Acid-resistant organic coatings for the chemical industry: a review

Industries that work with acidic chemicals in their processes need to make choices on how to properly contain the substances and avoid rapid corrosion of equipment. Certain organic coatings and linings can be used in such environments, either to protect vulnerable construction materials, or, in combination with fiber reinforcement, to replace them. However, degradation mechanisms of organic coatings in acid service are not thoroughly understood and relevant quantitative investigations are scarce. This review describes the uses and limitations of acid-resistant coatings in the chemical industry, with a comparison to alternative resistant materials based on metals or ceramics. In addition, coating degradation phenomena, caused by acid exposure, are mapped to the extent possible, and analysis methods for detecting coating degradation type and severity are listed and discussed. It is concluded that more knowledge on chemical and physical degradation mechanisms is required, and that improvements in resistance to elevated temperatures and abrasion would decrease the risk of use and increase the potential application areas of organic coatings exposed to acidic environments in the chemical industry.
Diffusion of surface-active amphiphiles in silicone-based fouling-release coatings

Amphiphiles (i.e. amphiphilic molecules such as surfactants, block copolymers and similar compounds) are used in small amounts to modify the surface properties of polymeric materials. In silicone fouling-release coatings, PEG-based amphiphiles are added to provide biofouling-resistance. The success of this approach relies on the ability of the amphiphiles to diffuse through the coating film and cover the surface of the coating. A novel method for the measurement of diffusion coefficients of PEG-based amphiphiles of different chemistries in PDMS-based coatings is presented here. The diffusion coefficient of the amphiphiles shows a weak dependency on their molecular weight, although this dependency is much less pronounced than for other rubbery polymeric materials. The biofouling-resistance properties in fouling-release coatings were also studied for these amphiphiles. It was found that the diffusion coefficient does not have any influence on the biofouling-resistance results for the studied compounds. Instead, the chemistry of the hydrophobic block of the amphiphiles is much more significant, with PEG-PDMS block copolymers showing the best properties among the studied compounds.

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Effect of Air Injection on Nucleation Rates: An Approach from Induction Time Statistics

From disruption of the supersaturated solution to improved mass transfer in the crystallizing suspension, the introduction of a moving gas phase in a crystallizer could lead to improved rates of nucleation and crystal growth. In this work, saturated air has been injected to batch crystallizers to study the effects on formation of the first crystal and subsequent turbidity buildup. To account for the typically large sample-to-sample variation, nucleation rates were evaluated for a large number of replicates using probability distributions of induction times. The slope and the intercept of the distributions were studied independently, allowing the simultaneous determination of the mean induction time and a certain detection delay related to the rate of crystal growth after formation of the first nucleus. When saturated air was injected in aqueous glycine
solutions, the average detection delay was reduced from 69 to 13 min, and the mean induction time decreased from 128 to 36 min. The effect on aqueous solutions of l-arginine was less apparent, with a detection delay reduction from 15 to 3 min, and no significant changes on the rate of primary nucleation. These results demonstrate the potential of this technique for reduction in nucleation induction time and improved mass deposition rates in crystallization operations.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), H. Lundbeck A/S, Massachusetts Institute of Technology
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Field study of the long-term release of block copolymers from fouling-release coatings

The addition of block copolymers (i.e. oils) is a common technique to enhance the biofouling-resistance properties of poly(dimethylsiloxane) (PDMS)-based fouling-release coatings. These copolymers diffuse from the bulk to the surface of the coating, thus modifying the properties of the surface and providing fouling-resistance properties. Upon release, dissolution or degradation of copolymer molecules at the surface, new molecules can diffuse from the bulk of the coating and cover the surface. Therefore, the long-term performance of these coatings is dependent on the stability and release rate of copolymer molecules from the surface. A method was developed to quantify the concentration of PDMS-based block copolymers from fouling-release coatings. About 300 experimental coatings exposed to seawater for up to 5.2 years were included in the analysis. The results showed that the loss of copolymer (in % on a weight basis) is significantly higher in warm waters, while the initial copolymer concentration in the coating does not have any effect for copolymer concentrations between 1 and 7 wt%. In short-term exposure, it was found that loss of copolymer was much higher in coatings containing small amounts of an organic biocide (copper pyrithione). Conversely, biocide-containing coatings displayed larger copolymer retention values in long-term experiments. Opposite results were obtained for biocide-free coatings, suggesting that the addition of the organic biocide alters the release profile of copolymers from fouling-release coatings. Finally, the potential of long-term field-studies is discussed, as compared to short-term laboratory experiments usually performed within fouling-release coatings studies.

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Mathematical modeling of pigment dispersion taking into account the full agglomerate particle size distribution

The purpose of this work is to develop a mathematical model that can quantify the dispersion of pigments, with a focus on the mechanical breakage of pigment agglomerates. The underlying physical mechanism was assumed to be surface erosion of spherical pigment agglomerates. The full agglomerate particle size distribution was simulated. Data from two previous experimental investigations were used for model validation. The first concerns two different yellow organic pigments dispersed in nitrocellulose/ethanol vehicles in a ball mill and the second a red organic pigment dispersed in a solvent-based acrylic vehicle in a three-roll mill. When the linear rate of agglomerate surface erosion was taken to be proportional to the external agglomerate surface area, simulations of the volume-moment mean diameter over time were in good quantitative agreement with experimental data for all three pigments. The only adjustable parameter used was an apparent rate constant for the linear agglomerate erosion rate. Model simulations, at selected values of time, for the full agglomerate particle size distribution were in good qualitative agreement with the measured values. A quantitative match of the experimental particle size distributions could be obtained using time-dependent fragment distributions, but this resulted in a very slight improvement in the simulated transient mean diameter only. The model provides a mechanistic understanding of the agglomerate breakage process that can be used, e.g., in the development of novel dispersion principles and for analysis of dispersion failures. The general applicability of the model, beyond the three pigments considered, needs to be confirmed.

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Polydimethylsiloxane (PDMS) resins are extensively used as binder in fouling-release coatings due to the low critical surface energy and low elastic modulus of PDMS. These properties result in poor adhesion of the fouling organisms, which are therefore detached by hydrodynamic forces during navigation [1,2,3]. Other compounds are usually mixed together with the binder (e.g., silica and pigments) in order to improve the mechanical, thixotropic and visual properties of the coatings. It has been shown, however, that these ingredients have a negative effect on the fouling-release properties of the coatings [1,2,4].

Together with the PDMS-system, non-reactive polymers have been used to improve the fouling-release properties of the coatings. Initially, hydrophobic siloxane-based polymers were used, which aimed to increase the hydrophobicity of the PDMS surface [5,6]. However, copolymers comprising hydrophilic, amphiphilic and zwitterionic chemistries have been recently introduced due to their resistance to protein adsorption [7,8]. As a result, most of the current commercial fouling-release coatings contain either amphiphilic or hydrophilic copolymers to improve the fouling release properties of the coatings [9,10,11].

This work shows the effect of an amphiphilic copolymer that induces hydrophilicity on the surface of the silicone-based fouling release coatings. The behaviour of these copolymers within the coating upon immersion and the interaction of these surface-active additives with other compounds of the coatings are addressed.
A Solvent-Free Base Liberation of a Tertiary Aminoalkyl Halide by Flow Chemistry

A flow setup for base liberation of 3-(N,N-dimethylamino)propyl chloride hydrochloride and solvent-free separation of the resulting free base has been developed. Production in flow profits from an on-demand approach, useful for labile aminoalkyl halides. The requirement for obtaining a dry product has been fulfilled by the simple use of a saturated NaOH solution, followed by isolation of the liquid phases by gravimetric separation. The flow setup has an E factor reduction of nearly 50%, and a distillation step has been avoided. The method exemplifies how flow chemistry can be exploited to simplify, improve, and optimize manufacturing processes.

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In the event of a fire, intumescent fire protective coatings expand and form a thermally insulating char that protects the underlying substrate from heat and subsequent structural failure. The intumescence includes several rate phenomena, which have been investigated and quantified in the literature for several decades. However, various challenges still exist. The most important one concerns mathematical model validation under realistic exposure conditions and/or time scales. Another is the simplification of advanced models to overcome the often-seen lack of a complete set of input and adjustable model parameters for a given coating, thereby providing models for industrial applications. In this work, these two challenges are addressed. Three experimental series, with an intumescent coating inside a 0.65 m³ gas-fired furnace, heating up according to so-called cellulosic fire conditions, were conducted and a very good repeatability was evident. The experiments were run for almost three hours, reaching a final gas temperature of about 1100 °C. Measurements include transient temperature developments inside the expanding char, at the steel substrate, and in the mineral wool insulation placed behind the substrate. A mathematical model, describing the intumescent coating behavior and temperatures in the furnace using a single overall reaction was developed and validated against experimental data. By including a decomposition front movement through the char, a good qualitative agreement was obtained. After further validation against experiments with other coating formulations, it has potential to become a practical engineering tool. This article is protected by copyright. All rights reserved.
Experimental investigation of the behaviour and fate of block copolymers in fouling-release coatings

Fouling-release coatings (FRC) were developed as an environmentally friendly alternative after the ban of highly toxic antifouling coatings based on tributyltin. Poly(dimethylsiloxane) (PDMS) has been the most widely used polymer for FRC, and its fouling-inhibition properties have been enhanced by addition of copolymers. Examples of these copolymers include phenyl-modified PDMS or poly(ethylene glycol) (PEG)-based copolymers (e.g. triblock PEG-b-PDMS-b-PEG). These copolymers diffuse from the bulk to the surface of the coating upon immersion and modify the physicochemical properties of the surface. FRC provide superior fuel savings to the shipping industry on the first stages of immersion compared to other current technologies, albeit its performance declines over time.

