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Solid-liquid phase diagrams in ternary mixtures of 1-chlorobutane + heptane + benzene : experimental data and prediction with DISQUAC model

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Solid liquid phase diagram was determined for ternary system of 1-chlorobutane with benzene and heptane. The three related binary systems were also measured. Ability of DISQUAC [1] model is here checked to predict ternary and binary experimental data.

Adaptive model-based control of fruit ripening processes

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Rising competition on the consumer market forces the food industry to improve production processes. To fulfill the increasing demands and to generate a cheap and homogeneous product, a model-based automation strategy for the banana ripening process is being developed. The automated process control comprises an assurance and improvement of product quality. Energy and personal costs can be reduced with the help of a uniform way of controlling the process.

The approach in the work presented here was to gather process understanding in a quantitative system analysis and the state of the art in an extensive technology analysis. The industrial ripening process is reproduced in a pilot plant, an experimental banana ripening box. Experiments in this box are used to search for a good indicator for the state of ripening. Plant parameters and significant process values must be assigned. Based on on-line measured values the actual state of the process will be estimated. Furthermore an applicable automation strategy must be worked out. Therefore, high-quality and highly efficient control loops are designed.

A mathematical model is developed on the basis of the biochemistry of ripening bananas and on the plant environment. It describes the dynamics of the banana ripening process in the form of a system of coupled differential equations. The model will be used for the estimation of important state variables which then will be used to control the process. The model allows rapid simulation of different scenarios and thus to find solutions for varying courses of processes. Such a model based process control scheme should lead to moderate and efficient production techniques.

The varying parameters in the banana ripening process require a high performance process control strategy that flexibly adapts to the variable and imprecisely described process. Adaptive process control with the OLFO-method has been successfully applied in biotechnology [1], [2], [3] and shall be applied, transferred and further developed to the banana ripening process, as a process in the food industry. It is expected that this model based adaptive and optimizing automation strategy could be transferred to other fruit ripening processes.

This innovative automation strategy should enable an advanced process control of the banana ripening process that flexibly adapts to changing conditions and process values.

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Highly automated laboratory plants for the education of process engineers

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Highly automated laboratory plants can be employed in numerous educational areas and for industrial training. One example is the academic education in the fields of environmental, chemical and process engineering.

In this paper, four laboratory plants automated with the process control system “WinErs” are presented. These plants differ in their processes and applications, however their built up is similar. All units are assembled within a metal frame with a switching cabinet for connection to the WinErs-process control system [1], they may also be combined with small scale training simulators [2].

The “LC20x0” is designed for the training of the design and parameterization of basic open- and closed-loop controls in the process industry. Control loops such as flow control, level control and temperature control are available. The unit consists of two storage tanks, pumps, level floating switches, a heater, a pressure sensor for level measurement and a control console, where all signals are provided as voltage signals.

With the “WinErs Lab Version” trainees can develop various binary sequence controls which can be directly tested on this unit. Control functions such as process start, stop and interruption or emergency shut-off etc. can be realised using switches and pushbuttons on the control panel.

The “BC1010” is an educational bioreactor for batch operation. The unit includes the reactor, a stirrer, flasks for three addition agents (e.g. acid and base for pH-correction, antifoam agent) with corresponding pumps. Temperature control of the reactor is realised with a heating rod, instead of a heating rod a double jacket reactor is available. The following process values are measured: pH-value, redox-value, oxygen content, conductivity (for antifoam control) and temperature.

The “LK 20x0” is a laboratory scale wastewater treatment unit that can also be used for environmental practicals e.g. the determination of the biodegradability of chemicals. It features control mechanisms for oxygen concentration and sludge recirculation. Additional upstream denitrification and a neutralisation stages are available.

The “LAC20x0” is a water treatment unit that can be used to study adsorption processes. The adsorption unit is equipped with three columns for sequential or “Merry-go-Round” operating mode. The plant can be used either for adsorption or deionisation processes. The flow path through the unit is determined by magnetic valves. In the continuous deionisation process the switching between the deionisation step, the regeneration step and the wash-up step is against the pH-value and the conductivity. Each column features a pH-value- and conductivity-probe at the inlet and outlet.

