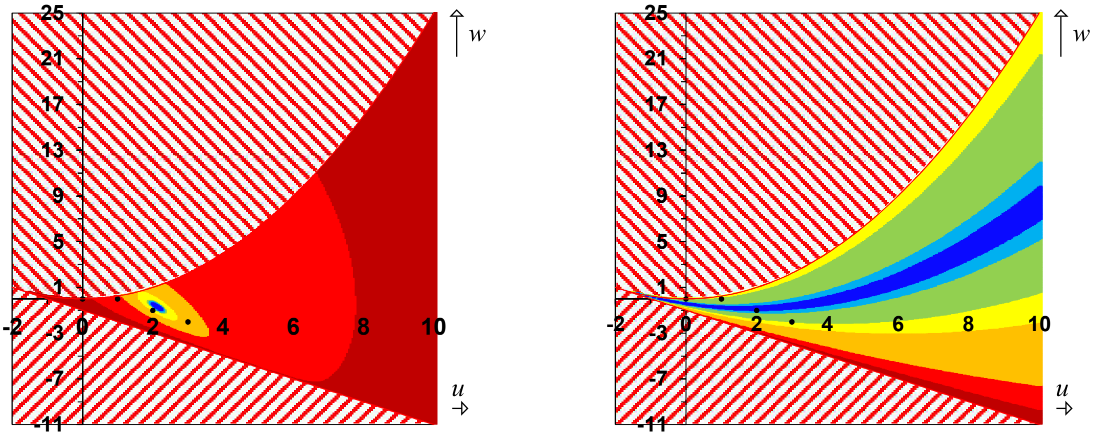

Figure 1. Objective function value as a function of the parameters u and w for an untranslated (left) and translated (right) EoS.

References

[1] A. Péneloux, E. Rauzy and R. Fréze, Fluid Phase Equilibria **8**, 7–23 (1982).
[2] J.-N. Jaubert, R. Privat, Y. Le Guennec, L. Coniglio, Fluid Phase Equilibria. 419, 88–95 (2016).
[3] R. Privat, J.-N. Jaubert, Y. Le Guennec, Fluid Phase Equilibria. 427, 414–420 (2016).
[4] Y. Le Guennec, R. Privat, J.-N. Jaubert, Fluid Phase Equilibria. 429, 301–312 (2016).
[5] J.D. Van der Waals, Over de continuiteit van den gas - en vloeistoftoestand, (1873).
[6] O. Redlich and J.N.S. Kwong. Chem. Rev. **44**, 233–244 (1949).
[7] D. Peng and D. Robinson. Ind. Eng. Chem. Fundam. **15**, 59–64 (1976)
[8] G. Schmidt and H. Wenzel. Chem. Eng. Sci. **35**, 1503–1512 (1980).

OC18

Sol - Gel Smart Materials: Characterization and Application

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The use of sol-gel technique to fabricate phospho-silicatenano-composite SiO_2- P_2O_5 based glasses containing 20 mol% P_2O_5 deposited on quartz silica substrate presented in this work particularly Erbium Er^{3+}, Neodemium $Nd^{3+}$and Yb^{3+} ions were doped in this phospho-silicate host matrial. The development of a planar waveguide based on silica phosphate doped with neodymium ions work on amplification of optical signal around 1360 nm directly without firstly converting it to electrical signal. Moreover nano-composite Phospho-Silicate (SiO_2 - P_2O_5) doped with Er^{3+} and hybrid-phospho-silicate-polyamidoamine-hyperbranched-polymer-Er^{3+}, respectively are considered as promising materials for photonic application specially planar wave guide too.

Where $BaTiO_{3,}$ $BaTiO_3$-Sn-RE were used for information storage application. Finally the ZnO nano-rod growing on the surface of plastic, silicon, silver wire (250 micrometer in diameter) and on the tip of a borosilicate glass capillary tube (0.7 micrometer in diameter) in order to act as biosensor used for measurement of extra/intracellular ions Figure (3).Variety of material studies were carried out for the investigation of the physical properties of these prepared materials; such as the X-ray diffraction (XRD), field emission scanning electron microscope (FESEM) and transmission electron microscope (TEM).

The aim of the present work is the development of phosphate, phospho-silicate-Er^{3+} and hybrid-phospho-silicate-polyamidoamine-hyperbranched-polymer-Er^{3+} nano-composites, co- activated with (Yb^{3+}) ions as sensitizer, towards planar optical waveguide applications. While the ZnOnano-rod can act as biosensor used for measurement of extra/intracellular ions.

OC20

Consequences of the Ni-enrichment in Co-based alloys designed to be TiC- or TaC-reinforced on their H.T. microstructures

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Although they appeared many decades ago the cast polycrystalline carbides-strengthened superalloys family remains of great interest for a number of high temperature applications inducing mechanical stresses, oxidation by gas mixtures and corrosion by melts. High levels of creep resistance can be achieved by obtaining eutectic MC-type carbides between matrix dendrites. Among them, script-like TaC and TiC are especially interesting but their characteristics may be threatened by the additions of nickel which are compulsory to stabilize the FCC cobalt matrix and to favor easy outwards Cr diffusion in hot oxidation conditions.

In this work we have explored how the introduction of more and more nickel in a Co(bal.)-25Cr-0.4C-6Ta alloy and in a Co(bal.)-25Cr-0.4C-1.6Ti one may influence the nature, fractions and morphology of the contained carbides. This was carried out by anticipating thermodynamic calculations using Thermo-Calc and by elaborating by foundry two series of alloys which were thereafter exposed at 1400K or 1510K for more than 20 hours before air quenching. Calculations and metallography results both show that adding Ni induces a progressive substitution of the TaC or TiC carbides by chromium carbides, which acts as soon as Ni becomes more present than cobalt in the chemical composition of the alloys.

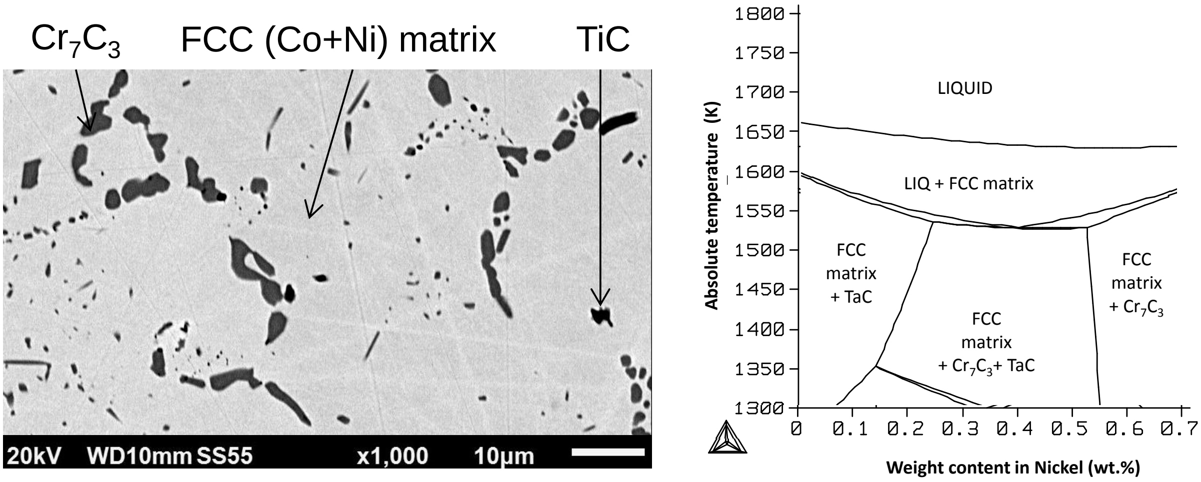

Figure 1. 1400K-aged Ti-containing Co(Ni)-based alloy (left) and phase diagram of Ta-containing Co(Ni)-based alloys (right)

References
[1] P. Berthod and L. Toubal, Materials Chemistry and Physics, **212**, 260-267 (2018).
[2] P. Berthod and Z. Himeur, Calphad **60**, 156-162 (2018).

OC21

Pinning mechanism and Pinning Force variation in $YBa_2Cu_3O_{7-\delta}$

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Abstract In this paper we interested to the variation of critical current density J_c and the variation of pinning force. Our objective is to study the relationship between the pinning force F_p and some critical parameters, for different value of magnetic field. These parameters are depending on the pinning mechanism. m is a parameter which represents the magnetic dependence when γ is a parameter depending on temperature . For the weaker value of magnetic field and in the absence of thermal activation, we obtained that the critical current density J_c exhibits with a behaviour according to $((1-(T/T_c))^{m'}$, where m' is an exponent varying with a variation of magnetic field. Mechanism pinning is also studied in this work, however different type of pinning are examined as function of magnetic field.

OC22

Carachterization and identification of the products formed from Moroccan phosphogypsum

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Phosphoric acid production (Reaction 1) worldwide generated millions of tons of phosphogypsum waste (120-300 Mt/year):

$$\underset{\text{Phosphate rock}}{Ca_5(PO_4)_3F(s)} + 5H_2SO_4(l) + 10H_2O(l) \rightarrow \underset{\text{Phosphoric acid}}{3H_3PO_4(l)} + \underset{\text{Phosphogypsum}}{5(CaSO_4.2H_2O)(s)} + HF(g) \quad (1)$$

These quantities are mostly disposed of without any treatment, usually by dumping in large stock piles or discharged directly into the sea. The Phosphogypsum contains various impurities (heavy metals, radionuclide ...), which has a harmful effect on the environment, especially the marine environment.

The main objective of this work is to contribute to the development of ways of recycling phosphogypsum for the production of valuable products. This method consists of dissolving phosphogypsum, considered as a source of calcium and sulfate, in an alkaline medium (KOH) for the sequestration of carbon dioxide CO_2 to produce calcite $CaCO_3$ and potassium sulfate K_2SO_4 (Reaction 2 and 3):

$$CaSO_4.2H_2O(s) + 2KOH(l) \rightarrow Ca(OH)_2(l) + K_2SO_4(aq) + 2H_2O(l) \quad (2)$$

$$Ca(OH)_2(aq) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l) \quad (3)$$

The morphology of the particles and their crystal structure were determined by different analyzes (MEB, EDX, XRD, FTIR and ATG/ATD). The pH-Conductivity measurements and the results of data analysis confirm the formation of the desired products.

Such investigation will be considered as a solution to reduce high amounts of phosphogypsum waste and the emissions of CO_2 by using the mineral carbonation process.

References

[1] A. Aagli, N. Tamer, A. Atbir, L. Boukbir, and M. El Hadek, *J. Therm. Anal. Calorim.*, **82**, pp. 395–399 (2005)

[2] C. Cárdenas-Escuderoa, V. Morales-Flórez, R. Pérez-Lópezc, A. Santose and L. Esquiviasa, J Hazard Mater **196**, pp. 431–435 (2011).

OC23

Co-precipitation synthesis of $CePO_4$ nanostructures: Correlation between the calcination temperature and structural properties

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Rare earth phosphates have recently been investigated as a potential ceramic material in view of their high-temperature phase stability, high melting point, low thermal conductivity, layered structural features, optical, photoluminescent and photocatalytic properties. The present work describes a method for synthesizing nanocrystalline cerium phosphate $CePO_4$ starting from cerium nitrate and ammonium hydrogen phosphate precursors by co-precipitation reaction. The obtained hydrated sample were dried and then calcinated at different temperatures for 3 hours. Thermogravimetry and Differential thermal analyses (**TGA–DTA**) of this hydrate allowed evidencing water elimination and other thermal transformations. The morphology of the calcinated samples were characterized by scanning electron microscope (**SEM**). The SEM results indicated that $CePO_4$ powders were in nano sized particles. The particle size and structures of the products were characterized by X-ray diffraction (**XRD**), the functional groups were confirmed by fourier transform infrared spectroscopy (**FTIR**).

Keywords: Cerium phosphate $CePO_4$, co-precipitation reaction, calcination route, thermal analyses, diffraction techniques, spectroscopy method.

Acknowledgments

This work was financially supported by project **PHC Toubkal** 18/64 – Campus France 28999WE and PPR project financed by the CNRST under number **PPR**/2015/32.

References

[1] K. Rajesh, P. Mukundan, P. Krishna Pillai, V. R. Nair, and K. G. K. Warrier, "High-Surface-Area Nanocrystalline Cerium Phosphate through Aqueous Sol-Gel Route," Chem. Mater., vol. 16, no. 8, pp. 2700–2705, 2004.