This project is mainly concerned with improving the understanding of FRC and identifying the causes that result in the worsening of the fouling-inhibition properties of these complex systems, specially focusing on the behaviour and fate of the block copolymers used as additives. The development of various methods to visualize and quantify processes involving these copolymers are presented. Chapter 1 provides an overview on marine biofouling, and the evolution and state-of-the-art in biofouling prevention. In Chapter 2, the scope, aims and hypotheses of this project are set. Chapter 3 studies the diffusion and biofouling-inhibition properties of PEG-based surfactants and copolymers added to PDMS and Chapter 4 analyses the distribution and behaviour of PEG-b-PDMS-b-PEG copolymers in PDMS coatings by fluorescence means. Chapter 5 investigates the degradation of PDMS-PEG-based copolymers in FRC immersed in seawater. Chapter 6 consists of a long-term field study regarding the release/loss of these block copolymers from fouling-release coatings. A coating based on a PDMS binder has been employed as model system in the thesis. The effect of the addition of various PEG-based surfactants and copolymers (i.e. amphiphiles) was investigated by a novel method developed in this project, and the diffusion coefficient and biofouling-inhibition properties of the different amphiphiles were studied. The results showed that there is a moderate dependence of the diffusion coefficient on the molecular weight of the molecule. The diffusion coefficients obtained were relatively high for all the investigated compounds with molecular weights (Mw) ranging from 600 to 4000 g/mol. Moreover, the biofouling-inhibition properties are not dependant on the diffusion coefficient of the amphiphiles, but mainly depend on the chemistry of the hydrophobic block, with PDMS-PEG-based copolymers providing the best results. Hence, the anchoring capabilities and stability of the copolymer on the surface of the coating are proven to be a central aspect of the performance of these FRC.

A novel fluorescent-labelled triblock PEG-b-PDMS-b-PEG copolymer was synthesized in this project to visualize the distribution and behaviour of PDMS-PEG-based copolymers in PDMS coatings. Images obtained by confocal microscopy proved that the copolymer molecules assemble in spherical domains inside the PDMS coating. The domains are smaller close to the surface and larger in the bulk of the film (with domains as large as 7 µm in diameter). The diffusion of copolymer from the bulk to the interfaces of the PDMS film could be observed by following the fluorescence intensity at different depths over time.

The chemical stability of PDMS-PEG-based copolymers in PDMS coatings immersed for up to 30 months in seawater in Singapore was also investigated. The copolymer remaining in the coatings after exposure was extracted and isolated, and its chemical composition was analysed. An increase in the relative content of PDMS was observed, probably due to the imperfect isolation process. However, no traces of degradation products were found, and it was observed that the molecular weight of the copolymer did not change over time. Therefore, it was concluded that the copolymer molecules remaining in the coating after 30 months of immersion did not suffer significant degradation. Conversely, the studied copolymers could be degraded in the laboratory under a range of conditions and the degradation products were successfully identified, mainly consisting of esters arising from the oxidative degradation of the PEG block. Further experiments showed that degradation can also occur in the bulk of the coatings depending on the physical properties and chemical composition of some of the constituents of FRC, both for coatings immersed in seawater and others kept in the laboratory in dry conditions.

The release/loss of copolymer from FRC was also studied, and the effect of different variables such as seawater temperature and the addition of biocide were addressed. Approximately 300 experimental coatings exposed to seawater for up to 5 years were analysed and the results exhibited a large scatter in the data, mainly attributed to differences in the coatings compositions. However, some comparable formulations suggest that seawater temperature has an important effect on the loss of copolymer from PDMS-coatings, while the initial concentration of copolymer has no influence for copolymer concentrations as high as 7 wt%. In addition, the initial concentration of biocide showed diverse effects, with biocide-containing coatings leading to higher copolymer losses in the first stages of immersion and larger copolymer retention values in long-term exposure, indicating that the addition of biocide strongly influences the release profile of these copolymers from FRC.

In summary, the addition of block copolymers is a successful method to impart biofouling-inhibition properties to fouling-release coatings. The development of new methodologies has allowed the investigation of the behaviour and fate of these block copolymers in FRC. While the performance of these copolymers is not limited by its diffusion properties in the film, attention should be put on the physical properties and chemical composition of the copolymer and other coating constituents. These variables have an important influence on the anchoring, release and degradation of these copolymers, which dictate the long-term performance of fouling-release coatings.

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Introduction to Applied Colloid and Surface Chemistry

Colloid and Surface Chemistry is a subject of immense importance and implications both to our everyday life and numerous industrial sectors, ranging from coatings and materials to medicine and biotechnology.

How do detergents really clean? (Why can’t we just use water?) Why is milk "milky"? Why do we use eggs so often for making sauces? Can we deliver drugs in better and controlled ways? Coating industries wish to manufacture improved coatings e.g. for providing corrosion resistance, which are also environmentally friendly i.e. less based on organic solvents and if possible exclusively on water. Food companies want to develop healthy, tasty but also long-lasting food products which appeal to the environmental authorities and the consumer. Detergent and enzyme companies are working to develop improved formulations which clean more persistent stains, at lower temperatures and amounts, to the benefit of both the environment and our pocket. Cosmetics is also big business! Creams, lotions and other personal care products are really just complex emulsions.

All of the above can be explained by the principles and methods of colloid and surface chemistry. A course on this topic is truly valuable to chemists, chemical engineers, biologists, material and food scientists and many more.
Long-term stability of PEG-based antifouling surfaces in seawater

Poly(ethylene glycol) (PEG) is a hydrophilic polymer that has been extensively used in the biomedical and marine environment due to its antifouling properties. In the biomedical field, PEG has been successfully used to functionalize surfaces due to its resistance to cell and nonspecific protein adsorption. However, the long-term stability of PEG has limited its use in some areas. In the shipping industry, there is a great need for long-term solutions to keep the hulls of the ships fouling-free. The long-term stability of PEG in polydimethylsiloxane (PDMS) fouling-release coatings is studied here, in both accelerated laboratory tests and real seawater conditions. This article shows how PEG-based copolymers, which have been exposed in fouling-release coatings to real-life seawater conditions, are isolated and compared to those exposed to accelerated laboratory testing with successful results. The influence of the chemistry of the PEG compounds, the chosen laboratory degrading agents, and the possible degradation pathways and products are discussed.

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Scopus rating (2010): SJR 0.571 SNIP 0.968
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Effects of biofouling development on drag forces of hull coatings for ocean-going ships: a review

This review presents a systematic overview of the literature and describes the experimental methods used to quantify the drag of hull coatings. It also summarizes the findings of hull coating's drag performance and identifies the main parameters impacting it. The advantages and disadvantages of the reported methods listed in this review provide an assessment of the most efficient methods to quantify the drag performance of hull coatings. This review determines that drag performance of hull coating technology varies depending on whether the coating condition is newly applied, after dynamic or static seawater exposure. The summarized data reveal that, while several methods have attempted to quantify drag performance of hull coatings, other methods must be explored in order to accurately measure the long-term drag performance of hull coatings in conditions mimicking those that ship hulls encounter during actual voyages.
Driven by the growth of the wind power industry during the last decade, the size of wind turbines has grown considerably and single-turbine power can nowadays reach a capacity of 8 MW with rotor diameters exciding 160 m. Rain erosion is a considerable threat to the mechanical integrity of the blades in such equipment. To reduce expensive blade maintenance repairs and to avoid out-of-service periods, energy-absorbing blade coatings are required to protect rotor blades from rain erosion. In this work we describe the design, construction and evaluation of a laboratory setup for fast screening of up to 22 coating samples that is based on water jet slugs. Our objective is to study the effect of the parameters involved in the rain erosion process and to correlate our experimental results with data obtained with the complex and expensive whirling arm rig, which has become the industry standard method of test for rain erosion. Our results showed that water slug velocity and impact frequency are the most influential parameters in the coating erosion rate. Coating defects, often present on the specimens tested, appeared to play an important role in the erosion mechanism. Two particular experimental blade coatings were investigated using the proposed experimental design. The evaluation of the coatings under conditions where impact frequency and water hammer pressure were “matched” could not be directly correlated with the results obtained with the whirling arm rig. This result may be attributed, among other contributing factors, to the different contact modes in the two setups, i.e. the movement of coated panels against rain drops versus the movement of water drops against coated specimens. Additional factors that require further investigation are the specimen geometries and the potential significance of the presence of a thin water film on the coated surfaces. Our results endorse the complex nature of the rain erosion phenomenon, which is the result of the simultaneous combination of complex mechanisms and as such, it is difficult to reproduce at the laboratory scale.