Each training unit is supplied with an individual, highly automated operating and monitoring system designed for process reliability and long-term data acquisition and storage. The process control system WinErs, which is employed for the automation of the training units, can be used to modify the operating and monitoring system to individual requirements. This gives the operator the flexibility to test new control algorithms or operating modes.

WinErs is an intuitively and easy-to-use tool that provides graphical programming interfaces using block diagram and GRAFCET editors. It also features a faceplate editor for the design of individual user interfaces and a data acquisition system in which historical data can be evaluated later on.

Several applications of the plants in the academic and industrial education show, that the concept of combining process technology as well as automation and control technology in well designed laboratory plants is of great benefit for the modern education of chemical engineers and plant operators. These new plants can be used to train plant operators and students not only in traditional steady state process operation but also in the field of process dynamics and control.

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An integrated view on business ethics and corporate culture in the 21st century, a sociological perspective

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In the context of ever-increasing news and media reports on corruption, there are concerns that it may become worse with devastating effects unless drastic action is taken. The problem is compounded when one considers the effects of unethical conduct on the ability of companies to deal with their corporate responsibilities including the mission to support social upliftment programmes and strengthen the social base for a vibrant corporate culture. In particular the soaring white collar crimes seem to be ravaging the limited economic resources of the country with impunity.

The paper outlines, in broad terms, the business environment so far as it allows the entrepreneur to contribute meaningfully to the advancement of economic interests in society. This growing menace to the economy depletes the scarce resources which are desperately needed by communities. It seems to manifest itself in rimes such as bribery, pilfering habits, tax evasion, extortion, dishonest advertising and other practices, and various instances of business ethics in building and supporting corporate culture that is responsive to the concerns and needs of society as a whole beyond contractual relations with employees.

However, the antithesis suggests that the corporate environment is not always conducive to engendering the required type of corporate culture. It is often alleged that unethical business activities represent one of the biggest threats to corporate stability and capability of business to achieve corporate objectives and engage in social investment programmes if nothing is done unethical behaviour, the corporate world finds it overwhelmed confronted with a number of options. reels with shock business and industry fraud, corruption finance and other forms of mismanagement in finance matters, organisations seek ways for redress. relating specifically to unethical financial dealings, white collar crimes and incipient culture of corruption, there is growing concern for

The contradictions that are embedded in the corporate environment undermine any attempts to establish a permanent value system to guide and consolidate corporate culture that is based on sound business ethics. The social imperatives of our country have shown that urgent action is required to bring about sanity and create conditions necessary for effective implementation of corporate programmes.

The paper then explores basic processes designed to achieve integration an the infusion of business ethics into corporate levels of the organization. Unless the connection is made the success of corporate programmes will remain a remote possibility. There must be strategic interventions at various levels of organizational structures to inculcate corporate values. A distinction is drawn between successful behavior modeling interventions and the less successful ones. In this way behavior traits and activities that pose a real threat can be isolated and dealt with accordingly.

The KPMG (an auditors' firm) report issued in 1999 on major South African businesses has confirmed that more than 60% companies recently experienced fraud and more than 80% respondents expected fraud to increase. Obviously, a corporate culture suited to the South African situation cannot prosper under such conditions. Research evidence has further established that management in enterprises is responsible for a large percentage of the total

number of cases reported on fraud. Surely, this raises questions about the integrity of the moral behavior that pervades upper echelons of business organizations.

Wherever corruption occurs it taints society in many ways and at all levels of social life, since it comes in different forms and sizes. The impact of economic crimes is devastating and right now there are no measuring instruments to accurately determine their total effect on human development. The tendency has been to loosely classify them and differentiates between minor and serious economic crimes. Latest figures indicate that incidents of unethical business activities have increased in number and gravity as already described. What is now needed are drastic measures to curtail the cancerous effects of these, since this type of behavior not only retards social and economic progress of society but also weakens the entire fabric of society and its institutions.

For example, the perpetrators of unethical economic activities and white collar crimes are often regarded as role-models by the youth and aspirant entrepreneurs in our society. It is society that must take action to discourage replication of unacceptable behavior. Society has numerous mechanisms to sanction the behavior of its members. The paper outlines strategies for the application of broadly defined interventions.

The absence of a strong institutional framework to prevent the spread of unethical business activities puts the economic future of the country in jeopardy in many ways. It retards social development and undermines efforts to raise living standards. The scarce resources to fight against diseases and poverty get depleted as few individuals are enrich at the expense of the majority. In short an upsurge of countless social evils can be noticed as a result of the inability of corporate responsibility programmes to cope with the needs of society.