[2] M. Kirubanithy, A. A. Irudayaraj, A. D. Raj, and S. Manikandan, "Synthesis, Characterization and Photoluminescence Behaviours of $CePO_4$ and Tb-doped $CePO_4$ Nanostructures," Mater. Today Proc., vol. 2, no. 9, pp. 4344–4347, 2015.

OC24

Experimental study of CO_2 solubility on NaCl and $CaCl_2$ solutions from 333.15 K to 373.15 K and pressures up to 400 bar

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On the scope of a project which aims to explore geothermal reservoirs in order to produce geothermal energy in France, it is important to have information about the thermodynamic behavior of the brines recovered from this geothermal reservoirs for process safety and efficiency raisons. Furthermore, one of the most important information required is the amount of gas solubilized on these brines at reservoirs pressures and temperatures as well as any other conditions one may find when the fluid is being pumped to the surface on the geothermal energy production plant. However, solubility data for most of the pressure-temperature-salinity conditions required for the project are not found on literature, mainly for pressures higher than 200 bar, for brines containing $CaCl_2$ and for salt mixtures brines ($NaCl-CaCl_2$).

Therefore, in order to be as close as possible to these conditions, experimental study of CO_2 solubility on NaCl and $CaCl_2$ brines (up to 2 mol NaCl/Kg H_2O and 1 mol $CaCl_2$/Kg H_2O) from 333.15 K to 373.15 K has been performed. Solubilities have been determined in the pressure range between 60 bar and 400 bar thanks to a 250 cm^3 Hastelloy C-2000 well stirred autoclave, in which thermodynamic phase equilibrium is obtained by putting the solution in contact with the gas phase under high pressure before sampling for analysis.

High pressures can be obtained with a compressor whereas band heaters allow us to have the high temperatures required for our experiments. In order to have a constant pressure on our autoclave, a hydraulic actuator can move upwards and downwards, which ensures an isobaric functioning while sampling.

For NaCl solutions, once the equilibrium is achieved, liquid samples are recovered with a sampling syringe that contains a trapping NaOH solution free of carbonate. The CO_2 is trapped by this solution and then analysed by acid-base titration. On the other hand, when $CaCl_2$ is dissolved in our solutions (either pure or mixed with NaCl), CO_2 solubility will be measured through conductometric titration besides the acid-base titration. These analytical methods have already been used at our team for lower pressures and different brine salinities [1],[2]. In the framework of this project, literature data were useful to validate our experimental protocol with a new device, in order to have new experimental points.

Results presented are the isotherms for the system $H_2O-CO_2-NaCl-CaCl_2$ on the temperature range of this project at each salinity studied, in which one may see the graphical evolution of CO_2 solubility with pressure (m_{CO2}-P). Experimental data were produced with good accuracy since uncertainties of our measurements were calculated with ANOVA method and are lower than 3%.

References

[1] H. Messabeb, F. Contamine, P. Cézac, J.P. Serin and E.C. Gaucher, Journal of Chemical Engineering Data **61(10)**, 3573-3584 (2016)

[2] H.Messabeb, F. Contamine, P. Cézac, J.P. Serin, C. Pouget and E.C. Gaucher, Journal of Chemical Engineering Data **62(12)**, 4228-5234 (2017)

OC25

Sea water desalination and remineralization steps in the south of Morocco

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Keywords : Desalination, Remineralisation, Reverse Osmosis, Lime, Calcite,

Abstract : Water is a fundamental element of ecosystems and very vital for people and their activities. The distribution of fresh waters is very uneven. In fact, ten countries share 60% of the fresh water reserves and twenty-nine others, mainly in Africa and the Middle East, are on the contrary confronted with a chronic shortage of fresh water. So, Due to its geographical location (arid and semi-arid zone) and its climatic conditions, Morocco is no exception to the rule, especially since water has become a major concern in the southern regions of Morocco. scarcity and poor quality of water resources can have a significant impact on the socio-economic sectors in these areas. Indeed, to face the shortage of water because of drought, the National Office of Electricity and Water (ONEE -water branch-) has lanced an ambitious program by the realization and installation of desalination plants in the south of Morocco. The produced water (osmosis water) is not equilibrated; it attacks pipelines and causes corrosion. In the other hand this water releases toxically substances that will provoke problems of health's clients.

Post-treatment of remineralization is necessary to achieve the calco-carbonic equilibrium of water. This work aims to study of the feasibility of remineralization's processes of osmosis water in desalination stations of sea water and demineralization station of brackish water to produce water meeting the Moroccan Standard for the Quality of Human Feeding Water NM 03.7.001 [2,3].

This work was complemented by a comparative study between three techniques of remineralization adopted in three plants installed in the south of Morocco. The results show that remineralization of osmosis water by passage through a calcite bed is the efficient and the easiest one. That's why; we have realized a calcite bed pilot on laboratory scale. We have examined the effect of water debit, the residence time E.B.C.T (Empty Bed Contact Time), the upward speed and bed length on the parameters of treated water. The knowledge and the control of these parameters at a laboratory scale are essential for the conception (design) of a process of optimal remineralization [4,5].

References

1. Direction centrale du pole industriel, Analyse et evaluation de l'expérience ONEP en dessalement membranaire, Mai 2010.

2. Qualité des eaux d'alimentation humaine, N° 221-06 du 2 Février 2006, publié au B.O N° 5404 du 16 Mars 2006

3. E Gabbrielli ,J.P Gerofi, , Desalination,49 (1984) 95–103.

4. M.G. Biyoune, A. Atbir, E. Mongach, H. Bari, A. Khadir, L. Hassnaoui, L. Boukbir, M. Elhadek, Comparative study between three methods of remineralization, J. Mater. Environ. Sci. 6 (5) , 1243 – 1252, (2015).

5. M.G. Biyoune, A. Atbir, H. Bari, E. Mongach, A. Khadir, L. Hassnaoui, L. Boukbir, M. Elhadek, Remineralization of desalinated water by adding lime Ca(OH)2 in the desalination plant of Laâyoune, J. Mater. Environ. Sci. 5 (S2), 2359 – 2364, (2014)

OC26

Experimental and predictive study of the effect of seawater composition on liquid-solid equilibrium: Application of cryoscopy on marine water in El Jadida Bay: Atlantic Ocean – Morocco

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Seawater is a complex multi-component system where almost all chemical elements are present in different concentrations (macro, micro and trace) and forms (simple and complex ions, dissolved gases, etc. . .). However, seawater can be used as a source of extraction of useful substances that can be resulting from different seawater desalination processes such as membrane desalination, reverse osmosis, evaporation processes, and evaporation–cooling processes [1]. Freezing is one of the efficient processes for separating dissolved brines from seawater. It allows the study of marine freezing systems. It has a similar effect to that of evaporation technologies [2]; it depends on operating conditions such as temperature (freezing and air), air movement, and salinity, with H_2O in the form of ice. It requires well-defined separation operations to obtain the extraction of specific mineral salts at different temperatures and composition, which makes this process relatively complex[3]. These properties make it possible to understand and predict the various interactions between the chemical elements dissolved in liquid and solid phases and to determine the optimal operating conditions for desalination.

This work focuses on the experimental and predictive study of the physico-chemical and thermodynamic properties of the liquid-solid equilibrium of seawater from El Jadida Bay. The experimental method of lowering the melting temperature of ice (cryoscopic method) was used to study the liquid-solid equilibrium of El Jadida seawater at different compositions. The results obtained experimentally from solid-liquid equilibrium, solutions at different concentrations of seawater, are in good agreement with the data in the literature. In addition, the Frezchem calculation code (FREeZing CHEMistry) based on Pitzer thermodynamic model was used to predict the ionic composition, salinity, solid phases that are formed and temperatures of the liquid-solid equilibrium. Thus, the thermodynamic study quantified the effect of seawater composition and salinity on the freezing and precipitation temperature of gypsum ($CaSO_4.2H_2O$) and mirabilite ($Na_2SO_4.10H_2O$), which would alter the purity of the ice by including it in our desalination process.

References

[1] A. Kovacheva, D. Rabadjieva and St. Tepavitcharova, Desalination 348, 66-73 (2014).
[2] SC.Stark, BV.O’Grady, HR.Burton and PD .Carpenter, Australian Journal of Chemistry 56, 181–186 (2003).
[3] B. M. Butler, S. Papadimitriou, A. Santoro and H. Kennedy, Geochimica et Cosmochimica Acta, 182, 40–54 (2016).

OC27

The inhibitory effect of a phosphate product on the sanitary waters of the tourist area of Agadir

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Abstract

The scaling of water transport pipes has become one of the major problems encountered in areas that exploit high hardness groundwater. Several methods can be used to prevent this phenomenon of scaling. Among these methods, the use of inhibitors remains one of the best techniques to prevent or delay the formation of scale deposits.

During our work on the phenomenon of scaling observed in the sanitary water transport pipes of the tourist sector in the city of Agadir, we carried out a one-year follow-up (January to December 2015) to determine the physical and chemical quality of these waters. Sampling was conducted from four sampling points, well distributed throughout the study area and involving 84 water samples. For each sample, the parameters measured are: temperature, pH, conductivity, total hardness and concentrations of HCO_3^-, Ca^{2+}, Mg^{2+}, Na^+, K^+, SO_4^-, NO_3^-, Cl^- and OH^- ions. Indeed, the physico-chemical quality monitoring shows that the hydrotimetric title varies between 25 °F and 55.63°F and the complete alkalimetric title varies from 7.5°F to 34°F.

For the kinetic study of the scaling power, which is the subject of this work, we selected four samples of high hardness from the 84 samples analysed. This study was carried out using the controlled degassing method "LCGE" and showed that the waters studied are scaling. The germination time Tg varies between 38 and 84 mn.

Thus, we were particularly interested in studying the inhibitory effect of scaling phosphate material. This study was carried out on synthetic water with a hardness of 40°F using the "L.C.G.E" method and concluded that this phosphate-based compound has a total efficacy on the formation of calcium carbonate.

Keywords: scaling power; sanitary water; Agadir; kinetic study; physico-chemical analysis; LCGE.

OC28

Optimization and modeling of degradation of orang G by sulfate radicals using a response surface methodology (RSM) based on the central composite design

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Abstract

The experimental design methodology was applied for modeling and optimizing the operation parameters on Orange G removal using persulfate activated with new magnetic material : Polyaniline coated hematite sand supported on graphene oxide (HS@PANI-GO). Four experimentals parameters (concentartion of persulfate (mM), dose of catalyst (g.L^{-1}), contact time (min), orange G concentration (mM)) were adopted to obtain the preliminary information. The multivariate experimental design was employed to establish a quadratic model as a functional relationship between the removal rate of OG and four experimental parameters. The interaction effects and optimal parameters were obtained by using Design Expert software. The optimum of OG removal is: [PS] = 4 mM, catalyst dose 2 g.L^{-1}, [OG] = 1 mM and 90 min. Under these conditions, the experimental removal of the orange G was found to be 98.14 %, while the value predicted by the model was 96.58%. This shows that there is no significant difference between the predicted and experimental responses. The values of R^2 (0.917) and R^2Adj (0.834) prove the existence of a good correlation between the data.

KEYWORDS: modeling, Optimization, removal of orang G, RSM

OC29

Study of the interaction between water and the red stigmas of saffron *Crocuse Sativus L.*, : Kinetic of the Drying Process by traditional method

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Abstract:

Saffron *Crocuse Satuvis L.*, is the most expensive spice in the world, it belongs to the irridaceace family, the drying of this spice is a decisive step to keep the saffron in good quality, this work aims to determine the optimal conditions for drying this spice by traditional method in the laboratory at temperatures between 40 and 60°C under atmospheric pressure and the masses are varied between 0,484 and 0.848, to study the influence of the initial mass and the temperature on the drying phenomenon, the results obtained show that the drying kinetics depends on the initial phase and the drying temperature according to the values of the relative rate constants at each temperature it was possible to determine the value of the activation energy Ea=47.073 Kj.mol^{-1}, the kinetic modelization performed in this study shows that the regime that describes this drying phenomenon is an interfacial progression in cylindrical symmetry.