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Estimation of long-term drag performance of fouling control coatings using an ocean-placed raft with multiple dynamic rotors

An experimental setup was designed and built to estimate changes in the skin friction of fouling control coatings (FCC) over an extended period of time in conditions simulating the vast majority of ship profiles (regarding speed and activity) in the present market. The setup consisted of two separate parts: one aged FCCs directly in seawater in a dynamic manner by simulating the exposure condition of a ship’s hull, and a second, laboratory part measured the torque (drag) of aged coatings in a rotary setup. From the spring to the autumn of 2013 and 2014, four commercial FCCs were exposed for 53 weeks in Roskilde Fjord, Denmark, which is characterized by relatively cold seawater and a salinity of approximately 1.2 wt%. The in situ immersion seawater conditions consisted of five-week cycles divided into 2 weeks of static immersion and 3 weeks of dynamic immersion, during which time the cylinders were rotated at a tangential velocity of 8.1 knots. The skin friction was found to generally increase more during the static period, compared to the dynamic ones. Over the course of the entire exposure period, the skin friction of the investigated FCCs decreased in the following order: fluorinated fouling release coating (FRC) (highest skin friction), hydrogel-based FRC without biocides, silylated acrylate self-polishing...
copolymer coating, and hydrogel-based FRC with biocides (lowest skin friction). However, the differences in skin friction between the latter three coatings were minor and often within the range of experimental uncertainty. The average surface roughness of the FCCs in the newly applied and mechanically cleaned condition, determined as the Rt(50) and Rz parameters, was evaluated as poor predictors of skin friction.

**General information**

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**Experimental investigation of coating degradation during simultaneous acid and erosive particle exposure**

When used in industrial processes, such as stirred acid leaching in the mineral industry, thermoset coatings are exposed to a combination of aggressive chemicals and erosive particle wear. While each exposure condition has been studied separately, no research has been presented on the effects of a simultaneous exposure. To investigate this, a pilot-scale stirred acid leaching tank, containing erosive particles and acidic solutions, has been designed and constructed. Resin
types considered are amine-cured novolac epoxy and vinyl ester. Transient coating degradation is mapped through visual inspection and changes in film thickness. The new set-up, capable of experimenting with erosive particles in acidic solutions, is presented. In addition, results from preliminary experiments, using abrasive particles and water in a high-speed disperser, are discussed.

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Fuel efficiency and fouling control coatings in maritime transport
First, this thesis concerns the drag performance of fouling control coatings (FCCs) used to protect hulls on ships against biofouling and, therefore, minimize any drag therefrom. A systematic overview of the literature and description of the experimental methods used to quantify the drag of FCCs has been made. Also, the advantages and disadvantages of the reported methods are listed; these provide an assessment of the most efficient methods to quantify the drag performance of FCCs. In addition, the main parameters impacting FCCs and the main findings for the drag performance of the mostly used FCC technologies are outlined. It was found that the drag performance of FCCs varies, depending on whether the FCC has been newly applied, has experienced dynamic exposure, or has experienced static seawater exposure. The summarized data revealed that the most common drag performance method currently used consists of measuring drag when coatings are newly applied and after static exposure. It was found that the main limitation of this method primarily arises due to incorrect exposure conditions, when compared to larger commercial ships that mainly are moving with few and shorter idle periods. As a result, it was determined that other methods must be explored in order to accurately measure the long-term drag performance of FCCs in conditions that mimic those encountered by ships' hulls during actual voyages.

In an experimental study, five commercial FCC systems were applied to smooth disks with a radius of 11.45 cm. The drag performances in the newly applied coating condition and after one month of static immersion in natural seawater were measured using a friction disk machine (FDM). The four best performing coatings were re-examined for their drag performance after an additional 2.5 months of immersion. The five FCCs in the newly applied coating condition when applied on completely smooth substrates revealed a small difference and, in most cases, one that was less than the experimental uncertainty. After one month of static immersion, the hydrogel-based fouling release coating (FRC) with biocides had the lowest drag, while the fluorinated FRC had the highest drag. The hydrogel-based FRC without biocides and the two self-polishing copolymer (SPC) coatings showed intermediate performances. After 3.5 months of static immersion, the two hydrogel-based FRCs showed superior drag performance, compared to the two SPC coatings. Furthermore, the drag performances of two different FCC systems with varying substrate roughness values (i.e., the roughness below the coating system) were measured in the newly applied condition. An increase in the substrate roughness led to increased drag for both FCC systems, but the FRC was impacted less by the higher substrate roughness than the SPC coating.

To overcome the limitations from investigating only the drag of newly applied coatings and coatings after static immersion, an experimental setup was designed and built to estimate the changes in the skin friction of four FCCs over an extended period of time in conditions simulating the vast majority of ship profiles (i.e., speed and activity) in the present market. The setup consisted of two separate parts; one part aged FCCs directly in seawater in a dynamic manner similar to that experienced by a ship's hull, and a second, laboratory part measured the torque (drag) of coated cylinders in a rotary setup. Four commercial FCCs were exposed for 53 weeks in Roskilde Fjord, Denmark, i.e., in relatively cold seawater (salinity of 1.2 wt%), from the spring of 2013 to the autumn of 2014. The in situ immersion conditions consisted of five-week cycles. Two weeks consisted of static immersion. This was followed by three weeks of dynamic immersion, in which the cylinders were rotated in natural seawater at a tangential velocity of 8.1 knots. It was found that the skin friction generally increased more during the static immersion, as opposed to the dynamic exposure, which revealed the need for exposure conditions that mimic those of larger commercial ships. Furthermore, with regard to the entire exposure period, it was found that the skin friction of the investigated FCCs decreased in the following order: fluorinated FRC (highest skin friction), hydrogel-based FRC without biocides, silylated acrylate SPC coating, and hydrogel-based FRC with biocides (lowest skin friction). However, the differences in skin friction between the latter three coatings were found to be small and often within the experimental uncertainty. After 25 weeks of immersion and mechanical cleaning, the differences in skin friction were, on average, less than 1%, i.e., within the experimental uncertainty, for velocities relevant for larger commercial ships. The roughness parameters, Rr(50) and Rz, were found to be poor indicators of the drag performance in the newly applied and mechanically cleaned coating condition.
Isolerende maling baseret på partikler af aerogel
I procesindustrien er der et stort behov for særligt fleksible og holdbare isoleringsløsninger. Det kan f.eks. være undersøiske rørledninger eller hulrum, hvor pladsen er meget begrænset. I de senere år er der kommet forskellige malinger med isolerende egenskaber på markedet. Men hvor store effekter kan man egentlig opnå med sådanne malinger?

Kinetic modeling of multi-component crystallization of industrial-grade oils and fats
Transient crystallization kinetics is investigated for complex, industrial-grade vegetable oils consisting of more than ten triacylglycerols (TAG). The classical nucleation model has been used to describe primary nucleation, while secondary nucleation has been described by a semi-empirical approach. Growth is modeled using a modified Burton-Cabrera-Frank (BCF) model. Surface tensions and growth constants have been determined using focused-beam-reflectance measurements (FBRM). The required adjustable parameters in the model have been fitted to overall crystallization curves obtained by solid-fat content (SFC) measurements for a given oil at different cooling rates and degrees of dilution. The developed model can accommodate more polymorphs simultaneously and performs well with respect to predicting crystallization onset, rate of crystallization and final SFC value. It can also qualitatively describe how higher cooling rates lead to formation of more meta-stable crystals and smaller mean-crystal sizes. : The model provides a good starting point for developing more realistic, transient models for TAG crystallization with the ability to accommodate processing conditions and complex chemical compositions. Such a predictive model may provide a powerful tool to screen and optimize oil formulations in industrial processes and allow product developers to evaluate recrystallization events.
Quantitative analysis of silica aerogel-based thermal insulation coatings

A mathematical heat transfer model for a silica aerogel-based thermal insulation coating was developed. The model can estimate the thermal conductivity of a two-component (binder-aerogel) coating with potential binder intrusion into the nano-porous aerogel structure. The latter is modelled using a so-called core–shell structure representation. Data from several previous experimental investigations with silica aerogels in various binder matrices were used for model validation. For some relevant cases with binder intrusion, it was possible to obtain a very good agreement between simulations and experimental data with shell thickness and/or thermal conductivity of the shell as adjustable parameters. However, the experimental data was not sufficiently detailed to allow a separation of the effects of the two parameters. In the ideal case of no aerogel binder intrusion, a comparison with a coating containing intact hollow glass or polymer spheres showed that silica aerogel particles are more efficient in an insulation coating than hollow spheres. In a practical (non-ideal) comparison, the ranking most likely cannot be generalized. A parameter study demonstrates how the model can be used, qualitatively, to get an indication of the effect of important model parameters on the thermal conductivity of an insulation coating. With relevant data available for service life exposure conditions and raw material costs, the model can also be used as an optimization algorithm.
Quantitative Mapping of Mechanisms for Photoinitiated Coating Degradation

This work concerns the mathematical modeling of photoinitiated coating degradation. Using experimental evidence available, some of the most important assumptions underlying existing models for the most common coatings are analyzed and suggestions for further work provided. A modeling approach that can be used to implement the various effects of water on the degradation mechanisms of cross-linked coatings is also presented and experiments to test the approach are suggested. Additionally, simulations with an existing degradation model for an epoxy–amine coating are used to map the influence of model parameters on the lag time (i.e., the time passing prior to the onset of erosion) and the stable erosion rate. The simulation results can be used in the optimization of UV radiation-induced intercoat adhesion losses, which are often observed in multilayer coating systems based on top coated epoxy coatings. Finally, potential directions for future experimental research in the field are outlined.
Rain erosion of wind turbine blade coatings using discrete water jets: Effects of water cushioning, substrate geometry, impact distance, and coating properties

Rapid and reliable rain erosion screening of blade coatings for wind turbines is a strong need in the coatings industry. One possibility in this direction is the use of discrete water jets, where so-called jet slugs are impacted on a coating surface. Previous investigations have mapped the influence of water jet slug velocity and impact frequency. In the present work, the effects on coating erosion of water cushioning, substrate curvature, and water nozzle-coating distance were explored. The investigations showed that in some cases water cushioning (the presence of a liquid film on the coating surface prior to impact) influences the erosion. Contrary to this, substrate curvature and the water nozzle-coating distance (<100 mm) did not influence the results to any significant degree. Mechanical measurements to characterize selected blade coatings, including tensile strength, flexibility, impact, hardness, and abrasion experiments, were also conducted. The ranking of abrasion resistance of the blade coatings was in agreement with the ranking of rain erosion resistance measured in the whirling arm rig (an industrial standard). Results of this work, with more pertinent parameters explored, confirm the conclusion from the previous investigation that a direct correlation of data from discrete water jet experiments with those obtained in the whirling arm rig does not seem possible (at least not for the blade coatings considered). The underlying mechanisms of rain erosion are substantially different in a setup based on impacting water jet slugs and a setup where a rotor arm impacts falling water drops.