In this paper, the author identifies the main cause for the lack of integration of business ethics and corporate culture arising from certain business practices of the twentieth century. The effects of these can be measured against specific criteria which provide guidelines for acceptable codes of business ethics. Selected case studies used demonstrate the universal nature of the problems associated with the lack of integration between business ethics and corporate culture. These also highlight the importance of drastic intervention to ensure sufficient control of deviant tendencies and the need to establish normative social structures to regulate the relationship between business ethics and corporate culture.

The assumptions made include the weakening of direct involvement of socialization agencies such as the judiciary system, the church and religious bodies, the education system and the work environment itself. It is hypothesized that failure to re-assert the central role of the above elements of the normative system of society will lead to disastrous consequences and the possible demise of the value system governing business ethics as understood for decades before the twenty first century.

The paper concludes with implications for sustainable economic growth, globalization, peace and democracy worldwide. Various scenarios depicted help to reconstruct factors that could contribute to nurturing an appropriate corporate culture for viable business ethics in the context of current sociological issues including participation, globalization and sustainable industrial development in developing economies, culture and democracy. For an in-depth analysis of the above conceptual framework for the paper, it is necessary to examine the total impact of concerns raised in the paper towards resolving the issues confronting the embattled corporate sector in South African and in other parts of the world experiencing similar developmental problems. For example, the lack of consensus between labour, the state and business around unethical business activities responsible for the downward spiral in the economy.

Finite-element solutions for laminar flow in sinusoidal corrugated-plate channels

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Using the finite-element computational fluid dynamics program POLYFLOW[®], fully developed laminar flows (no-swirl regime) of Newtonian fluids in sinusoidal corrugated-plate channels (Metwally, 2002; Metwally and Manglik, 2000, 2002, 2004) are analysed in the present work. Friction curves equations $fRe = K$ were proposed for different values of the channel aspect ratio ($0 \leq \gamma \leq 1$). The coefficient K can be related with the shape factor, K_0 , and tortuosity coefficient, τ , by $K = K_0 \tau^2$ (Fernandes et al., 2007). It was found that K , K_0 and τ increase with the increase of γ , relations $\tau(\gamma)$ and $K_0(\gamma)$ being proposed. The local behaviour of the interstitial velocity is also studied.

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Nanocrystalline TiO₂: Parameters and effectiveness

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Titanium dioxide nanoparticles was prepared by hydrolysis of titanium isopropoxide alcoholic solution and two important characteristics, i.e. pH of the hydrolysis catalyst and reactant concentration. In first case an aqueous solution of varied pH and peptizing the resultant suspension was used. In second experiment different water/titanium molar ratio(r) was used in synthesis of TiO₂ nanocrystalline and the crystallite size and phase transformation of the resultant powder was investigated. Synthesized powder was characterized by X-ray diffraction, scanning electron microscope (SEM) and transmission electron microscope (TEM). In first experiment the as prepared powders, prepared at temperatures lower than 100°C, consist of very fine anatase crystallites ranges from 7.6 nm at pH 2 to 13.3 nm at pH 9. Different thermal behaviors are experienced while annealing at elevated temperature which is believed to be due to the nucleation and growth process. It was also found that In case of powders with high r value; nucleation plays the main role in the formation rate of new crystallites when the temperature rises from 400 °C to 550 °C. It is concluded that for a constant r value, an increase in TTIP molarity of the prepared sol, increases the average particle size while the growth ability within 400 – 550 °C is enhanced.

Keywords: Hydrolysis, Titanium isopropoxide, nanocrystallite, TiO₂, reactant, pH

High pressure technologies - market trends and technical developments

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In recent years numerous developments were asked for by demanding industries (e.g. automotive, chemical, petrochemical, food, etc.). These developments comprise remarkable increase in single train capacities of production plants and/or rise in operating pressure.

In particular the increasing dimensions require a new mindset, e.g. when forging pre-materials and due respect of physical properties of materials when designing equipment for sufficient heat transfer. Consequences had to be shouldered by manufacturers of high pressure equipment, systems or plants consisting of changes in manufacturing techniques and production sequence, the application of high strength materials, etc.