Keyword: *Crocuse Satuvis,.L*, drying kinetics, rate constant, activation energy, the kinetic modelization

OC31

THERMAL AND STRUCTURAL ANALYSIS OF CELLULOSE PHASE FROM MOROCCAN CACTUS CLADODES AND ITS POTENTIAL APPLICATIONS AS A REINFORCING AGENT IN PET COMPOSITES

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Abstract

The purpose of this study is related to the use of cellulose phase isolated and characterized from Moroccan cactus (O*puntia ficus indica*) cladodes, and its effect on polymer composite with varying fiber reinforcement content to improve the adhesion between polymer matrix and surface fiber.

Cellulose fibers were isolated by alkaline treatment, using three distinct stages. Firstly cactus cladodes was subjected to a hot water (70°C) treatment to remove hemicellulose, then to an alkaline aqueous solution (15% of sodium hydroxide (NaOH), 98°C) treatment to separate lignin from cellulose, and finally to a washing (distilled water) and drying stage. Cactus cellulose fibers were analysed by different complementary analysis (DRX, FT-IR; ^{13}C NMR and TGA-DTA) [1, 2, 3].

The reinforcing capability of cellulose fibers extracted from cladodes was examined using polyethylene terephthalate (PET) as matrix. The effects of the fiber loading on physical properties of the composites, in terms of tensile strength, Young's Modulus and Flexural Modulus before and after water absorption were studied. Composites containing 15 wt% fiber loading, exhibited the best mechanical properties before and after water absorption, as a result of a good interface adhesion between cellulose fibers and matrix.

Keywords : Cactus ; Cellulose phase ; Alkaline treatment ; Composites ; Mechanical properties.

References:

[1]- Sun JX, Sun XF, Zhao H, Sun RC. Isolation and characterization of cellulose from sugarcane bagasse. Polym Degrad Stab 2004;84:331–9.
[2]- Bhattacharya D, Germinario LT, Winter WT. Isolation, preparation and characterization of cellulose microfibers obtained from bagasse. Carbohydr Polym 2008;73:371–7
[3]- Moubarik A, Grimi N, Boussetta N, Pizzi A. Isolation and characterization of lignin from Moroccan sugar cane bagasse: Production of lignin-phenol-formaldehyde wood adhesive. *Ind Crops Prod.* (2013);45:296-302..

OC32

Modelling and optimization of ultrasound-assisted competitive and simultaneous adsorption of toxic dyes onto activated carbonaceous anaerobically digested

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In this paper, an effective methodology was used to modeled the ultrasound-assisted adsorption of Congo red (CR) and Crystal violet (CV) in binary mixture. The ultrasonic adsorption of CV/CR on activated carbonaceous anaerobically digested (TDAW) were investigated using central composite design coupled with response surface methodology (CCD-RSM). Elaborate models were evaluated after some statistical tests including analysis of variance (ANOVA), the correlation coefficient (R^2), the adjusted correlation coefficient (R^2_{Adj}) and the test of significant coefficients. Results shows that models were present was high significant (P-value < 0.0001) and the values of R^2 and R^2_{Adj} prove the existence of a good correlation between the data. In addition, all coefficients models present a P-value high than 0.05 were eliminated from fitting model. The data showed that the TDAW has strong selective adsorption of CV dye in comparison to CR, and optimum conditions were found to be natural pH, 11.19 mg of adsorbent, (55%:45%) of CV:CR ratio, a contact time of 25 min and initial dye concentration of 30 mg/L at adsorption temperature T=25 °C ± 1. In these conditions, both dyes (CV and CR) are easily regenerated using HCl (0.1 N).

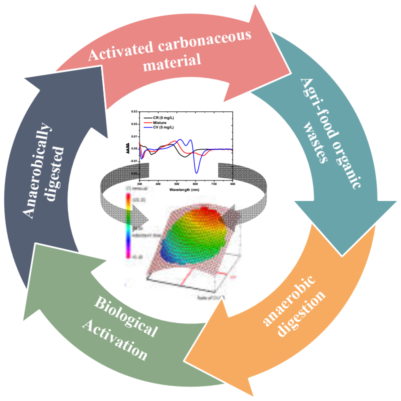

Figure 1. Modellig and optimization of ultrasound-assisted competitive and simultaneous adsorption of toxic dyes onto activated carbonaceous anaerobically digested

Acknowledgement: This work was supported by MNEFPESRS, CNRST, SCAC, IFM, Institute of Materials Science Mulhouse - University of Upper Alsace and the Materials and Environment Laboratory (LME) - University Ibn Zohr in the framework of Franco-Moroccan cooperation, research projects CEDocs 2018 - under No. 08/00057.

Posters

Measured densities and derived thermodynamic properties of waste cooking oil biodiesel from 298.15 K to 393.15 K and pressures up to 140MPa

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Abstract

As an alternative for petrodiesel, biodiesel can easily become the crucial solution for environmental problems. Biodiesel is the common name for a variety of ester-based oxygenated fuels from renewable biological sources. It can be made from processed organic oils and fats. To date, many vegetable oils have been used to produce biodiesel namely waste cooking oil. In this regard, the knowledge of the thermodynamic properties of biodiesels and their derived properties becomes crucial not only for developing optimal biodiesel production and purification processes, but also for enhancing biodiesels performance in engines. In this work, we report Density data (685 points) for waste cooking oil biodiesel at several temperatures between (298.15 and 393.15) K and pressures up to 140 MPa . The experimental density data were fitted with a Tait-like equation in the same range of pressure and temperature with low standard deviations. The Tait-correlation parameters, along with the AAD (0.03 %), MD (0.06%), Bias (3.4 10-2 %), and standard deviation, σ ($3.16 \cdot 10^{-4}$ $g.cm^{-3}$).

The derived thermodynamic properties, i.e. isobaric thermal expansion coefficient and the isothermal compressibility coefficient, were then calculated from the experimental density data using thermodynamic equations.

Determination of the limits of ternary phases based on the compounds of the binary system Ni-Ti at high temperature

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Abstract

The purpose of this paper is to establish a new values of enthalpies of formation of the ternary intermetallic compounds ($Al_xNi_{0.75}Ti_{0.25-x}$ $0.04 \leq x \leq 0.07$; $Al_xNi_{0.50}Ti_{0.50-x}$, $0.04 \leq x \leq 0.08$; and $Al_xNi_{0.33}Ti_{0.67-x}$, $0.03 \leq x \leq 0.09$) of ternary phases based on the system Ni–Ti, measured by direct calorimetry at high temperature. After each calorimetric measurement, the reaction products are analyzed by X-ray powder diffraction (XRD) and electron probe microanalysis (EPMA) to check their structures, compositions and to determine the limits of each phase. The calorimetric results are compared with literature data and with predicted values based on semi-empirical and theoretical models.

Keywords: Transition metal alloys; Enthalpy of formation; Calorimetry by direct reaction; ternary phase equilibria; limits of solubility of the ternary phases.

P 6

Numerical study of the evaporation of a thin film dripping along the active walls of a vertical channel

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Abstract

The phenomena of heat and mass transfer during the flow of a liquid film on a heated wall has a considerable interest in the engineering field, which was translated into many applications, such as in desalination, distillation, drying, and the cooling of electronic components.In this work, we present a numerical study on coupled heat and mass transfers with phase change in an adiabatic vertical channel formed by two parallel flat plates. The lower plate of the channel is covered by a film of thin liquid water dripping by gravity and maintained at a constant temperature while the upper one is adiabatic and dry. A Volume of fluid method is employed to solve the coupled governing equations for liquid film and gas flow together with the interfacial matching conditions. The results show that the temperature of the film increases slightly for the heating zone and then decreases over most of the plate for the evaporation zone. A comparison between our numerical and experimental results shows a very satisfactory agreement.

Keywords: heat and mass transfer*, evaporation, numerical and experimental study.*

P 8

New thermodynamic assessment of the Gallium-Aluminum binary system

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Thermodynamic modeling of the Al-Ga binary system was carried out with the help of the CALPHAD method [1]. In this method, the thermodynamic models for the Gibbs energy of all the individual phases are studied using the Parrot module in the Thermo-Calc Software package [2,3]. The excess terms of the Gibbs energy of the solution phases (liquid and fcc_A1) were assessed with the recent exponential temperature dependence of the interaction energies by Kaptay [4-6] and compared with the linear dependence by Redlich-Kister [7]. In the two cases, additional constraints to avoid the appearance of unwanted inverted miscibility gap in the liquid phase during the phase diagram calculation up to 6000 K were imposed. All of the experimental data (phase diagram and thermodynamics information) available in the literature were used for the optimization of the thermodynamic parameters. The calculated phase diagram and the thermodynamic properties of the system are in satisfactory agreement with the majority of the experimental data.

Keywords: New thermodynamic assessment, Al-Ga system, Calphad method, phase diagram

References

[1] L. Kaufman, H. Bernstein, New York, NY : Academic Press, (1970)
[2] B. Jansson, Ph. D. thesis, Division of Physical Metallurgy, Royal Institute of Technology, Stockholm, Sweden, (1984)
[3] B. Sundman, B. Jansson, and J.-O. Andersson, Calphad. 9, 2, 153-190, (1985)
[4] G. Kaptay. Calphad. 28–2:115-24 (2004)
[5] G. Kaptay. Calphad. 32–2:338-52 (2008)
[6] G. Kaptay. Mat SciEng A. 495:19-26 (2008)
[7] O. Redlich, A.T. Kister, Ind. Eng. Chem, (1948)

P 10

CALPHAD Description of the Manganese-Antimony Binary System

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Abstract:

This is the main text of the abstract. Your abstract should fit on one A4 size page. The text of Based on the critical review of the available experimental data reported in the literature, including phase diagram, crystallographic data and thermodynamic data, the Manganese-Antimony binary system was assessed thermodynamically using the CALPHAD (CALculation of PHAse Diagram) approach with the aid of the Thermo-Calc software. The solid solution phases, including liquid, α-Mn, β-Mn, γ-Mn, δ-Mn, and Sb are modelled by the substitutional solution model, while the intermetallic compounds such as MnSb and Mn_2Sb, which have a homogeneity range, are treated as (Mn%, Sb)m(Mn, Sb%)n by a two-sublattice model. A set of self-consistent thermodynamic parameters obtained finally to describe the Gibbs energies of various phases in the Manganese-Antimony binary system can be used to reproduce well phase equilibria and thermodynamic data.

P 12

Thermodynamic evaluation of the Gallium – Lutetium binary system

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Abstract:

The $Ga-Lu$ binary system have been optimized by using the experimental data available on the phase diagram and thermodynamic functions by the CALPHAD approach [1]. The $Ga-Lu$ system [2] contains five intermetallic compounds (figure), which have been found: Ga_3Lu, Ga_2Lu, Ga_5Lu_3, $GaLu$ and Ga_3Lu_5 . These phases are stoichiometric except for the compound Ga_3Lu_5, which has a range of homogeneity, and has been processed by the two-subnet model [3] with substitution in each subnetwork. The solution model was used to describe the excess term of Gibbs energy $({}^{ex}G)$ for the liquid phase and the solid solution. The $Ga-Lu$ system was examined using the description of the liquid phase: linear dependence (Redlich-Kister model) [4].Calculations based on thermodynamic modeling are in good agreement with the data of the phase diagram and the experimental thermodynamic values available in the literature. The modeling process allows us to calculate for the first time the phase equilibria and the thermodynamic properties of the liquid phase and the intermetallic compounds. The results obtained will be reported in a series of figures and tables in a poster or a slide during the communication.

Key words: Ga-Lu system, CALPHAD technique, Thermodynamic evaluation, Redlich–Kister equation.