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Thermodynamic Modeling of Multi-phase Solid–Liquid Equilibria in Industrial-Grade Oils and Fats

Compositional thermodynamic phase separation is investigated for industrial-grade vegetable oils with complex compositions. Solid–liquid equilibria have been calculated by utilizing the Margules 2-suffix activity-coefficient model in combination with minimization of the Gibbs’s free energy of the system. On the basis of quasi-equilibrium solid-fat content (SFC) measurements, a new approach to the estimation of the interaction parameters, needed for the activity-coefficient model, has been developed. The parameters are fitted by matching the SFC of two oils at various degrees of dilution and isothermal temperatures. Subsequently, the parameters are successfully validated against three oils, rich in asymmetric and symmetric triacylglycerols (TAG), respectively. The new approach developed is shown to be very flexible, allowing incorporation of additional TAG and polymorphic states. It thereby provides a simple way to dealing with multi-component, multi-phase TAG mixtures without having the required binary interaction parameters at hand a priori. This ultimately provides a powerful, predictive tool which may serve as a starting point for laboratory screening and creation of tailor-made products because many different oil mixtures can be evaluated quickly with respect to specific properties, prior to more time-consuming experimental evaluation.

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Use of Fillers, Pigments and Additives in Fouling-Release Coatings: a Literature Review

Polydimethylsiloxane (PDMS)-based fouling-release coatings represent a non-toxic alternative in the area of marine protection. Many researches and testing procedures are dedicated to the challenge of exploring of effective, reliable and high-performance constituents of the coatings – fillers, pigments and additives – in order to achieve the desired and long-lasting fouling-release properties.

Primarily, coating formulations are prepared on the basis of PDMS with inorganic fillers such as fumed silica (SiO₂), calcium carbonate (CaCO₃), pigments – titanium dioxide (TiO₂), iron oxide (Fe₂O₃) or carbon black (C), and other additives (e.g., silicone oils) [1, 2]. Silica and calcium carbonate can be used as agents to improve mechanical strength of the elastomeric material and provide superior thixotropic behavior to the coating formulations. Despite the fact that currently silica is more widespread in coating applications, calcium carbonate can also be competitive due to observed reduction of the surface modulus as a consequence of the dissolution under exposure to water [3]. Moreover, in many cases, calcium carbonate is added as extending filler in order to diminish expenses for silicone elastomers. As an additional option, pretreatment operations for silica can be considered as they ensure necessary hydrophilic/phobic properties alongside with easy dispersion in the PDMS matrix and lower moisture content. However, in this case, impaired reinforcement is observed [2].

One of the challenges in this field is to determine the right filler loading value. In case of a high filler content, the crucial fouling-release characteristics tend to deteriorate due to lower intrinsic hydrophobicity of the PDMS matrix, despite the fact that the tensile strength and toughness are on the suitable level [1]. This result is obtained without dependence on type of the filler [3]. It also should be mentioned, that several recent researches opened promising perspectives of embedding of natural sepiolite nanofibers (Mg₄Si₆O₁₅(OH)₂·6H₂O), single- or multi-walled carbon nanotubes (CWNTs and MWNTs), modified graphite and graphene as fillers to maintain durability alongside with simultaneous fouling-release performance [1]. The explanation lies in the fact that addition of MWNTs in low amounts helps to improve the properties mentioned above because of energetically favorable CH-π interactions between methyl groups of the PDMS and aromatic rings of the MWNTs [5]. One of the major advantages of utilization of nano-structured fillers is that the particles are capable of providing significant interface area (by means of modifying the topography of the base) for interactions with the polymer matrix. This phenomenon gives an opportunity of potential enhancement of the mechanical strength without negative influence on the fouling-release properties. Another benefit of the nanoparticles is in altering of wetting abilities with forming self-cleaning or superhydrophobic surfaces [5]. Effect of the filler presence was tested by pseudobarnacles adhesion in order to estimate the tensile strength and fouling-release characteristics. It was discovered that the higher content of filler was, the greater pseudobarnacles adhesion strength and the lower fouling-release performance [1–3, 6]. As it is well known, besides giving color and opacity, pigments also influence mechanical (tensile strength, abrasion resistance, elastic modulus, tear energy) and adhesion properties in condensation-cured PDMS-based coatings [2]. In addition to this, pigments can enhance biofouling resistance. For instance, titanium dioxide possesses a capability of switching from hydrophobic to hydrophilic under UV-light exposure. The photocatalytic effect of TiO₂ gives an advantage in keeping the coating surface clean via weakening of the adhesion forces between fouling species and the surface of the coating [7]. As a drawback, using pigments in some cases demands higher PDMS loading due to hindrance of the self-stratification effect of bringing the PDMS to the coating surface [6]. Normally, in order to estimate the influence of pigments, pull-off test is conducted revealing the adhesion strength of the coating on the underlying tie-coat [2].

According to the conducted experiments, it was concluded that silicone oils used as additives provide outstanding fouling-release properties due to appropriate critical surface tension and molecular mobility alongside with interfacial slippage and friction [3]. The principle of action of this additive type is in gradual migration of the molecules to the interface and leaching phenomenon which leads to the detachment of marine organisms and plants by slipping [4]. In other words, the fouling species settle onto the oils instead of the coating surface with a consequent release of the additive into the seawater. Usually, the amount of the additive in a coating formulation is relatively small (1-10 wt. %) as exceeding the limit of the additive content shortens service time span, causing surface damage and increasing coating susceptibility to biofouling [2]. Besides aforementioned silicone oils, several other types of the additives such as carboxyl-functionalized organosilicon polymers, low-molecular weight polysisobutylene, liquid paraffin-petrolatum, perfluorinated polymers or oligomers can be used to improve fouling-release properties [2]. In order to assess the efficiency of additives, immersion tests are typically conducted. During the tests, plates covered with coatings are put into seawater and cleaned after the specified period of time evaluating biofouling detachment characteristics [1, 2, 5, 8, 9]. Contact angle measurements are generally done by using the sessile drop technique giving a picture of the surface properties (hydrophobicity/hydrophilicity) of coatings [5, 7, 8].

Summarizing the information stated above, it is should be noted that for the current coating formulations a lot of experiments and tests are required with the purpose of establishing the most effective and optimal ratio between the components. Further research must be done in the area of silica action alongside with the nano-structured compounds as a future replacement of traditional fillers. Likewise, the negative impact of a high filler loading on the fouling-release performance, must be thoroughly examined.

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Accelerated rain erosion of wind turbine blade coatings

During operation, the fast-moving blades of wind turbines are exposed to continuous impacts with rain droplets, hail, insects, or solid particles. This can lead to erosion of the blades, whereby the electrical efficiency is compromised and expensive repairs may be required. One possible solution to this problem is elastic blade coatings, which are able to absorb the impact energy without crack formation. The purpose of the work presented in this thesis has been to design and construct a laboratory experimentation device, which allows an accelerated and reliable evaluation of existing or novel blade coating formulations. Results of experiments are compared to data obtained in the larger-size whirling arm rig, which is the present industrial standard for blade coating evaluation. The whirling arm rig consists of three fastmoving horizontal rotors rotating in a heavy artificial rain fall. There are four chapters in the thesis. In chapter 1, a literature survey provides background information to the field. Topics discussed are the global wind energy development, possible wind turbine constructions, blade structures and materials, blade coatings, and liquid erosion mechanisms. In chapter 2, the design, construction and evaluation of a new laboratory setup for fast screening of 22 coating samples simultaneously is described. The device is based on a principle of discrete water jet slugs. A review of previous rain erosion testing equipment is also included. To provide a basis for comparison of the new setup with the whirling arm rig, a dimensional analysis was conducted and experiments with two polyurethane-based blade coatings carried out. Results showed that water jet slug velocity and impact frequency are the most influential parameters on the coating erosion rate. Furthermore, very small coating surface defects, often present on the specimens tested, appeared to play an important role in the erosion mechanism. The evaluation of the coatings under conditions where impact frequency and water hammer pressure were “matched” could not be directly correlated with the results obtained with the whirling arm rig. This may be attributed, among other contributing factors, to the different contact modes in the two setups, i.e. the movement of coated panels against rain drops versus the movement of water drops against coated specimens. The results endorse the complex nature of the rain erosion phenomenon, which is the consequence of the simultaneous combination of complex mechanisms and as such, it is difficult to reproduce at the laboratory scale. In chapter 3, the experimental investigation was expanded to a study on the effects of three important process parameters on coating erosion: water cushioning, substrate curvature, and water nozzle-coating distance. In addition, to map the influence of physical properties on rain erosion, mechanical measurements to characterize selected blade coatings, including tensile strength, flexibility, impact, hardness, and abrasion experiments, were conducted. The investigations showed that in some cases water cushioning (the presence of a liquid film on the coating surface prior to impact) is important. Contrary to this, substrate curvature and the water nozzle-coating distance (< 10 cm) did not influence the results to any significant degree. The ranking of abrasion resistance of the blade coatings was in agreement with the ranking of rain erosion resistance measured in the whirling arm rig and is an interesting indication for future work. Finally, in chapter 4, conclusions are drawn and suggestions for further work provided.