The paper deals with a set of examples from commercial applications of high pressure technologies in production of fertilizer and LDPE, in food processing as well as with the transfer of know-how of high pressure processing into new fields like pharmaceuticals and semiconductor industry.

For extraction applications a trend to higher pressures is visible which can be demonstrated by the design pressure of recently delivered plants. The paper will describe said developments briefly and lead to explanations of the advantages of supercritical fluid processing under “real” high pressure like new product developments and economic production of high value products.

Keywords High Pressure, Development Trends, Market Trends, Plant Capacities, SFE (Supercritical Fluid Extraction), HPP (High-Pressure Pasteurisation), LDPE (Low-Density Polyethylene)

PRISM: Towards knowledge-based processing systems

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PRISM is a Marie Curie Research Training Network funded by the European Commission. It aims at the development and application of modelling, simulation and optimisation methodologies, and computer-aided tools for sustainable process integration and/or intensification opportunities in order to reduce cost, waste and energy while taking into account realistic operating objectives (controllability, productivity, reliability, robustness of performance etc). The activities of this Research Training Network (RTN) are four Research Clusters. Research Cluster 1 concentrates on the Model-Building Technologies and tools. Research Cluster 2 focuses on the variety of approaches in Model-Based process systems engineering. Research cluster 3 addresses Real-time Optimisation. Research Cluster 4 considers real life industrial case studies and development of software prototypes. The University of Manchester is involved in Cluster 2, in particular the design of flexible processing with development of modelling framework and validation studies, and Cluster 4 activities – real industrial case studies in chemical and petrochemical industries.

The PRISM network is based on a multidisciplinary partnership including: (i) specialists in process systems engineering (simulation, design, control, and synthesis of chemical, petrochemical, and oil & gas processes), (ii) experts in theoretical optimisation and advanced solution techniques, (iii) experimentalists to verify the theoretical work, (iv) SMEs providing engineering services for the process industries with software development activities and (v) industrial end-users to provide real industrial case studies for the application of the developed methodologies, algorithms and tools.

The network is responsible for a well structured multidisciplinary training and knowledge transfer programme. Early-stage researchers attend advanced courses (on process simulation, design, control, optimisation, hybrid separations, material design, process synthesis and flexible plant operation) run by the participating institutions in order to assist the development of new skills. The organisation of workshops, summer schools, participation in international conferences are also key elements of the overall training programme where young researchers have the opportunity to communicate their results. Experienced researchers organise workshops and interact with the industrial partners and participating SMEs. Intensive research exchange schemes between the teams of the network provide an effective means for knowledge transfer and sharing of experience. The ultimate goal of the network training programme is to contribute to a new generation of process engineers, aware of modern advances in computer-aided process simulation, design, optimisation, control and synthesis techniques. The University of Manchester has had two researchers involved in the PRISM network training: an early-stage researcher and an experienced researcher.

The multidisciplinary consortium of the PRISM network, covering most activities of theoretical and applied research in the process systems engineering field, (modelling, simulation, design, synthesis, control, and optimisation of chemical/petrochemical, and oil & gas engineering systems) is made up of one research institutes, nine academic institutes, two industrial partners and one engineering SME providing simulation, control and optimisation services to the industrial sector. The main idea of the consortium is that no single partner would have the recourses and expertise to organise a well structured research and training programme in the process systems engineering field.

The training programme takes advantage of the international nature of the network and the complementarily of its teams. PRISM is therefore expected to expose researchers to different schools of thoughts working in the same research field. Thus, for the successful implementation of PRISM the consortium will employ an effective and well structured scheme for training and interchange of information by promoting exchanges between the industrial partners, SMEs and the academic/research partners. The exchange scheme will provide early stage and experienced researchers with the complementary information for solving their individual tasks. The network also allows a large degree of interaction between theoretical and applied researchers, which will lead to a greater understanding of the challenges in computer-aided design, control and optimisation of process systems.

Each academic team of the network consortium allocates both early stage and experienced researchers to achieve the specific project's objectives. The main role of experienced researchers is two fold:

- To participate in network-wide events which enable the transfer of knowledge between the members of the research teams. Such events will include joint lecture courses, summers schools, workshops, etc. Exchange of knowledge with the members of other teams will be also a key activity for experienced researchers through undertaking visits and secondments.
- Mentoring of early stage researchers within PRISM in order to pass on experience and specialised knowledge.