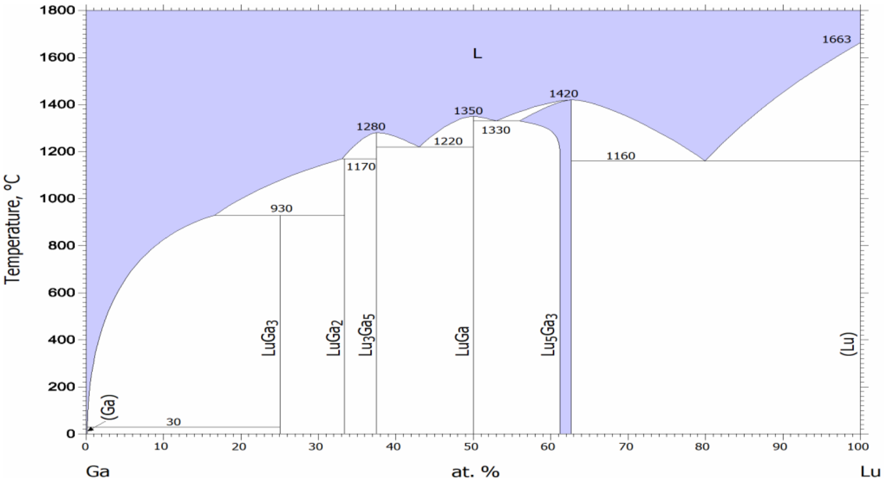

Figure: The experimental phase diagram of the $Ga-Lu$ system [2]

References

[1] L. Kaufman and H. Bernstein, Computer Calculations of Phase Diagrams, Academic Press, New-York, NY, (1970).

[2] T.B, Massalski. (editor-in chief): "Binary Alloy Phase Diagrams", Second Edition, Vol. 2, Materials Information Soc., Materials Park, Ohio (1990)

[3] Temkin, M. 1945. Mixtures of fused salts as ionic solutions. Acta Physicochim. URSS, 20(4), 411–420.

[4] O. Redlich, A. Kister, Ind. Eng. Chem. **40**,345 (1948).

P 13

Disquac prediction of solid−liquid phase equilibria diagrams for systems PHA with octacosane.

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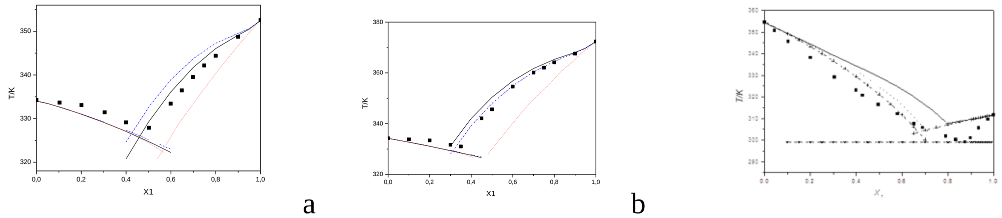
Abstract

The knowledge of thermodynamic properties of systems containing polycyclic aromatics and long chain alkanes is important in numerous petroleum industrial applications. While molecular interactions between small molecules and between molecules of widely different sizes has been exhaustively studied, interactions in systems formed by heavy hydrocarbons are not well documented [1].

Solid–liquid equilibria (SLE) measurements of mixtures containing polyaromatics and heavy alkanes are very rare. Group contribution models like Asog, Unifac and Disquac can be used to predict the thermodynamic properties and have proved fairly successful in predicting SLE[2]. In this work, the experimental phase diagrams available in the literature[3]. naphtalene, phenanthrene, pyrene and +octacosane were correlated using Disquac model [4]. Knowledge of solubility is essential for the design and development of separation process involving crystallization. PHA with octacosane are regarded as possessing two types of surfaces: type a, alkane (CH_3 or CH_2 group), and type b, benzene (C_6H_5- group) Values of the required geometrical parameters have been given elsewhere [4].

In this work, we have represented the combinatorial term using the Flory–Huggins equation (DQF). Huyskens equation [5] (DQH) was also employed to correlate the solid–liquid equilibria data. Both two equations can accurately represent the nonideality of the liquid-phase for the systems[6]. The correlated results are also in good agreement with the experimental data (Figure 1).



a b c

Figure 1. SL phase diagram for a -naphtalene (1) + nC_{28} (2) b - phenanthrene(1) + nC_{28} (2) c - pyrene (1) + nC_{28} (2): ▪ experimental points; ——, DQF; .... DQH; – – – –, idéal; – — –,eutectic temperature

References

[1] P.B. Choi, and E.McLaughlin, Ind.Eng. Chem. Fundam., **22**,46 (1983b).
[2] NM.Djordjevic, Thermochimica Acta, **177**,109 (1991).
[3] A. Aoulmi, M. Bouroukba, R. Solimando and M. Rogalski Fluid Phase Equilibria **110**, 283(1995).
[4] H.V.Kehiaian, Pure Appl. Chem., **57**, 15 (1985).
[5] K.Kniaz, Fluid Phase Equilibria, **68**, 35(1991).
[6] P. L.Huyskens and M. C. Haulait-Pirson. J. Mol. Liquids **31,**135 (1985).

Thermodynamic assessment of The Ytterbium-Gold with the Kaptay equation for the excess Gibbs energy of the liquid phase

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The rare-earth/ gold alloys have been widely studied because of their greatest properties which makes them a fundamental component in a great number of new technologies. Hence AuYb presents the Kondo effect which describes the change in electrical resistivity with the temperature [1]. This property makes this alloy widely used in the nanoelectronics as transistors and for improving cell photovoltaic panels…Those alloys are also used as anti-theft markers for the sensing of physical parameters (pressure, temperature…) [2].

To utilize the full technological potential of these metals, it was essential to have a fundamental knowledge about their properties. In this sense the aims of this work is to compile all the available experimental information [3], to confirm its consistency and to create an optimized set of data by using the CALPHAD (CALculation of PHAse Diagram) approach [4]. The excess term of the Gibbs energy of the solution phases (liquid, b.c.c. and f.c.c.) was assessed with the Kaptay equation [5] and compared with results obtained by using Redlich and Kister [6] polynomial equation. The intermetallic compound βYbAu in this binary system which has a homogeneity range was treated by a two-sublattice model [7]. The others compounds were modeled as stoichiometric. A consistent set of thermodynamic parameters was optimized to give account of the available experimental and thermodynamic data.

[1] G.Creuzet, I.A Campbell, J.Magn. Magn Mater., 27(1982) 221-226.

[2] C.A. Grimes, S.C.Roy, S.Rani, Q. Cai, Sensors, 11 (2011), 2809-2844.

[3] A. Iandelli, A Palenzona, J. Less-common Met., 18 (1969) 221-227.

[4] L. Kaufman, CALPHAD , 7 (1977)

[5] G. Kaptay, Comp. Coupling of Phase Diagrams and Thermo., 28 (2004) 115-124

[6] O. Redlich, A.T. Kister, Ind. Eng. Chem., 40 (1948) 345-355.

[7] M. Hillert et L. I. Staffanson, Acta Che. Scand., 24 (1970) 3618-3626.

Calphad-Type Assessment of the Al-Ti-Au Ternary System

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Binary alloys involving gold, aluminium and titanium are of considerable interest in metallurgy and have been extensively used in aerospace engineering and processing equipment. For instance, the Ti-based alloys are known for their high strength-to-weight ratio, good toughness, and corrosion resistance. Ti_3Au was reported [l] to absorb significant quantities of hydrogen. Ten years ago Jorda et al. [2], investigated at temperature of 775 K by means of X-ray powder diffraction, optical metallography, microhardness measurements and differential thermal analysis, the phase equilibria of the Ti-Au-Al ternary system. Later study, identified two ternary compounds, TiAuAl which melts congruently at 1453 K and $TiAu_2Al$ which forms by peritectic reaction at 1273 K. The sub-binary systems Al-Ti, Ti-Au, and Al-Au are reviewed and adopted from the previous assessments, the thermodynamic analysis of the Al-Ti-Au ternary system is performed by the CALPHAD approach, and a set of self-consistent thermodynamic parameters of the ternary system are obtained. Furthermore, the isothermal sections of this system at different temperatures and the ternary invariant equilibria are calculated and compared with the corresponding experimental data, and all are in good agreement with most of the experimental results. Thus, the optimized thermodynamic parameters in this study may provide more accurate guidance to develop the new alloys involving it.

Keywords: Thermodynamic assessment, Al-Ti-Au ternary system, Calphad method, phase diagram.

References

[1] E. A. Aitken, in J. H. Westbrook (ed.), Intermetallic Compounds, R. E. Krieger, Huntington, NY, (1977) 512.

[2] J. L. Jorda, J. Muller and H. F. Braun, Journal of the Less-Common Metals, 134 (1987) 99 -107.

Study of the interaction between water and the red stigmas of saffron *Crocuse Sativus L.*, : kinetics of process of drying under microwave irradiation

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Abstract:

Drying is defined as a process of moisture removal due to the simultaneous transfer of heat and mass. It is also a classic method of preserving food, the drying of stigmas red of Saffron *Crocuse satuvis., L* is performed under irradiation microwave technical is a more used in many industrial processes in order to optimize the consumption of energy in the drying process. This study also aims to study the influence of microwave power, which can impose a different microwave power ranging from 50 to 200 w on the kinetics of drying, the experiments were also carried out by varying the initial mass from 0.5 g until 2g for determining the influence of the initial mass on the drying kinetics, by fixing the microwave power on 200w. The analysis of the experimental data shows that the initial masses and the microwave power have an important effect on the drying kinetics of this spice, the comparative study of conventional drying and under microwave irradiation shows that the drying mechanism is depends on the technique used in drying of this spice.

Keyword: *Crocuse Satuvis,.L*, drying kinetics, rate constant, activation energy, the kinetic modelization

P 18

Biodiesel density: experimental measurements of ternary blends of ether, alcohol and hydrocarbon

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The increase in ecological pollution, as well as the unpredictable price of crude oil has led in recent years to a renewed importance for biofuels. As demand in the transport sector is consistently expanding and considering the advantages of biofuels, it is expected that market demand for biofuels will increase in the near future. In this specific situation, it will be interesting to study whether new types of biofuels that could be used in blend for other fuels in internal combustion engines.

Density measurement is very important to the biofuel as it impacts on the engine injection systems. The amount of fuel to the engine must be precisely adjusted to ensure complete combustion while reducing greenhouse gas emissions. In addition, the experimental densities of biodiesel at high pressure and high temperature is missing in the literature.

In this work, new density measurements ρ of dibutyl ether (1) + heptanol (2) + heptane (3) ternary mixtures were presented at various compositions and temperatures. In addition, the experimental density data were fitted with a Tait-like equation with low standard deviations.

Keywords: Dibutyl Ether, 1-Heptanol, Heptane, Density, High Pressure, PC-SAFT.

P 19

Study of clogging of the transport pipes of treated wastewater and sprinklers of Agadir Golf Ocean

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Abstract

In Agadir region, the reuse of treated wastewater for irrigation of green spaces has been hampered by the problem of scaling of the water passage circuits.

This study aims at identifying and characterizing these scale deposits of tartar formed in these pipes at the level of the sprinklers of the golf ocean of Agadir.

In this study, tartar samples were taken from various points in the treated wastewater transport pipes and sprinklers of Agadir Golf Ocean. The characterization of the different recovered tartar samples were performed by different analytical techniques such as: chemical analysis, X-ray fluorescence spectrometry analysis, thermal analysis, X-ray diffraction analysis and scanning electron microscopy.

The results of these various analyses revealed the presence of calcium carbonate mainly in the form of calcite variety and other chemical components such as: silicon, quartz, calcium silicate and phosphate calcium carbonate.

Keywords: Scaling, wastewater, irrigation, calcium carbonate, calcite variety, Ocean Golf of Agadir.

P 20

Abstract:

the interest of the phase diagrams in the Study of Structural hardening mechanisms of alloys Pb-Te , Pb-Te-Sn , Pb -Te -Ag For battery grids

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In order to meet the economic requirements of electrical energy storage lead-acid battery's, we undertook research to improve the mechanical strength of the battery grids

This work has therefore been devoted to the study of the mechanisms of hardening of binary alloys Pb0,003wt% Te; Pb0,005wt% Te; Pb0,0062wt%Te And the ternary alloys : (Pb0,005wt%Te 0,24wt%Sn , Pb0,005w%Te0,64wt%Sn , Pb 0,005wt%Te1,09wt%Sn) ; (Pb-0,005wt%Te 0002wt%Ag Pb 0,005wt%Te0,007wt%Ag).

The evolution of the quenched structure of each of these alloys to its equilibrium state was followed by various techniques: hardness, microhardness, optical microscopy, scanning electronic microscopy and microanalysis EDAX, two structural states are considered: raw casting alloys and rehomogenized. Temperatures are explored 20 ° and 80 ° C.

The aging of these alloys (Pb-Te, Pb-Te-Sn, Pb-Te-Ag) is characterized by a continuous and a discontinuous precipitation processing. Their over ageing is characterized respectively by such precipitates PbTe, $PbTe_x Sn_{1-x}$, and ((Pb,Te,Ag) , PbTe). Relating to the maximum hardness obtained is still low; it is about 7, 5 HV 10 HV and 7,75 HV respectively.