Design of Continuous Reactor Systems for API Production

The pharmaceutical industry has experienced many changes over the last few decades. Continuous production has been promoted as one of the more promising methods for making the industry more efficient and sustainable. The primary focus of this thesis is on the performance of Grignard chemistry in continuous reactor setups. Grignard chemistry encompasses a very powerful reaction type frequently applied in the pharmaceutical industry, for the formation of new carbon-carbon bonds. Three Grignard addition reactions have been studied, all having very different behaviors related to aspects of
reaction engineering. A double Grignard addition (two different Grignard reagents) to a lactone was studied with continuous production in mind. The complexity of the reaction was investigated kinetically in order to optimize a potential flow setup. The investigation indicated that reaction temperatures below -40 °C could suppress the formation of an undesired bis-addition product by stabilizing the mono-addition adduct. A Grignard addition to a poorly soluble tricyclic ketone, previously studied in the laboratory, was transferred to full-scale production. Successful upscaling of the laboratory setup to full-scale production equipment enabled complete replacement of the existing batch production of this intermediate. The crowning achievement in this work was the realization of continuous laboratory reactor setups capable of manufacturing the entire GMP portion of the synthesis of melitracen HCl at H. Lundbeck A/S. The formation of a carbon-carbon bond between a tricyclic ketone and a Grignard reagent was the primary objective, this being the first step in GMP synthesis. The process was optimized to include one-step hydrolysis and dehydration, followed by phase separation of the product-containing organic phase, which was then precipitated with hydrogen chloride to obtain the final API. The Grignard reagent was also produced in a continuous laboratory setup involving handling of solid magnesium turnings. Likewise, the alkyl halide used in the formation of the Grignard reagent was produced continuously. The three segmented units were able to be coupled to construct a single continuous reactor facility for manufacturing melitracen HCl. The study of Grignard addition reactions to the three different substrates investigated in this thesis has culminated in a methodology by which reaction engineering decisions can be guided. The methodology provides suggestions on when and how decisions should be made on continuous production methods for Grignard chemistry within pharmaceutical manufacturing. Physicochemical properties, such as solubility, were found to be critical. However, from a business perspective, issues such as the current lifecycle of the API and GMP can make a potential reactor setup non-feasible. If the pharmaceutical industry is to adapt to recent trends towards end-to-end and on-demand pharmaceutical production, access to standard reactor units for commonly-used chemical transformations and methods for timely decision-making are essential. The methodology described herein provides an approach to fulfilling this need for Grignard chemistry in flow reactors.

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Diversity screening for novel enzymes degrading synthetic polymers
The objective of this PhD study was to evaluate the feasibility of enzymatic degradation of synthetic polymers used as binder materials in marine coatings. Enzymatic modification of synthetic polymers like epoxy resin, polyurethanes and various acrylics is desirable in several industrial processes: waste management, production of biofuels and valuable biochemicals. Secondly, the goal was to identify new ways in which relevant enzymatic activities may be identified. Finally, the aim was to contribute to the known diversity of biocatalysts with potential to: oxidize a number of low-molecular phenolics – including some of low-molecular coating binder models, perform the kinetic resolution of selected epoxides and to enzymatically fucosylate various oligosaccharide molecules.

In this work discovery and characterization of a wide diversity of novel enzymes of bacterial and fungal origin is reported. First, a collection of fungal strains was screened for the capability to degrade several compounds of synthetic origin. Strains with the ability to modify colloidal polyester polyurethane, as well as various commercial emulsions of acrylates were identified. Secondly, we have used metagenomic library from heavily polluted soil – one of the most challenging habitats and source of potent enzymes, potentially degrading a range of recalcitrant xenobiotics from oil and paint industries. It is well-established that ‘you get what you screen for’, therefore the major challenge was the availability and the choice of proper substrates for identification of promising enzyme candidates. Several genes coding for enzymes with the capability to oxidize various natural and synthetic substrates were identified, expressed heterologously and characterized. Three multicopper oxidases (MCOs) were identified encoded by genes identified in a metagenomic library constructed from soil contaminated with heavy metals and various paint residues. Mco1 is a three domain CopA-like protein and Mco2 and Mco3 are representatives of bacterial twomaind copper oxidases (MCOs). The enzymes catalyzed oxidation of 2,2’-azino-bis(3- ethylbenzothiazoline-6-sulphonic acid) (ABTS) and 2,6-Dimethylenophenol (2,6-DMP) under diverse reaction conditions and catalyzed the conversion of majority of aromatic alcohols tested. Under conditions tested, the enzymes catalyzed decolorization of common industrial wastewater dye contaminants. Mco2 was identified as being a hyperthermostable enzyme with a remarkable half-life of 21 hours at 80 OC.
Cloning and heterologous expression of a potent laccase from the fungus Ganoderma lucidum was also performed. Interestingly, the recombinant LacGL1 enzyme was able to promote higher yields of glucose during cellulase-catalyzed hydrolysis of pretreated sugarcane bagasse.

We have further utilized the constructed metagenomic library for functional identification of epoxide hydrolase activities using a new agar-plate assay. Using this method, clones with epoxide hydrolase activity were identified. mepox1 gene was re-cloned for heterologous production of recombinant epoxide hydrolase. Despite low enantioselectivity, the purified enzyme exhibited a broad substrate specificity and wide pH range.

Finally, the discovery of novel metagenome-originating α-L-fucosidases and evaluation of their potential to catalyze the transglycosylation reaction to produce fucosylated human milk oligosaccharides is reported in this work. Seven fucosidases were identified, all belonging glycosyl hydrolase family 29, that exhibit different hydrolytic capacity for 2'-fucosyllactose, 3-fucosyllactose and various fucosylated plant cell wall polymers. Several enzymes catalysed transglycosylation either using lactose or pNP-Fuc as acceptor and Mfuc6 exhibited an unusually high transglycosylation/hydrolysis ratio. Using 25 mM pNP-Fuc as donor and under conditions tested, the maximum yields of 1.6 ± 0.1 mM 2'-fucosyllactose and 0.9 ± 0.01 mM of 3-fucosyllactose were achieved.

In conclusion, results included in this work further substantiate that the functional mining of a metagenome can lead to the successful discovery of diverse biocatalysts. This work paves the way for efficient identification of novel enzymatic catalysts and generates enzymes as well as small molecules with valuable biological properties and market potential.
Steel is an incombustible substrate, but at elevated temperatures structural steel suffers from a drastic reduction in mechanical strength. In the event of a fire, the reduced strength may lead to collapse of the structure. A method to prolong
the time before steel reaches the critical temperature (450 - 600 °C), at which the collapse may occur, is the use of a fire protective intumescent coating, which swells when exposed to temperatures above about 200 °C. The swelling of the intumescent coating happens according to a complex sequence of chemical reactions, whereby the coating forms a porous char, which thermally insulates the substrate. In addition to the coating itself, several process parameters influence the performance of the intumescent coating. Such parameters may for instance be the interaction with an underlying anticorrosive primer, the heating rate employed, or the oxygen content in the fire. In this work, focus has been on process parameters for an intumescent coating for so-called cellulosic fires. The thesis contains five chapters, where Chapter 1 is a literature survey providing background knowledge on coatings, intumescent coatings in particular, and fire scenarios. In Chapter 2, the effects of coating thickness and gas-phase oxygen concentration on two epoxy primers used in an intumescent coating system were investigated. It was found that primers with a too high thickness failed in the presence of oxygen. In nitrogen, the primer did well, except for a single case, which showed a minor delamination at the edges. In addition, it was shown that the thermogravimetric behavior of the primer and intumescent coating alone could not be used for explaining the entire coating system performance. A novel experimental method, which may potentially be developed into a fast screening method of primers for intumescent coatings, is also described. Upon heating in nitrogen, a color change of the primer from red to black was observed. Potentially, this may be used as an indicator to whether a primer under an intumescent coating has been exposed to oxygen or not in gas-fired furnace experiments. In Chapter 3, a mathematical model of an intumescent coating exposed to heating in a pilot-scale gas-fired furnace is presented. The model takes into account convective heat transfer to the char surface, conduction inside the char, and the char expansion rate. Model validation was done against experimental char expansion rates and temperatures of the steel substrate and at intra-char positions. The model was solved in a discretized and non-discretized version and a good qualitative description of the temperature curves was found. An important learning was that temperatures measured inside the char are very important for a proper model validation. Due to its simplicity and few input parameters, the model (non-discretized version) shows a good potential as a practically applicable engineering model. Results suggest that oxygen mass transport is not a limiting factor for the char oxidation reactions. An investigation of the repeatability of the experimental temperatures showed that temperatures close to the char surface were somewhat more uncertain than the steel temperature and char temperatures close to the steel substrate. Chapters 4 and 5 are concerned with the development of a fast screening method for the extent of expansion and char strength of intumescent coatings. The method is relevant for investigation of special cases, where the char is damaged by moving objects during a fire. The method uses the concept of shock heating to avoid long heating up and cooling down times of a furnace. In Chapter 4, it was found that for measuring char strength reliably at room temperature, dried samples were required. Chapter 5 discusses shock heating in various oxygen concentrations and verified that the expansion is affected by the gas composition. Experimental data showed that under a high heating rate, the char strength could not meaningfully be correlated to the degree of expansion. Furthermore, it was found that at the high heating rates employed thin films (147 μm) would contract horizontally while expanding vertically. This was not the case with a coating thickness of 598 μm. The strength of the char in the vertical direction was also investigated. It was found that the outer crust of the char had the highest mechanical strength and a weak zone, in the central region of the char, was identified.
observed in nitrogen, while the color remained red in the oxygen-nitrogen mixture. In summary, the results suggest that an adequate choice of primer, primer thickness, and intumescent coating is essential for a good performance of an intumescent coating system. (C) 2014 Elsevier B.V. All rights reserved.