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Chemisorption undesirable substances from power gas for high temperature solid oxides fuel cell

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In the paper is described a research of purification of a gas mixture containing H₂S, HCl and HF by sorbents based on limestone and dolomite. This gas mixture simulates the real emissions of an industrial biomass (sustainable fuel) gasification process. Which means that the typical concentration levels of the compounds mentioned above are 100 ppm, 150 ppm and 20 ppm, respectively.

The sorption process takes place under high temperatures e.g. 500° C. Hot purified gases can be used in High Temperature Solid Oxides Fuel Cell (HTSFC). The research takes place in a quartz laboratory reactor. For the analytical determination of the HCl and HF acids is used an ion chromatography method. To analytically determine H₂S is used ion selective (S²⁻) electrode. To indicate the break through point is used litmus and plumb papers.

Keywords

High temperature, sorption, H₂S, HCl, HF.

Preparation and characterization of the NaA-Me zeolites catalysts in the n - paraffins isomerization

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Several works have shown the possibility to modify the NaA zeolite by the cations such as Li, K, Mg, and other [1]. On the other hand metals like [2] : Ni, Co, Mo, Cr, Cu; Th and W haven't been studied in recent works, it would be therefore interesting to study the behaviour of these cations in the NaA zeolite. This study has been carried on the NaA zeolite designated prolabo small balls zeolite \varnothing 1-4 mm;.The acidic attack has been done in presence of (HCl, HNO₃, H₂SO₄, CH₃COOH) in the pH= 2 ÷ 5,5 , beyond the pH>5.5, the zeolite is practically steady. The zeolite is activated by a salt oxalate of ammonium in aqueous environment, according to the composition (X fluorescence), the acidic attack drives to the solubilisation of present bivalent cations being in the zeolite cages. The second stage consists on adding the saline solution with the murexide to the NaA zeolite previously treated. The complex introduced at a pH = 10-11, encourages the stability of the metals complex then it is necessary to bring back the medium to the pH = 6-6,2 the complex yields to liberate the Me^{+Z} cations progressively according to the time (kinetic decomposition of the complex in acidic environment). The obtained results showed that:

- the NaA zeolite containing Me is acid-proof for a pH <2, the one that contains the copper didn't present a stability to acids.

Electrochemical oxidation of olive mill wastewater over DSA electrodes

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The electrochemical oxidation of olive mill wastewater (OMW) and model compounds over a Ti/IrO₂ anode was studied by means of cyclic voltammetry and bulk electrolysis. Experiments were conducted at 1300 mg/L initial COD, 0-1.23 V vs SHE and 1.4-1.54 V vs SHE potential windows, 50 mA/cm² current density, 0-25 mM NaCl, 60-80°C temperature and acidic conditions. The reactivity of model compounds decreases in the order phenol \approx p-coumaric acid > cinnamic acid > caffeic acid. Partial and total oxidation reactions occur with the overall rate following zero-order kinetics with respect to COD and increasing with temperature. Oxidation of OMW at 43 Ah/L, 80°C and in the presence of 5 mM NaCl leads to complete color and phenols removal, elimination of ecotoxicity but moderate (30%) COD reduction. Similar performance can be achieved at 6 Ah/L in the presence of 15 mM NaCl. In the absence of salt, the respective color and phenols removal (at 6 Ah/L) is less than 10%. Excessive salinity (25 mM), although does not change color, phenols and COD removal, has an adverse effect on ecotoxicity.

Keywords: cyclic voltammetry; DSA; electrolysis; OMW; phenols; Ti/IrO₂

Electrochemical characterization of the Co-Ni/Cu multilayer system

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Metallic multilayers are fabricated in a sulfate solution by controlling the current and potential for the deposition of cobalt and copper layer respectively. In present study, cyclic voltammograms and current transients were employed to characterize the multilayer structure. The results indicate that electrodeposition of cobalt layers is controlled by a kinetically controlled process while the reduction of copper ions is a diffusion-controlled process. AFM images of the Co-Ni/Cu multilayers also confirm the instantaneous nucleation mechanism, where it is expected that the growth of multilayer films would be form as equally-rounded grains with plan structure. The EDX analysis together with AAS analysis shows the composition of layers.