This study therefore concluded that the mechanical properties obtained are very small and probably will not get battery grids that require improved strength , electrochemical study is needed before a final decision in the battery industry grids.

Keywords: *battery, alloy grid, structural hardening, precipitation continues, discontinuous transformation*

Références :

[1] A.Aguizir ; thèse doctorat « Etude des mécanismes de durcissement structural des alliages Pb-Te,Pb-Te-Sn et Pb-Te-Ag pour les grilles de batterie » université ibn Zohr ; année 2013.

P 21

Thermodynamic assessment of the Scandium-Gold binary system

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Abstract

The phase diagram and thermodynamic properties of the Sc–Au system was carried out by means of the CALPHAD (Calculation of Phase Diagrams) method through Thermo–Calc software package on the basis of the experimental data of phase equilibria and thermodynamic proprieties from the published literature data. The excess Gibbs energies functions of the solution phases including liquid, face–centered cubic fcc_A1, body–centered hexagonal close–packed hcp_3 and cubic bcc_A2, modeled with Redlich–Kister polynomials functions. While all intermetallic compounds have been treated as stoichiometric compounds. The thermodynamic parameters describing various phases in the Sc–Au binary system were finally obtained, and a good agreement is achieved between the calculated results and the reported experimental data.

Sc–based alloys have been used as aero–structures materials [1] and Sc addition on wrought alloys has positive effects on weldability and welding properties [2]. The phase equilibria in the Sc–based alloys systems are of importance for design of new Sc–based alloys. Hence, the purpose of the present work is to assess the Sc–Au binary system for which the experimental phase diagram was reexamined by Palenzona et al. [3] and to develop a precise thermodynamic description by means of the calculation of phase diagram (CALPHAD) technique described and presented by [4, 5] and successfully applied in various computer programs in order to give a more complete and consistent description of the phases existing in the studied system and their stability. The thermodynamic optimization of the Sc–Au system is part of a research program, actually carried out in our laboratory, and it focuses on the study of the interaction between REEs and the noble metals.

Keywords: Phase diagram; Thermodynamic assessment; CALPHAD method; thermodynamic modeling

References

[1] J.T. Staley, J. Liu, W.T. Hunt Jr, Adv. Mater. Proc. 152 17(1997).
[2] S. Lathabai and P.G. Lloyd, Acta Mater. 50 (17) (2002) 4275–4292
[3] A. Palenzona and P. Manfrinetti, J. Alloys Compd. 257 (1) (1997) 224–226.
[4] L. Kaufman and H. Bernstein, Computer Calculation of Phase Diagrams, Academic Press, New York. 1970.
[5] I. Ansara, Int. Metals Rev. 24 (1) (1979) 20–53.

P 22

DEVELOPMENT AND VALIDATION OF A METHODE FOR DETERMINATION OF ANTIBIOTIC METRONIDAZOLE USING MODIFIED CARBON PAST ELECTROD BY SILVER

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Abstract

Metronidazole, 1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole (**Fig.1**) is the most important nitroimidazole derivative and is well-known for its anti-microbial properties. Because it is effective against anaerobic bacteria ,trichomonas ,amoeba and giardia ,nowadays it has been extensively used for the treatment of anaerobic bacterial diseases and protozoal diseases .However ,Metronidazole can be genotoxic and carcinogenic the accumulated dose of MTZ exceeds a 2g daily dosage in human beings 9-11 presenting with some toxic reactions like seizures peripheral neuropathy .Therefore it is important and necessary to develop a highly sensitive and rapid method for the determination and quantification of Metronidazole .

Methods for the assay of metronidazole are usually based on high performance liquid chromatographic (HPLC) and spectrophotometric techniques. For such applications, however, the analyses are time consuming and are of high cost. Therefore, the electro analytical methods are simple, economical and sensitive to reach lower detection limits. In this work, we report an efficient method for the electro-catalytic detection of metronidazole at carbon paste electrode modified with (Ag) using the electrochemical methods. The electrode modified with (Ag) were characterized by X-ray diffraction (XRD), scanning electron microscopy (MEB), and infrared spectroscopy (IR).Shows the formation of nanoparticles the silver. The best responses were obtained with cyclic voltammetry in phosphate buffer **(Fig .2)** as supporting electrolyte. The validation of the proposed method compared to HPLC as reference for Metronidazole detection was assessed.

Keys words: Silver, cyclic voltammetry, metronidazole, carbon paste electrode, medicament.

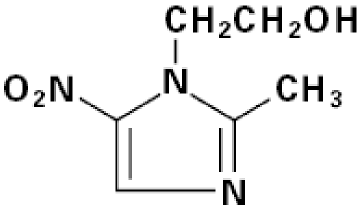

Fig .1 : Chemical Structure of Metronidazole

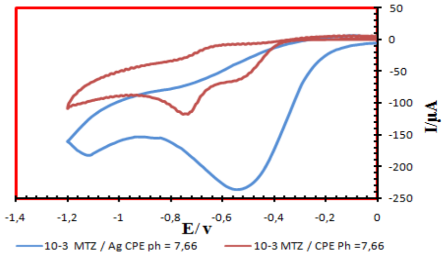

Fig .2: MTZ / CPE and MTZ /Ag CPE

Survey of thermal performances of a solar system used for the heating of agricultural greenhouse and the improvement of tomato production in Morocco

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The use of thermal solar energy for heating greenhouse in winter period, where climatic conditions are unfavorable for the plant, is an important issue. In this paper, the performance of a rock-bed heating system is analyzed and discussed in a conventional Canarian type greenhouse in Morocco. An experimental comparative study is conducted in two East-West orientated greenhouses for solving the problem of conventional greenhouses that are facing overheating problems during the day and excessive cold at night, and improving the quality and quantity of agricultural production. The geometry, building materials and date of planting are identical for studying the impact of the heating system on the temperature and humidity inside greenhouse, as well as their influence on the crop development. Results show that the temperature at night inside the greenhouse equipped with the rock-bed exceeds that of the control greenhouse by 2.6 °C. The relative humidity is found to be 10% lower at night inside the heated greenhouse. This improvement in the microclimate during night has a very positive impact on the quality of fruit and the yield increased by almost 29%.

P 25

Transforming Moroccan phosphogypsum into potassium sulfate and precipitated calcium carbonate (PCC)

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The world production of phosphogypsum, i.e: a by-product which is generated from phosphoric acid industry is evaluated at about 150 Mt per year. Faced with this environmental problem, management and storage of such quantities of phosphogypsum, it is necessary to propose new processes to valorize the by-product into valuable products.

In this study, we have used KOH to convert Moroccan phosphogypsum to K_2SO_4 and $CaCO_3$:

$$CaSO_4.2H_2O(s) + 2KOH(aq) \rightarrow Ca(OH)_2(s) + K_2SO_4(aq) + 2H_2O(l) \quad (1)$$

$$Ca(OH)_2(s) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l) \quad (2)$$

The potassium sulfate can be utilized as a fertilizer or in other mineral carbonation processes to produce K_2CO_3. The precipitated calcium carbonate (PCC) can be used in various industries: plastic, paper, adhesive, paints, …

In order to optimize the conversion of Moroccan PG in KOH solution, we have studied the influence of several parameters; the temperature, the volume of CO_2 injected, the KOH/PG ratio and the concentration of $Ca(OH)_2$ on the purity of the products formed and the conversion yield (%).

References

[1] A. Aagli, N. Tamer, A. Atbir, L. Boukbir, and M. El Hadek, J. Therm. Anal. Calorim., 82, pp. 395–399 (2005)

[2] C. Cárdenas-Escuderoa, V. Morales-Flórez, R. Pérez-Lópezc, A. Santose and L. Esquiviasa, J Hazard Mater 196, pp. 431–435 (2011).

Hydro-chemical characterization with a statistical approach of groundwater quality in EL MERK region, south-eastern Algeria

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Abstract

The objective of this work is to evaluate the quality of groundwater at EL MERK through the evaluation of the physicochemical characteristics of water and dissolved elements in order to determine their origins. The identifying of the structures of the variables and quantifying the water families by the analyzes of the individuals with a multidimensional statistical approach. The suitability of groundwater for irrigation and other uses was assessed by determining the sodium adsorption ratio, soluble-sodium percentage, total dis- solved solids and total hardness of water samples. This analysis indicated that the chemical composition of groundwater in the study area is of Cl–SO4–Mg–Ca mixed facies with concentrations of chemical constituents correspond known guideline values of W.H.O except the Na. Piper diagrams shows that there is no dominant cation neither no dominant anion. Geospatial mapping of hydro-chemical parameters analysed with Wilcox diagram show distinctive areas of irrigation suitability.62.5 % of samples fall in the suitable category and indicate that the study area is suitable for irrigation.

keywords : physicochemical, groundwater, EL MERK, dis- solved solids

References

[1] A. Sebei, T. Slama and M. A. Helali, Environ. Earth Sci **77**, 557 (2018).
[2] C. M. Bethke and T. M. Johnson, Annu. Rev. Earth Planet. Sci **36**, 121–152 (2008).
[3] C. Bakouan, B. Guel and A. Hantson, Afrique Sci **13**, 325–337 (2017).
[4] T. Subramani, L. Elango, and S. R. Damodarasamy, Environ. Geol **47**, 1099–1110 (2005).
[5] H. S. A. F Atta, A. W. M Amer, Water Sci **32**, 1–15 (2018).
[6] C. Sadashivaiah, C.R. Ramakrishnaiah,and G. Ranganna, India. Int. J. Environ. Res. Public Health **5**, 158–164 (2008).
[7] K.E. Ahoussi, Y.B. Koffi, A.M. Kouassi, G. Soro, and J. Biémi, J. Appl. Biosci **63**, 4703–4719 (2013).
[8] S. Kateb, K. Baouia, R. Zegaite and N. Mekhloufi, RJPBCS **9**, 43–51 (2018).
[9] N. Nasri, R. Bouhlila, M.W Saaltink and P. Gamazo, Appl. Geochemistry **55**, 160–169 (2015).
[10] A. Rezaei and H. Hassani, Environ. Geochem. Health **40**, 583–608 (2018).

P 27

Concentration and distribution of fluoride in Touggourt region (Algeria)

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Abstract:

Dental fluorosis is one of the most common health problems in North Africa, in South Algeria, we are witnessing a "silent" fluorosis among citizens, considering that under-ground water is the only source for drinking however, the concentration of fluorine ion exceeds the value allowed by the World Health Organization (**1,5 ppm**). For the temperate areas, dental fluorosis occurs when the concentration of fluoride in water exceeds 1.5 to 2 ppm. for this reason, we wish to present this work of definition and mapping of a fluorotic risk in the region of Touggourt in Ouargla ‘s county to identify the spots with highest concentration in fluoride.

The work will be done in two phases: first in the laboratory of the university Kasdi Merbah of Ouargla we determine the different concentration of samples taken from 13 under-ground water wells currently exploited, and compare the results obtained by the old results which the ADE (ALGERIENNE DES EAUX) got as it is shown in the following table:

Table: Results of Analysis (ADE).

APC	Number of drilling	Locality	Depth of Drilling	in Service	stopped	*max value of Fluor (ppm)*
Touggourt	1	F Sidi Mehdi 2 TGT	1799	x		0,75
	2	F Sidi Mehdi3	1760	x		0,67
	3	Complexe Sidi mehdi2			x	1,1
	4	F Ain Sahra		x		0,46
	5	Forage Secour Complexe	78	x		1,91
	6	F Bilair	85	x		0,84
	7	F- Sidi Slimane		x		0,72
	8	F Albien Sidi Slimane	1755	x		0,7
	9	F ONID Sidi Slimane				0,35
	10	Forage Beni Assoud TGT	95	x		1,17
	11	Forage Zaouia TGT	75		x	1,07

Then we use in the second phase Geographic Information System (GIS) to represent these percentages and concentration obtained.

Keywords: Fluoride, Water, Health, Fluorosis, South, Concentration.

References

[1] B. Forsman, Early supply of fluoride and enamel fluorosis, p 22-30 (1977).

[2] D. Marcel, Chimie des oxydants. Traitement des eaux, p 505 (1989).