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Mathematical Modeling of Vegetable-Oil Crystallization

In recent years the food sector has experienced a great boost in demand for tailor-made fats and oils to produce so-called functional foods, where ingredients have been carefully modified to yield products with specific, valuable properties. Depending on market segment and product, it may be desirable to enhance specific properties such as shelf life, viscosity, texture, sensory aspects and physical appearance. Vegetable oils and fats constitute a considerable part of many food products such as chocolate, margarine, bread, spreads and ice cream. Several attractive properties found in these products, including flavor release, melting profile and appearance, are governed by the oils and fats added. Consequently, altering the fat phase may lead to enhanced properties of the products.

The primary focus of the present work is vegetable oils and fats originating from different sources covering the most abundant fatty-acid moieties encountered in industrial productions of food and confectionary products. The oils usually contain more than 95% triacylglycerols (TAGs), a family of molecules which is shown to govern many of the aforementioned properties of oils and fats. With few exceptions natural oils and fats comprise an abundant number of TAGs giving rise to complex chemical compositions. In this research the focus will mainly be on TAGs, disregarding minor components.

To date improvements of oils and fats have largely been based on empirical laboratory tests designed by skilled experts and specialists drawing on many years of experience and knowledge. With this in mind, the aim of the present project was...
to develop a transient mathematical model, describing crystallization of vegetable fats and oils, based on physicochemical phenomena. The model itself can provide the industry with a valuable tool to design and optimize products. It can also serve as a fundament for testing proposed hypotheses and facilitate realizations with respect to oil and fat crystallization. The research carried out in this project is schematically described in Figure 2. The mathematical model is developed by combining the 5 sections. The actual work is primarily concerned with sections 2-4, while the outputs (section 5) are used as a measure of the model's performance. Section 2 deals with the thermodynamic foundation needed to correctly understand and describe the driving force toward crystallization of TAGs from a liquid. As a consequence of the polymorphic nature of TAGs and their ability to mix non-ideally in the solid state, special measures are to be exercised to develop a versatile, predictive model describing multi-component, multi-phase solid-liquid equilibria.

With reference to research reported in literature, solid-liquid equilibria for complex systems are calculated by minimization of the Gibb's free energy of the system. Possible phase splits are taken into account by employing the tangent-plane criterion. Non-ideal mixing leads to excess Gibb's free energy, which can be described by an activity-coefficient model, in this case the Margules 2-suffix model. This model requires binary-interaction parameters for each pair of TAGs. Obtaining these parameters for pure binary mixtures would be extremely time-consuming, expensive and in some cases impossible due to unavailability of the pure TAGs. A new approach to simultaneously determine all interaction parameters for complex, industrial oils is developed. A series of solid-fat-content (SFC) measurements are performed for different oil blends and temperatures and the experimental SFC values are matched by the model by varying the interaction parameters. The final model with the fitted interaction parameters performs excellently and is validated against independent oil blends. This SLE model shapes the foundation needed in the following kinetic and mechanistic assessments.

Section 3 extends the developed SLE model to deal with TAG crystallization under non-isothermal conditions and deals with appropriate description of nucleation and growth phenomena. The developed model is fitted and tested against SFC curves recorded for various oil blends and temperature profiles while some necessary kinetic constants are obtained via focusedbeam-reflectance measurements (FBRM). The model includes primary and secondary nucleation and growth being governed by both integration and diffusion kinetics. Both growth constants are temperature dependent and the integration constant is allowed to change value as a function of TAG type (tri-saturated, di-saturated, etc.) due to the different degrees of conformational order needed for integration to take place. The diffusion constant is related to the viscosity of the system which in turn is a function of the solid-volume fraction. In total five adjustable parameters are indentified and fitted to experimental SFC curves. Using the fitted parameters the transient model can describe the course of crystallization for a number of oil blends and accommodates the effect of varying the cooling rate.

Section 4 refines the model behavior by introducing a population balance (PB), keeping track of the chord-length distribution (CLD) (derived from particle-size distribution (PSD)) and providing a more realistic picture of the surface area available for growth. A discretized PB, based on the moving-pivot technique, is introduced. The PSD is divided into a number of segments and this approach is numerically easy to handle and well-behaved. The method proves fast, precise and flexible with respect to mechanistic dependencies. All particles are assumed to exhibit spherical geometry and nucleation, growth and aggregation events are accommodated in the PB. Five adjustable parameters are fitted by comparing the model output with experimental CLDs recorded using FBRM. Good results are obtained taking only nucleation and growth into account and disregarding aggregation. The model describes the experimental CLDs well, not only in terms of the overall shape but also with respect to trends. The model correctly describes broader distributions as the concentration of crystallizing TAGs is increased and more narrow distributions as the cooling rate is increased.

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**Model-based analysis of thermal insulation coatings**

Thermal insulation properties of coatings based on selected functional filler materials are investigated. The underlying physics, thermal conductivity of a heterogeneous two-component coating, and porosity and thermal conductivity of hollow spheres (HS) are quantified and a mathematical model for a thermal insulation coating developed. Data from a previous experimental investigation with hollow glass sphere-based epoxy and acrylic coatings were used for model validation. Simulations of thermal conductivities were in good agreement with experimental data. Using the model, a parameter study was also conducted exploring the effects of the following parameters: pigment (hollow spheres) volume concentration (PVC), average sphere size or sphere size distribution, thermal conductivities of binder and sphere wall material, and sphere wall thickness. All the parameters affected the thermal conductivity of an epoxy coating, but simulations revealed that the most important parameters are the PVC, the sphere wall thickness, and the sphere wall material. The model can be used, qualitatively, to get an indication of the effect of important model parameters on the thermal conductivity of an HS-based coating and thereby be used as a specification tool or as a help in the planning of relevant experiments to conduct. Further work with the model must involve additional experiments to secure a general verification of important
Offshore wind energy developments
This chapter will give a brief overview of a few of the activities within offshore wind energy research, specifically 1) Support structure optimization, 2) Blade coatings for wind turbines; 3) Scour protection of foundations, 4) Offshore HVDC and 5) Offshore wind services.

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Quantitative analysis of thermal insulation coatings
This work concerns the development of simulation tools for mapping of insulation properties of thermal insulation coatings based on selected functional filler materials. A mathematical model, which includes the underlying physics (i.e. thermal conductivity of a heterogeneous two-component coating and porosity and thermal conductivity of selected fillers) was recently developed. The model has been validated against data from a previous experimental investigation with hollow glass sphere-based epoxy and acrylic coatings. In this presentation, a concise introduction to the model and some of the simulation results are provided. A practical case story with an insulation coating applied to a hot water pipe is included. Further development of the simulation tool to other types of fillers will be shortly discussed.

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Separation of Enantiomers by Preferential Crystallization: Mathematical Modeling of a Coupled Crystallizer Configuration
A mathematical model describing the separation of enantiomers by simultaneous preferential crystallization in a coupled crystallizer configuration is developed. The model was validated against experimental data for a chemical model compound, the conglomerate forming system of asparagine monohydrate in water. The kinetic parameters required were taken from available literature sources and simulations compared to experimental data. Simulations were found to be in good agreement with experimental data. Additional model simulations suggest that the separation process can be improved by increasing the mean residence time of the liquid phase in the crystallizers, and the mass of seeds supplied. Reducing the size of seed crystals will also lead to an improved separation. The model can also be used to simulate the
performance of the crystallization process for a racemic compound forming system. The racemic compound and the pure enantiomer can be separated simultaneously in each crystallizer, having sufficient enrichment of the pure enantiomer in the feed solution. The model can also be extended to represent a fully continuous separation process taking into account the continuous supply of enantiopure seed crystals and liquid feed solution and the continuous removal of solid product and mother liquor.