[3] D. Raymond, le traitement des eaux, 2émé édition, p 231 – 235. (1990).

[4] N. Nasri, R. Bouhlila, M.W Saaltink and P. Gamazo, Appl. Geochemistry 55, 160–169 (2015).

[5] OMS, Critères d’hygiène de l’environnement 36, fluor et fluorures, Genève (1985).

[6] S. Acharya, Dental caries, 55: 359 - 364 (2005).

[7] S. Kateb, K. Baouia, R. Zegaite and N. Mekhloufi, RJPBCS 9, 43–51 (2018).

P 28

Di-hydrofolate reductase inhibitors: can 2,4-diaminopyrimidine be a model for co-crystal screening?

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Pharmaceutical co-crystals are multicomponent solids made up of an API and of one or more co-formers, joined together in a stoichiometric ratio in a new crystalline structure. The co-crystal components, all solid when pure at ambient conditions, are most commonly linked by hydrogen bond interactions, in supramolecular synthons [1,2].

Dihydrofolate reductase (DHFR) inhibitors, such as trimethoprim, Figure 1.a, and pyrimethamine, Figure 1.b, share a common 2,4-diaminopyrimide (24DAPM) core structure, Figure 1.c [3]. In a co-crystallization experiment, it is interesting to investigate if 24DAPM can be a good a model for DHFR co-crystal screening: the same type of supramolecular synthons is expected for DHFR inhibitors and for 24DAMP, although the molecular complexity of the formers may also play a role in the co-crystallization trial outcome.

In order to get insight on these effects, in this work results are presented and discussed for the ongoing investigation of co-crystallization of trimethoprim, of pyrimethamine and of the core fragment 24DAPM with two types of co-formers, capable of giving rise to different supramolecular heterosynthons with the target molecules: the two xanthines, theophylline and caffeine, and the three isomeric pyridinecarboxamides, picolinamide, nicotinamide and isonicotinamide, Figure 1.

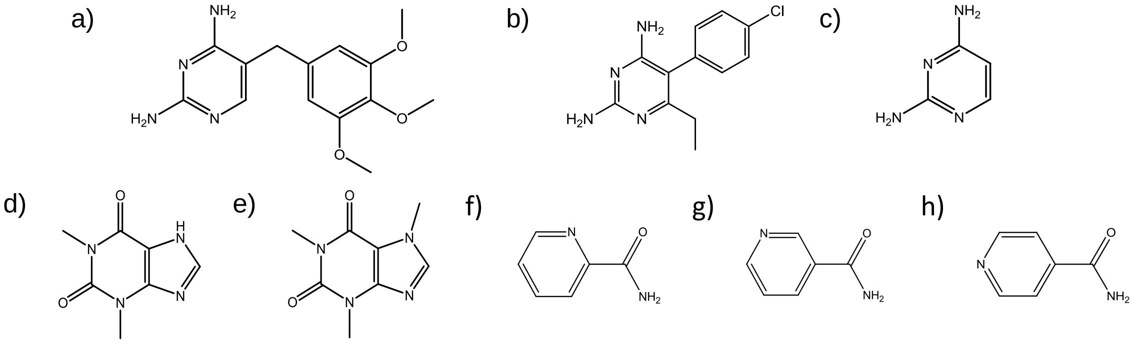

Figure 1. Molecular structures: a) trimethoprim, b) pyrimethamine, c) 2,4-diaminopyrimidine, d) theophylline, e) caffeine, f) picolinamide, g) nicotinamide, h) isonicotinamide.

References

[1] N. Duggirala, M. L. Perry, O. Almarsson and M. J. Zaworotko, Chemical Communications **52**, 640 (2016).
[2] E. Grothe, H. Meekes, E. Vlieg, J.H. ter Horst and R. de Gelder, Crystal Growth & Design **16**, 3237 (2016).
[3] R. G. Nelson and A. Rosoesky, Antimicrobial Agents and Chemotherapy **45**, 3293 (2001).

P 29

Investigation on solid forms of iguratimod: co-crystals and polymorphs

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Iguratimod (IGU), developed in Japan, is a novel methane sulfonamide derivative, a disease-modifying anti-rheumatic drug with anti-inflammatory action. It was recommended for the treatment of rheumatoid arthritis at the 2012 European League Against Rheumatism meeting and in the 2014 Asia Pacific League of Associations for Rheumatology guideline, and is currently approved for treatment of rheumatoid arthritis in Japan and China [1]. Iguratimod has poor aqueous solubility and co-crystals offer potential advantages in terms of improving the solubility and dissolution rate of APIs.

In this work, cocrystallization of iguratimod with pyridinecarboxamide isomers was investigated. Cocrystallization was successfully undertaken with nicotinamide (NIC) and picolinamide and not with isonicotinamide, which is not typical. The synthesis was achieved by liquid assisted grinding and the solids obtained were characterized by differential scanning calorimetry, infrared spectroscopy, powder X-ray diffraction, single crystal X-ray diffraction and polarized light thermomicroscopy.

The crystalline structure of the iguratimod:nicotinamide (1:1) co-crystal was solved. Single crystal X-ray diffraction data reveal the presence of iguratimod dimers linked by the sulfonamide groups, as well as nicotinamide dimers where the amide···amide homosynthon present in one of the metastable nicotinamide polymorphs is observed [2]. Both dimers are linked together by $\mathrm{N\text{-}H_{NIC}\cdots O{=}C_{IGU}}$ amide···amide supramolecular synthon. The aromatic nitrogen in nicotinamide is not involved in intermolecular interactions. This co-crystal can be of particular relevance as nicotinamide, a water-soluble vitamin and a member of the vitamin B group, has been shown to enhance the solubility of many poorly water soluble drugs through cocrystallization [3,4].

Additionally, in order to supplement the lack of literature information, an investigation on the polymorphism of iguratimod was also carried out.

References

[1] T. Mimori, M. Harigai, T. Atsumi, T. Fujii, M. Kuwana, H. Matsuno, S. Momohara, S. Takei, N. Tamura, Y. Takasaki, S. Ikeuchi, S. Kushimoto and T. Koike, Modern Rheumatology **27**, 755 (2017).
[2] J. Li, S. A. Bourne and M. R. Caira, Chemical Communications **47**, 1530 (2011).
[3] X. Sun, Q. Yin, S. Ding, Z. Shen, Y. Bao, J. Gong, B. Hou, H. Hao, Y. Wang, J. Wang and C. Xie, Journal of Chemical Thermodynamics **85**, 171 (2015).
[4] P. Sanphui, V. K. Dev, D. Clara, N. Malviya, S. Ganguly and G. R. Desiraju, Molecular Pharmaceutics **12**, 1615 (2015).

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Integration of photovoltaic energy and food production systems for the Mediterranean countries

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Abstract

Photovoltaic energy has been particularly successful in many domestic and industrial settings where opaque photovoltaic covered roofs provide renewable electricity. Modern farming, for an ever growing population, employs vast areas of greenhouses consuming considerable amounts of energy. Photovoltaic is one of the cleanest sources of alternative energy. Due to high energy demand in one hand and environmental negative impact of fossil fuels, on the other hand many countries consider the alternative energy sources as a suitable and feasible option in industry and domestic usage.

The use of photovoltaic energy for greenhouse environment control to replace or reduce the consumption of fuel and power-line electricity is an important objective for sustainable greenhouse crop production. The photovoltaic greenhouse is a new technology for a double use of the resource land, because it generates energy in the form of biomass (crops, or flowers…) and, also, electric energy.

The goal of our research is to study the microclimate inside a Canarian greenhouse, 40% of their roof were occupied by photovoltaic panels. The results show that the shading provides by the photovoltaic panels has a little effect on the microclimatic variables inside a photovoltaic greenhouse.

Keywords: photovoltaic panels, greenhouse, microclimate, tomato plants, yield.

P 31

On the Dimorphism and the Pressure-Temperature State Diagram of Gestodene, a Steroidal Progestogen Contraceptive

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The pressure-temperature phase diagram of the dimorphism of contraceptive drug gestodene [1] is constructed using the temperature and enthalpy of fusion of form I (469.5 K, 107 J g^{-1}), and those of the endothermic transition from form II to form I (311 K, 8.52 J g^{-1}). At ordinary pressure, the sign of the enthalpy of this transition indicates that these polymorphs are enantiotropically related and that form II, whose melting temperature is calculated to be about 452 K, is the stable form at room temperature. Taking into account the inequality in the specific volumes, it is shown that the two forms remain enantiotropically related on increasing the pressure since the slope dP/dT of the I-II equilibrium line is found to be negative while that of the I-liquid equilibrium is positive as usual.

In addition, it is also shown that the heats of dissolution, inferred from solubility measurements, lead to virtually the same value of the heat of transition from II to I as differential scanning calorimetry measurements [2].

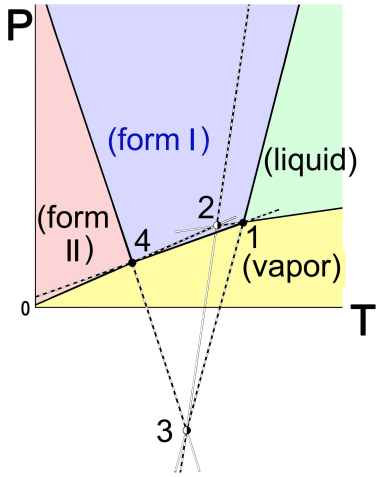

Figure 1. Topological P,T diagram for the dimorphism of gestodene. 1= stable I-liq-vap, 2 = metastable II-liq-vap, 3= metastable I-II-liq, 4 = stable I-II-vap.

References
[1] F.Z. Stanczyk, D.F. Archer. Contraception **89, 187** (2014).
[2] L. Zhu, L-Y. Wang, Z.L. Sha, Y.F. Wang, L.B. Yang, X.C. Li, X.Y. Zhao, W. Du. Cryst Growth Des **17, 4582** (2017).

P 32

Interactive software for modelling of binary or ternary salt - water phase diagrams.

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Abstract

Programming is a necessary step for modelling and critical evaluation of data, especially since the exploitation of diagrams must be computer-assisted.

The modelling programs, which we have written, are specially designed and adapted to binary or ternary salt-water phase diagrams. They are used to describe solubility surfaces of the polythermal ternary phase diagram type water-salt phase, as long as they involve stoichiometric phases anhydrous or hydrates.

Several models exist in the literature, including that of Pitzer [1], which is based on the calculation of ionic interaction parameters in solution. The binary calculations are based on semi-empirical equations [2]. The model used is that proposed by R. Cohen-Adad et al. [3], which can be adapted to binary, and higher order systems. The chosen model is well adapted to calculations of these solubility surfaces and gives very good results.

The binary model program is used to calculate binary diagrams, Ternary model written under the Windows environment models ternary diagrams. The choice of this environment is made for writing a software easy to use and control in an intuitive way.

The program is independent of the experimental data. Several modules make up the program: data module (system, compositions, solubility, temperature, nature of phases, precision, references) [4], isotherm module, field module and exploitation module. The graphical interface can set several parameters: the type of coordinates (molar, mass or Jänecke), the type of the graphical representation (right triangle, equilateral or representation of Jänecke)... The exploitation of the results of the modelling makes it possible to compute and display the monovariant lines, to determine the temperatures or the coordinates of the liquidus.

The programs are constantly updated and new releases programs will emerge with other features as needed.

References

[1] K. S. Pitzer, J. Phys., Chem., **77**, 268 (1973)

[2] R. Tenu and J. J. Counioux, J. Chem. Phys., **78**[10], 823 (1981)

[3] R. Cohen-Adad, M. Th. Cohen-Adad, R. Ouäni, F. Getzen, J. Chim. Phys., **87**, 1441(1990)

[4] R. Cohen-Adad, J. W. Lorimer, S. L. Phillips, M. Salomon, J. Chem. Info. Comp. Sci., **35**, 675 (1995)

P 33

The new description of the Bi-Cu-I ternary phase diagram

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In this work, we give a new description of the ternary phase diagram Bi-Cu-I. We have tried to give more precision on the extent of the different three-phase domains and the different existing ternary equilibria.

The methods used in the study of this ternary are: differential thermal analysis, X-ray diffraction and metallography.

Two intermediate known compounds Cu_2BiI_5 and $CuBiI_4$ that undergo peritectic decomposition are observed. Nine ternary invariants points are found: three eutectics, two peritectics, three transitory peritectics, and one metatectics. A large ternary liquid-liquid miscibility gap originating from the BiI_3-Bi binary was demonstrated with a maximum C_M at 897 ° C.

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Compatibility study between acebutolol and excipients

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Introduction: The study of compatibility of active pharmaceutical ingredient (API) with excipient is an important stage in the development of pharmaceutical dosage forms. Although excipients are pharmacologically inert, they can interact with API.The aim of the present study was to evaluate physical and chemical interactions between acebutolol and some excipients (magnesium stearate (MagSte), polyvinulpyrrolidone (PVP), microcrystalline cellulose (MCC), Acid ascorbic (AS), Acid citric (AC) and butylated hydroxyanisole (BHA)) in solid binary mixtures.

Material and methods: Binary mixtures of Acebutolol and excipients were prepared (1:1). Differential scanning calorimetry analysis (DSC) was used as screening technique for assessing the compatibility between API and pharmaceutical excipients. Fourier transform infrared spectroscopy (FT-IR), HPLC and X Ray powder diffraction (XRD) were used as complementary techniques to implement and assist in interpretation of the DSC results.The influence of storage at relative humidity of 75% (21 days) on physico-chemical stability on binary mixture was also evaluated.

Results: Mixtures whose DSC thermograms showed a slight shift of the melting peak compared to acebutolol alone, were considered as compatible. On the basis of DSC results, a strong interaction was found between acebutolol and PVP and antioxidant (AC and AS). Theseinteractions were confirmed by HPLC which revealed a degradation of acebutolol.FT-IR was able to identify the bonds C = O and NH, as being the most concerned by the establishment of hydrogenbonds between components.The endothermic peak change and the enthalpy value decrease observed in DSC curves could be explained, by XRD result, with the amorphizing effect of the excipients on the crystalline active ingredient.

Conclusion: Thecorroborative results of calorimetric, spectrometric and chromatographic analysiscould offer a scientific support to a drug formulator in his strategy of developing finished products.

[1] SBharate., B Sandipand N.Bajaj, Journal of Excipients and Food Chemicals 1, 3-26 (2010).
[2] F.Ali,R. Kumar, P. Sahu and G. Singh, J. Therm. Anal. Cal**130**, 1627-1641 (2017).

Impact of thermal treatment on the physicochemical properties of a natural material (diatomite)

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Abstract

The aim of this study was to characterize a natural diatomite before and after modification through heating treatment. The diatomite was collected in Tighza deposit, in the northeastern region of Morocco. The considered material was submitted to heating treatment at three different temperatures: 550, 750 and 950°C, in order to assess the inherent modifications. The characterization of all materials (raw and calcined) was performed by a whole series of analysis: *e.g.* X-ray diffraction, FTIR, , thermogravimetric analysis (TGA), SEM, Brunauer-Emmett-Teller (BET) surface area techniques, confirms the general diatomaceous earth character of the collected sample. The study showed different behavior according to the considered material. Furthermore, the effectiveness of calcination on improving diatomite properties, as well as to choose the best range of heating treatment for such an enhancement.

Keywords: diatomite, thermal treatment, characterization

Compatibility studies between pilocarpine and three excipients

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Introduction: Preformulation studies are a crucial step in the development of stable and effective solid dosage forms. Considered as pharmacologically inert, excipients are used to optimize the release and bioavailability of a drug substance. However, physicochemical interactions with a drug substance may occur and affect dramatically the quality and the stability of drugs. The present work aimed to evaluate physical and chemical interactions between pilocarpine (PIL) and three excipients namely microcrystalline cellulose (MCC), magnesium stearate (MgSte) and crospovidone (CRO).

Methods: Interactions between the drug substance and excipients were screened both in the solid and in aqueous state. Binary mixtures of PIL and excipients were prepared in at least two ratios 50:50 and 5:95 (% *w/w*). Solid mixtures and aqueous suspensions were exposed to a high temperature in sealed glass (60°C). The main experimental methods were HPLC and DSC.

Results: For mixtures containing MCC and CRO, no physical interactions have been observed. Chromatographic analysis showed a chemical stability of PIL in presence of both excipients. The DSC showed a significant shifting of the melting peak of PIL in the binary mixture containing MgSte. Chromatographic analysis showed a significant degradation of PIL which grows proportionally with the amount of MgSte in the mixtures.

Conclusion: The results demonstrate the absence of significant interaction between PIL and the two excipients MCC and CRO under the experimental conditions.The results suggest a stabilizing effect of these excipients. A chemical incompatibility with MgSte has been confirmed.

References

[1] F. Nishath, M. Tirunagari, K. Husna, A. Nandagopal and R. Jangala, Journal of Applied Pharmaceutical Science **01**, 66-71 (2011).
[2] T. Bogdan, J. Tunde and T. Dumitru, J. Therm. Anal. Cal **113**, 291-299 (2013).

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Physicochemical stability of atorvastatin amorphous dispersion in PVP

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Introduction : Solubility of the oral form is one of the major challenges for the pharmaceutical industry. Today, 60-70% of new chemicals discovered are poorly soluble, leading to low bioavailability and therapeutic inefficiency. The dispersion of an active substance in a polymer is increasingly used to improve its solubility. However, monitoring the thermal and structural stability of such a formulation is a crucial step to ensure the chemical integrity of the active molecule during pharmaceutical development.

Material and methods: In this work, we proceeded to the formulation of amorphous solid dispersion of atorvastatin (ATR) in polyvinylpyrrolidone (PVP) with respective compositions of 10, 25 and 50% PVP. For this purpose, a planetary Ball Mills was used to grinding ATR and PVP. The main experimental methods used to characterize the amorphous formulations obtained were DSC, FTIR, XRD and proton NMR.

Results: The DSC showed a significant shifting of the melting peak of ATR which grows proportionally with the amount of PVP in the mixtures. The proportion of PVP of 10% was sufficient to fully amorphize the ATR and inhibits its devitrification in the presence of moisture (HR = 90% for 1 month). On the other hand, it has been found that the dispersion of ATR (50% PVP) exposed under moisture leads to the formation of a new amorphous and hydrated form. This was confirmed by FTIR and proton NMR.

Conclusion: Despite the establishment of hydrogen bonding that is formed between the ATR and PVP preventing the drug re-crystallization, the solid dispersion containing 50% PVP (w/w) undergoes a phase separation following exposure to moisture at increasing relative humidity. In order to design a more physically stable SD, it is important to consider the interplay between PVP proportions, % humidity and storage duration.

Reference

[1] J Patel, D. Rathod, N. Patel and M. Modasiya, Int. J. of Pharm. & Life Sci. **3**, 1459-1469 (2012).
[2] Y. Huang, W. Dai, Acta Pharmaceutica Sinica B **4**, 18-25 (2014).

P 38

Characterization of scale deposits formed on the surface of reverse osmosis membranes

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Reverse osmosis is the process used in desalination plants, it requires only electrical energy, has low specific energy consumption, and can be associated with renewable energy sources such as wind and photovoltaics. The water contains several suspended ions intended to cross the reverse osmosis membranes and as concentrations increase, these ions precipitate as salts. Consequently, this membrane process is limited in concentration factor due to the osmotic pressure of seawater, which increases with salt concentration.

The city of Tan Tan is supplied with drinking water by the brackish water demineralization plant. This station, located in the north of the city, commissioned in 2003, based on reverse osmosis technology, has a production capacity of 1700 m^3 per day. The identification of a new method for controlling salt precipitation in membranes requires the characterization of the tartars formed.

In this study, tartar was collected from several reverse osmosis membranes and at different locations on these membranes. The characterization of the various recovered scale samples was performed by X-ray diffraction (XRD), thermogravimetric analysis (ATG) and differential thermal analysis (ATD). The results obtained showed that the different limestone samples taken are of different natures and show in all cases the presence of calcium carbonate.

Keywords: Scale, Reverse osmosis, thermal analysis, desalination.

P 39

Thermal and mechanical properties of plaster mixed with polystyrene for building thermal insulation.

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Abstract

Recently, thermal building insulation has become one of the most challenging issues that face the humanity. Growing concern has required buildings to become significantly more energy efficient. One of the main ways of achieving this aim is through the use of innovative materials to improve the thermal building insulation. In this prospect, this work dscribes the use of Polystyrene (PS) additive, in composites of hemihydrated calcium sulfate (Plaster) to improve the thermal efficiency of buildings. Prismatic pieces prepared by mixing the calcium sulphate with different amount of polysterene.

To check the microstructure transformations the x-ray diffraction and scan-ning electron microscopy were used. The thermal proprieties (thermal conductivity, thermal diffusivity, thermal effusivity and specific heat) as well as the mechanical pro-prieties (the flexural strength, the compressive strength, and Young's modulus) were experimentally determined and analyzed according to the chemical composition of the resulting composite. Results show that the addition of polystyrene with different amount and strongly influence the thermophysical and mechanical properties. Compared to the standard properties of plaster, the inclusion of polystyrene in the composition shows a significant improvement in thermal properties with a slight reduction in strength although this was compensated by a high level of flexibility and thoutness. Consequently, an innovative composite polystyrene-plaster material has prepared with better thermal performance and can contribute to improving the thermal comfort of buildings.

Keywords:
Thermal properties, Mechanical properties, Polystyrene, Composite and building materials.

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Synthesis of $CoFe_2O_4$ thin films by pulsed-electrodeposition technique

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Abstract:

In the present work, cobalt ferrite thin films were synthesized using electrodeposition technique in pulsed mode onto (FTO) substrate. The co-deposition of Co-Fe alloy films was performed in an aqueous bath by applying potentials alternating between −1 V and -1.2 V. The numbers of applied cycles are 4 to 20 cycles. Then, an annealing treatment in air at 500 °C for 24 h of the film leads to the oxidization and crystallization of the films toward the $CoFe_2O_4$ spinel ferrite phase. Their structural, morphological, chemical compositions and optical properties were investigated by X-ray diffraction, Scanning electron microscope (SEM), Energy dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FTIR), and UV-Visible measurements, respectively.

References

[1] A. Lisfi, C. M. Williams, L. T. Nguyen, J. C. Lodder, A. Coleman, H. Corcoran, A. Johnson, P. Chang, A. Kumar, and W. Morgan, PHYSICAL REVIEW **B 76**, 054405 (2007).

[2] Zhen He, Jakub A. Koza, Guojun Mu, Andrew S. Miller, Eric W. Bohannan, and Jay A. Switzer, Chem. Mater, **25 (2)**, 223–232 (2013)

P 42

Solid-liquid equilibria of the Binary system ($Mn(NO_3)_2 + H_2O$) and the ternary system ($Mn(NO_3)_2 + Co(NO_3)_2 + H_2O$) at -15 °C

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Abstract

Nanostructured Cobalt-Manganese oxides have attracted great attention due to their many applications in the industry [1,2]. To synthesis this nanostructure materials, several methods have been suggested like co-precipitation [3], sol–gel methods [4], polymers [5], hydrothermal method [6], spray pyrolysis [7], and so on. However, in this work, we studied the possibility of synthesizing precursors from corresponding metal salts using the phase equilibrium method.

Moreover, this method, under controlled conditions, is convenient for the rapid and accurate delimitation of the stability limits of each phase in the water-salts systems. Therefore, the study of solid-liquid equilibria between Mn(NO3)2 and Co(NO3)2 in water is an attractive route for the synthesis of corresponding metal oxides.

The solid-liquid equilibria of the binary system ($Mn(NO_3)_2 + H_2O$) from -36 °C to 35 °C and the ternary system ($Mn(NO_3)_2 + Co(NO_3)_2 + H_2O$) at -15 °C were studied under air pressure using a synthetic method based on conductivity measurements. The characterization of solid phases formed in the two isotherms of the ternary system was conducted using chemical analysis, atomic absorption spectroscopy (AAS), X-ray diffraction (XRD) and was confirmed by Schreinemaker's method of wet residue and the 'ensembles' method.

Keywords: Solid-liquid equilibria; Phase diagram; Conductivity method; Solubility; Manganese Nitrate; Cobalt Nitrate.

References

[1] A. Rousset, R. Legros, A. Lagrange, Recent progress in the fabrication of ceramic negative temperature coefficient thermistors, J. Eur. Ceram. Soc. 13 (1994) 185–195.