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Foaming in wet flue gas desulfurization plants: Laboratory-scale investigation of long-term performance of antifoaming agents

Spontaneous foaming can cause a range of operational problems in industrial processes such as wet flue gas desulfurization (FGD). This work investigates the performance of selected antifoaming agents (Nalco FM-37, Foamtrol 2290, and rapeseed oil) on foams generated by egg white albumin (protein), sodium dodecyl sulfate, and adipic acid at conditions of relevance for wet FGD plants. The addition of antifoaming agents breaks any existing foam and causes an induction period without foaming, after which the foam gradually will begin to reappear. Foaming by egg white albumin (2 g/L) at 0.014 m/s could be controlled by both commercial antifoaming agents (6.4 g/L), but not by rapeseed oil addition. Foaming by pure commercial antifoaming agents has also been demonstrated: up to 7 × 10⁻² m foam was observed with 6.4 g/L Nalco FM-37. © 2013 American Institute of Chemical Engineers AIChE J, 59: 3741–3747, 2013
A reactor setup consisting of two reactors in series has been implemented for a full-scale, heterogeneous Grignard alkylation. Solutions pass from a small filter reactor into a static mixer reactor with multiple side entries, thus combining continuous stirred tank reactor (CSTR) and plug flow reactor (PFR) technologies. Through the use of the reactor train in combination with in-line NIR analysis, on scale a 35% reduction in solvent volume was realized, and the formation of a key impurity was suppressed. The mini-reactor solution achieved many of the economic advantages attributed to microreactor technology, while avoiding the difficulties associated with handling of solids in microreactors.

**Full-Scale Continuous Mini-Reactor Setup for Heterogeneous Grignard Alkylation of a Pharmaceutical Intermediate**

A reactor setup consisting of two reactors in series has been implemented for a full-scale, heterogeneous Grignard alkylation. Solutions pass from a small filter reactor into a static mixer reactor with multiple side entries, thus combining continuous stirred tank reactor (CSTR) and plug flow reactor (PFR) technologies. Through the use of the reactor train in combination with in-line NIR analysis, on scale a 35% reduction in solvent volume was realized, and the formation of a key impurity was suppressed. The mini-reactor solution achieved many of the economic advantages attributed to microreactor technology, while avoiding the difficulties associated with handling of solids in microreactors.

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Investigation of char strength and expansion properties of an intumescent coating exposed to rapid heating rates

An efficient and space saving method for passive fire protection is the use of intumescent coatings, which swell when exposed to heat, forming an insulating char layer on top of the virgin coating. Although the temperature curves related to so-called cellulose fires are often referred to as slow heating curves, special cases where the protective char is mechanically damaged and partly removed can cause extremely fast heating of the coating. This situation, for a solvent based intumescent coating, is simulated using direct insertion of free films into a muffle oven. The char formed is evaluated with respect to the mechanical resistance against compression, degree of expansion, and residual mass fraction. Experimental results show that when using this type of shock heating, the mechanical resistance of the char against compression cannot meaningfully be correlated to the expansion factor. In addition, char properties, measured at room temperature, were dependent on the preceding storage conditions (in air or in a desiccator). The char was found to have the highest mechanical strength against compression in the outer crust facing the heat source. For thin (147μm) free coating films, a tendency to contract in the horizontal plane was observed. The experimental approach is relevant for testing of intumescent coatings used in buildings where moving or falling objects may damage the char during a fire.

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Mathematical modeling of photoinitiated coating degradation: Effects of coating glass transition temperature and light stabilizers

A mathematical model, describing coating degradation mechanisms of thermoset coatings exposed to ultraviolet radiation and humidity at constant temperature, was extended to simulate the behavior of a coating with a low glass transition temperature. The effects of adding light stabilizers (a UV absorber and a radical scavenger) to the coating were also explored. The extended model includes photoinduced oxidation reactions, intrafilm oxygen permeability, water absorption and diffusion, reduction of crosslink density, absorption of ultraviolet radiation, a radical scavenger reaction, and simulates the transient development of an oxidation zone. Simulations are in good agreement with experimental data for a fast degrading epoxy-amine coating with a glass transition temperature of −50°C. It was found that the degradation rate of the non-stabilized coating was influenced significantly by the diffusion rate of oxygen in the oxidation zone, whereas light absorption by the photoproducts formed was only a secondary effect. On the other hand, the degradation rate of the stabilized coating was mainly influenced by the light absorption capability of the coating and in this case there was no oxygen diffusion resistance. Finally, simulations showed that the rate constants of the photoinitiating and oxidation reactions, taking place within the epoxy-amine family of coatings, are strong functions of the specific crosslinker used and must be estimated, in each case, by calibration of the model against adequate experimental data series.
Separation of Chiral Active Pharmaceutical Ingredients: A First Step towards Continuous Preferential Crystallization in the Pharmaceutical Industry

The objective of this PhD project is to experimentally and theoretically investigate the separation performance and to improve the process understanding of a newly developed continuous preferential crystallization (PC) process for the separation of enantiomers forming conglomerates. This PC process is regarded as a first step towards a fully continuous PC process. The current knowledge of the importance of crystallization processes in the pharmaceutical industry and the complex thermodynamic and kinetic phenomena accompanied with the separation of chiral compounds are addressed. The experimental work covers laboratory studies and the theoretical work is based on the experimental data and observations.

A large fraction of active pharmaceutical ingredients (APIs) are enantiomers and the desired biological activity is provided only by one of the enantiomers. Strict regulatory requirements, increasing public demand, and fierce competition have forced the pharmaceutical industry to redevelop existing methods or develop completely new methods to produce pharmaceuticals consisting of APIs of the desired enantiomer. PC is one of several methods used industrially to obtain pure enantiomers by separation of a racemic mixture. The potential application of PC is strongly dependent on requirements to the thermodynamics and crystallization kinetics of the considered solute-solvent(s) system, and the
desired operating conditions. Meeting these requirements are essential to achieve predefined physical attributes of the final product and process economical targets. In this respect, an increasing interest in converting from the conventional batch to continuous PC has initiated the search for new process development opportunities of PC processes. The reason is the many advantages of continuous operation, especially in the case of separation of enantiomers. A newly developed lab-scale continuous PC process, so-called continuous coupled preferential crystallization (CC-PC) process, consisting of two mixed flow crystallizers coupled via crystal-free mother liquor exchange streams and with only the liquid phases operated continuously, was built as the main part of this PhD project. Experiments in triplicate were conducted for the experimental investigation to assess the robustness of the CC-PC process and to investigate the achievement of simultaneous separation of the enantiomers of the conglomerate forming system of the amino acid asparagine monohydrate by crystal growth of seed crystals. The achievement of a racemic liquid phase composition consisting of nearly equal distribution of enantiomers in solution was also investigated. Finally, the performance of the CC-PC process and its potential for further development to a fully continuous PC process was discussed. A nearly racemic composition of the liquid phase in the crystallizers was obtained. Successful enantioseparation by crystal growth was verified, with the repeatability being within 10% deviation. Productivities, yields, and purities of solid products were influenced by the morphological differences in the seed crystals. Due to irregularly shaped seed crystals of L-asparagine monohydrate (L-AsnH₂O), increase in the productivities and yields were achieved in the L-Tank, i.e. the crystallizer in which L-AsnH₂O crystals grow. Lower purities of solid products from the L-Tank compared to solid products from the d-Tank, in which seeds of d-asparagine monohydrate (D-AsnH₂O) were used, were obtained. This could be due to surface nucleation of D-AsnH₂O ascribed to the surface structure of the seeds of L-AsnH₂O supplied. An additional experiment was also carried out using seed crystals of a smaller average particle size having a smoother surface structure than used in the reference experiments. Productivity, yield, and purity were slightly improved in the L-Tank, for the same process duration. It should be emphasized, however, that it was found that the growth rate of the desired enantiomer was very low at the given experimental conditions and therefore practically no consumption of the enantiomer in the feed occurred in the crystallizer. This was ascribed to the nature of the controlling mechanism for crystal growth comprising slow surface integration of the asparagine monohydrate molecules onto the surfaces of the supplied seed crystals. The main advantages of the CC-PC process compared to other separation processes are low capital cost, high crystal purity and yield, ease of upscaling, increased safety, and reduced environmental impact due to reduction in amount of solvent used. Currently, the application is, however, limited to conglomerate forming systems. Nevertheless, the separation concept may open new possibilities for process improvements for enantioseparation of racemic compound forming systems as well. The theoretical investigation of the CC-PC process consisted of the establishment of a dynamic one-dimensional model describing the continuous separation of enantiomers by simultaneous preferential crystallization. The evolution in the moments of the crystal population balances in combination with the liquid phase mass balances for the enantiomers were presented. The model was validated against experimental data for the conglomerate forming system of asparagine monohydrate in aqueous solution. The kinetic parameters required were taken from available literature sources and simulations compared to experimental data. The simulations were found to be in good agreement with the experimental data. The sensitivity analysis conducted suggests that the separation process can be improved by increasing the mean residence time of the liquid phase in the crystallizers, the crystallization temperature, and the mass of seeds supplied. Reducing the size of seed crystals will also lead to an improved separation. The model can be used to simulate the performance of the continuous crystallization process for a racemic compound forming system. The racemic compound and the pure enantiomer can be separated simultaneously in each crystallizer having sufficient enrichment of the pure enantiomer in the feed solution. The model can also be extended to represent a fully continuous separation process taking into account the continuous supply of enantiopure seed crystals and liquid feed solution and the continuous removal of solid product and mother liquor.