[2] H. Abdoli, P. Alizadeh, Electrophoretic deposition of (Mn,Co)3O4 spinel nano powder on SOFC metallic interconnects, Mater. Lett. 80 (2012) 53–55.

[3] H. Bordeneuve, S. Guillemet-Fritsch, A. Rousset, S. Schuurman, V. Poulain, Structure and electrical properties of single-phase cobalt manganese oxide spinels Mn3−xCoxO4 sintered classically and by spark plasma sintering (SPS), J. Solid State Chem. 182 (2009) 396–401.

[4] H. Arabi, F. Ganjali, Structural and magnetic properties of cobalt and manganese doped Ni-ferrite nanoparticles, J. Supercond. Nov. Magn. 26 (2013) 1031–1035.

[5] F.M.M. Borges, D.M.A. Melo, M.S.A. Câmara, A.E. Martinelli, J.M. Soares, J.H. de Araújo, F.A.O. Cabral, Magnetic behavior of nanocrystalline MnCo2O4 spinels, J. Magn. Magn. Mater. 302 (2006) 273–277.

[6] L. Li, Y. Zhang, F. Shi, Y. Zhang, J. Zhang, C. Gu, X. Wang, J. Tu, Spinel manganese-nickel-cobalt ternary oxide nanowire array for high-performance electrochemical capacitor applications, ACS Appl. Mater. Interfaces. 6 (2014) 18040–18047.

[7] A. Restovic, E. Rios, S. Barbato, J. Ortiz, J.L. Gautier, Oxygen reduction in alkaline medium at thin MnxCo3-xO4(0≤x≤1) spinel films prepared by spray pyrolysis. Effect of oxide cation composition on the reaction kinetics, J. Electroanal. Chem. 522 (2002) 141–151.

P 43

The water quality after remineralization by limestone bed in the Daoura's plant

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Abstract

The quality and the rarity of water resources have a significant impact on the socio-economic sectors in the Morocco's southern provinces. Desalination of sea water and brackish water is an alternative solution in these arid zones. As In the sothern of Morocco (zone arid), the National Office of Electricity and Drinking Water (ONEE) has installed many plants of desalination. However the produced water after desalination (osmosis water) is unbalanced and has an aggressive character. Therefore, a post-treatment of remineralization is necessary to return to water its calco-carbonic balance and to protect the distribution network from corrosion degradation. There are many techniques of remineralization of osmosis water [1,2]. Following results on bed remineralization within Daoura station [3], this article tries to valorize this technique by examination the effect of many parameters on water quality in the scale of laboratory by using a bed of calcite pilot. We examined the effect of water debit, the residence time E.B.C.T (Empty Bed Contact Time), the upward speed and bed length on the parameters of treated water. The knowledge and the control of these parameters on laboratory scale are indeed essential for the conception (design) of a process of optimal remineralization. With the results of this study as well as other economic considerations, it would be possible to optimize the choice of the conditions needed for remineralization operation through calcite bed to minimize its costs of sizing and extrapolation in the industrial scale.

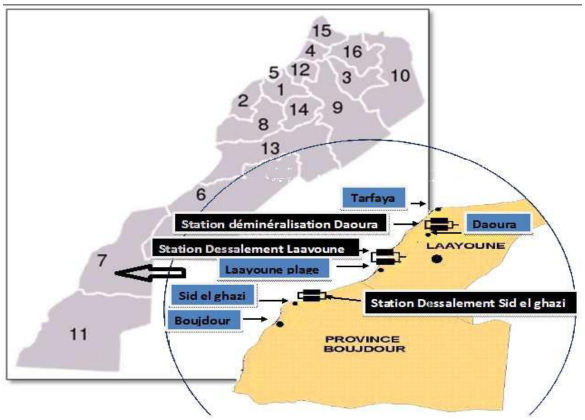

Figure 1. Geographic location of installed seawater desalination plants

References

1. A. Withers, Options for Recarbonation, Desalination, 179, 11-24 (2005).
2. J. C. Gude, J. F. Schoonenberg Kegel, W. J. C. Van De Ven, P. J. De Moel, J. Q. J. CVerberk and J. C. Van Dijk, J. Water Supply: Research and Technology – AQUA , 60, 469-477 (2011).
3. M.G. Biyoune, A. Atbir, E. Mongach, H. Bari, A. Khadir, L. Hassnaoui, L. Boukbir, M. Elhadek, , J. Mater. Environ. Sci. 6 (5) , 1243 – 1252, (2015)

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One step electrodeposition and Characterization of $CuSbSe_2$ Thin Films for PV applications

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Abstract

CuSbSe2 belongs to the Copper antimony chalcogenides CuSbCh2(ch=S,Se). An emerging family of absorbers studied for thin-film solar cells. It could be an alternative of CuInSe, whose manufacture is quite expensive, and kesterite, whose synthesis is quite problematic. CuSbSe2 thin films have been prepared by one-step electrodeposition followed by the annealing process in tubular furnace at 300°C for 5min under N2 atmosphere. The reduction potentials region was determine by cyclic voltametry and linear sweep voltametry. Then the samples have been elaborated by chronoamperomery at different potentials during 1h. The structural, morphological and optical properties of CuSbSe2 thin films were studied by X-ray diffraction, SEM and spectrophotometer respectively.

Key words: $CuSbSE_2$, electrodeposition, Characterization

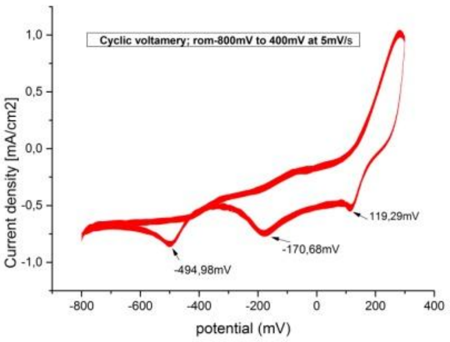

Figure1: Cyclic voltammetry curve: scanning from -0.8V to 0.4V (vs.SCE)

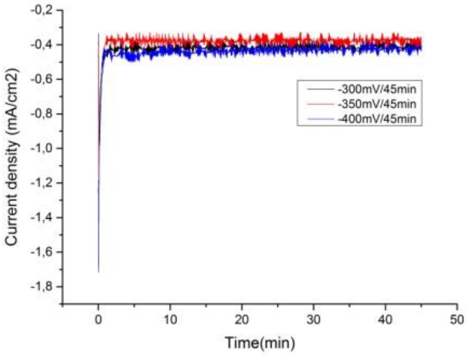

Figure2: Chronoamperomtry curves of CuSbSe2 thin films deposited at -0.3V,-0.35V and -0.4V/1h

References

[1] Ding Tang et al , Electrochemical and Solid-State Letters, 15(2) D11-D13 (2012)

[2]Ding tTang et al, Electrochimica Acta 76 (2012) 480–486

[3] F. W. de Souza Lucas, APL MATERIALS 6, 084501 (2018)

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Effect of applied potential on the properties of electrochemically prepared Cu_2O thin films

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In this work, we report on the synthesis of Cu_2O thin films by electrodeposition technique. The obtained thin films were analyzed by X-ray diffraction (XRD), scanning electron microscope (SEM) and UV-VIS measurements. The density functional theory using the plane-wave-self-consistent field (PWSCF) was carried out for Cu_2O to determine some of their electronic properties. The as-electrodeposited films at different potential are well crystallized in cubic structure, with <111> as preferential orientation and with lattice parameter a= 4.26 Å. Scanning electron microscope (SEM) images explored significant variation on morphology of Cu_2O thin films. The transmittance of Cu_2O films reveals that they have high optical transmission (> 70%) and the energy band gap on the order of 2.23 eV. Theoretical analyses show that Cu_2O have a direct band gap with value 2.01 eV, which is consistent with the experimental results.

Keywords: Cu_2O thin film, Electrodeposition, Structural property, DFT

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Thermodynamic description of the Gadolinium-Cadmium phase diagram

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Abstract

The thermodynamic optimization of the Gd-Cd binary system was carried out with the help of CALPHAD (CALculation of PHAse Diagram) method., $GdCd_3$, $Gd_{13}Cd_{58}$ and $GdCd_8$ have been treated as stoichiometric compounds while a solution model has been used for the description of the liquid, HCP_A3 (αGd), BCC_A2 (βGd) and HCP_A3 (Cd) phases. The intermetallic compounds GdCd, α-$GdCd_2$, β-$GdCd_2$, $Gd_{11}Cd_{45}$ and $GdCd_6$, which have homogeneity ranges, were treated by a two-Sublattice model. The calculations based on the thermodynamic modeling are in a good agreement with the phase diagram data and experimental thermodynamic values.

Keywords:
Gd-Cd system, Phase diagram, CALPHAD method, Redlich–Kister equation.

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Integration of solar technology into agricultural greenhouses

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A greenhouse is a structure with transparent walls, allowing plants to be grown in a warmer or better controlled environment than outside [1]. Culture can be made in the original soil or soilless, hydroponics, in pots or rock wool bags. A greenhouse is intended to protect plants against climatic hazards and to promote the growth of crops by creating climatic conditions more favorable than outside. Heating is required during winter periods to maintain the air temperature and humidity inside greenhouse in the optimum range for the good growth of the plantation [2]. To heat the greenhouse we need to install heating systems that we will generate the heat required to increase the temperature of the greenhouses to the optimal temperature, These systems consume a lot of energy [3].

Increasing fossil fuel prices and their adverse effects on the environment and human health have forced farmers and researchers in this field to use alternative heating sources. Renewable energies are the most promising sources, especially solar energy [4-6].

The most economical and efficient process to heat the greenhouse is to store excess heat during the day to use it to heat the greenhouse overnight. Usually, this storage is done in water, air or rocks tanks distributed in the greenhouse. The use of rocks for thermal storage offers advantages such as non-toxic, non-flammable and inexpensive [7- 9]. Many heating systems has been studied and developed by many researchers in the world but the majority of these systems are too expensive and difficult to achieve.

In order to keep the optimum growing environment in greenhouse, two greenhouses are constructed and installed in the MELK Zhar, Experimental center of Regional Centre of Agricultural Research of Agadir (INRA). The first is equipped with rock-bed heating system, and the second one devoid of a heating system erected for control purposes.

In this work we have studied the effect of a greenhouse heating system by a tank filled rocks placed on the ground of the greenhouse, during the day these rocks store the heat coming from the air of the greenhouse and release it into the air inside the greenhouse overnight to increase its temperature.

References

[1]. N.L. Panwar, S.C. Kaushik, S. Kothari, Renew Sustain Energy Rev. 15 (2011) 3934.
[2]. J. Xu, Li Y., Wang R.Z., Liu W. Energy 67 (2014) 63.
[3]. M. Lazâar, Kooli S., Hazami M., Farhat A., Belghith A., Desalination. 168 (2004) 391.
[4]. C. Von zabeltitz, Energy in Agriculture, 5 (1986) 111.
[5]. M. Kıyan, Bingöl E., Melikoglu M., Albostan A., Energy Convers Manage. 72 (2013) 147.
[6]. V.P. Sethi, Sharma SK., Energy 32 (2007) 1414.
[7]. V.P. Sethi, Sharma S.K., Sol Energy. 82 (2008) 832
[8]. H. Singh, Saini R.P, Saini J.S., Renew Sustain Energy Rev. 14 (2010) 1059.
[9]. D.L. Zhao, Li Y., Dai Y.J., Wang R.Z., Energy Convers Manage. 52 (2011) 2392.

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Application of jujube shell extract as green and effective corrosion inhibitor for copper in acidic medium

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Abstract

Natural Jujube shell extract (JSE) has been used as a copper corrosion inhibitor in hydrochloric medium 1M. This study was conducted by weight loss, polarization curves and electrochemical impedance spectroscopy (EIS) measurements. Scanning electron microscopy (SEM), energy dispersive X-ray spectrometry (EDS) and atomic force microscopy (AFM) studies were used to characterize the surface of uninhibited and inhibited copper specimens. The inhibition efficiency tends to increase by increasing the inhibitor concentration. The values of inhibitor efficiency estimated by different electrochemical and gravimetric methods indicate the performance of copper in HCl medium containing JSE. The obtained results indicate that JSE can be act as a good green corrosion inhibitor for copper in 1M HCl.

Keywords:
Corrosion; Inhibition; Copper; Green chemistry; Zizyphus Lotus; jujube shell.

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