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**Separation of enantiomers by continuous preferential crystallization: Experimental realization using a coupled crystallizer configuration**

The experimental realization of a continuous preferential crystallization process, consisting of two mixed-flow crystallizers coupled via crystal-free liquid exchange streams and with only the liquid phases operating continuously, is addressed. Experiments in triplicate, using the conglomerate-forming system of dl-asparagine monohydrate in water, were conducted, and the achievement of nearly racemic composition of the liquid phase in the crystallizers was verified. An experiment was
also carried out using seed crystals of a smaller average particle size than used in the reference experiments. Successful enantioseparation by crystal growth, with the repeatability being within ±10% deviation, was obtained. However, slow crystal growth, due to a low surface integration rate, led to a negligible consumption of the desired enantiomer added in the feed solution, resulting in low productivities. Productivities, yields, and purities of solid products were influenced by the morphological differences in the seed crystals. Due to irregularly shaped seed crystals, increase in the productivities and yields were achieved in the L-Tank. Lower purities of solid products from the L-Tank compared to purities of the solid products from the D-Tank were obtained. This could be due to surface nucleation of d-asparagine monohydrate, ascribed to the surface structure of the seeds of L-asparagine monohydrate supplied. Improvements in productivity, yield, and purity in the L-Tank, for the same process duration, were realized using seed crystals of lower average particle size having a smoother surface structure. The main advantages compared to other separation processes are low capital cost, high crystal purity and yield, ease of upscaling, increased safety, and reduced environmental impact due to reduction in the amount of solvent used. The application is currently limited to conglomerate-forming systems, but the separation concept may open new possibilities for process improvements regarding enantioseparation of racemic compound-forming systems as well. © 2013 American Chemical Society.
Simulering af fotoinitieret nedbrydning af maling
Beskyttende malingslag udsat for sollys, ilt og vand forvitrer gennem en række komplicerede fysiske og kemiske processer. Glasovergangstemperaturen af malingen og tilstedeværelsen af små mængder lysstabilisatorer har stor indflydelse på nedbrydningshastigheden.

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Authors: Kiil, S. (Intern)
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Stimuli-Adaptable Materials
The work presented in this Thesis deals with the development of a stimuli-adaptable polymer material based on the UV-induced dimerisation of cinnamic acid and its derivatives. It is in the nature of an adhesive to adhere very well to its substrate and therefore problems can arise upon removal of the adhesive. This is also known from skin adhesives where it is very undesirable to cause damage to the skin. The overall idea of this project was to resolve this problem by developing a material which could switch between an adhesive and a non-adhesive state. Switchable adhesion is known in the literature but the presented work has a new approach to the field by basing itself on the idea of developing a network into
which a photo-active polymer is mixed and which function as an adhesive. Upon irradiation with UV-light for a short time a non-adhering inter-penetrating network material would be formed. Two simple models for the extent of reaction for the system are presented and show that the timescale for the reaction is minutes to hours. This was further investigated with IR-spectroscopy and UV-absorbance spectroscopy. UV-spectroscopy confirmed that a change in the material occurs upon irradiation with UV and that the reaction time is in the range of minutes. A number of polymer derivatives with cinnamic acid or cinnamylidene acetic acid were prepared and the material properties of these were studied before and after irradiation with UV-light. For the cinnamylidene acetic acid derivatised polymers a macroscopic change was observed upon dissolution of the irradiated compound. The irradiated polymers formed threads or fibres when exposed to water while the unexposed polymers dissolved as a hygroscopic powder. Cinnamic acid derivatised poly(ethylene glycol) (PEG) was studied in detail and three different polymers were derivatised, namely a 4-armed star PEG (Mn = 2000 g/mol), a short linear PEG (Mn = 1000 g/mol) and a long linear PEG (Mn = 4000 g/mol). The derivatised polymers were mixed to create three different photo-active materials and these were investigated with rheology before and after irradiation with UV-light for one hour. It was observed that the largest change occurred for the system consisting solely of the cinnamic acid derivatized 4-armed star PEG. The development of the material properties of this material was studied in details by exposing the compound to UV radiation for up to 120 h and determining the rheological properties after the exposure. It was found that approx. 24 hours was needed to form a manageable film and that approx. 70 hours were needed to obtain stable rheological properties. The exposure times were larger than expected but it was assumed that this would be resolved by preparation of the inter-penetrating network materials. A number of inter-penetrating network materials where both the permanent Network as well as the switching segment was made up of PEG-polymers were prepared. It was found that for a material with relatively long chains in both permanent Network (Mn = 10000 g/mol) and switching segment (Mn = 15000 g/mol) no changes occurred upon exposure to UV-light. It is expected that this is because Mn of polymers is above the molecular entanglement weight. Inter-penetrating network materials with Mn = 4000 g/mol in the permanent network were prepared. Initially a linear photo-active PEG was mixed into the material. This material exhibited a decrease in the values for G and G after irradiation with UV-light for 30 minutes. The reason for the decrease in the two rheological parameters is unclear but the change encouraged further work with this type of systems. Two inter-penetrating network materials with the star-shaped cinnamic acid derivatised PEG as switching segment were prepared and irradiated with UV-light for 72 hours. The network with r = 0.75 in the permanent matrix proved the expectations by clearly showing a solvent effect when the photo-active polymer was introduced into the permanent network. In addition a significant increase of G and G was observed after 72 h of irradiation with UV-light proving the formation of a second network consisting of the photo-active polymers. A network with r = 0.5 in the permanent matrix was also investigated but gave very different results due to the lower value for r. The applied r-value is significantly closer to the critical rc-value and thus resulted in problems with the film formation. The data showed that the secondary network dominates the rheological properties of this network. A material with shorter chains in the permanent network (Mn = 1000 g/mol) was also investigated but showed no change after irradiation with UV-light for 15 minutes. This is related to the stiffness of permanent matrix. First steps to creating an inter-penetrating network with two different polymers were taken by incorporating the cinnamic acid derivatised PEG-stars into a poly(propylene oxide) network. However exposure to UV-light did not result in any changes of the material properties. It was also tested if the photo-active PEG could be incorporated into a poly(dimethyl siloxane) network, but the addition of the photo-active PEG resulted in complete hindrance of the cross-linking of the poly(dimethyl siloxane). A number of problems were identified throughout the work, primarily concerning the mismatch between the expected exposure time needed to induce changes in the materials and the exposure time observed experimentally. This can partially be explained by mobility of the polymers and concentration of the photo-active cinnamic acid. Studies presented in the literature show that the position of the cinnamic acid groups is important for the dimerisation to occur. The nature of polymers makes encounters between end groups less likely and this affects the dimerisation. Furthermore, an NMR-study showed formation of the cis-isomer of cinnamic acid. The isomerisation of cinnamic acid only occurs if dimerisation is hindered. This underlines that the circumstances are not ideal for dimerisation.

General information
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Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Center for Energy Resources Engineering, CHEC Research Centre
Authors: Frankær, S. M. G. (Intern), Skov, A. L. (Intern), Kiil, S. (Intern), Daugaard, A. E. (Intern)
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Electronic versions:
Sarah Maria Grundahl Frankær.pdf
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Active pharmaceutical ingredient (API) production involving continuous processes – A process system engineering (PSE)-assisted design framework

A systematic framework is proposed for the design of continuous pharmaceutical manufacturing processes. Specifically, the design framework focuses on organic chemistry based, active pharmaceutical ingredient (API) synthetic processes, but could potentially be extended to biocatalytic and fermentation-based products. The method exploits the synergic combination of continuous flow technologies (e.g., microfluidic techniques) and process systems engineering (PSE) methods and tools for faster process design and increased process understanding throughout the whole drug product and process development cycle. The design framework structures the many different and challenging design problems (e.g., solvent selection, reactor design, and design of separation and purification operations), driving the user from the initial drug discovery steps – where process knowledge is very limited – toward the detailed design and analysis. Examples from the literature of PSE methods and tools applied to pharmaceutical process design and novel pharmaceutical production technologies are provided along the text, assisting in the accumulation and interpretation of process knowledge. Different criteria are suggested for the selection of batch and continuous processes so that the whole design results in low capital and operational costs as well as low environmental footprint. The design framework has been applied to the retrofit of an existing batch-wise process used by H. Lundbeck A/S to produce an API: zuclopenthixol. Some of its batch operations were successfully converted into continuous mode, obtaining higher yields that allowed a significant simplification of the whole process. The material and environmental footprint of the process – evaluated through the process mass intensity index, that is, kg of material used per kg of product – was reduced to half of its initial value, with potential for further reduction. The case-study includes reaction steps typically used by the pharmaceutical industry featuring different characteristic reaction times, as well as L-L separation and distillation-based solvent exchange steps, and thus constitutes a good example of how the design framework can be useful to efficiently design novel or already existing API manufacturing processes taking advantage of continuous processes.
Continuous Hydrolysis and Liquid–Liquid Phase Separation of an Active Pharmaceutical Ingredient Intermediate Using a Miniscale Hydrophobic Membrane Separator

Continuous hydrolysis of an active pharmaceutical ingredient intermediate, and subsequent liquid–liquid (L–L) separation of the resulting organic and aqueous phases, have been achieved using a simple PTFE tube reactor connected to a miniscale hydrophobic membrane separator. An alkoxide product, obtained in continuous mode by a Grignard reaction in THF, reacted with acidic water to produce partially miscible organic and aqueous phases containing Mg salts. Despite the partial THF–water miscibility, the two phases could be separated at total flow rates up to 40 mL/min at different flow ratios, using a PTFE membrane with 28 cm² of active area. A less challenging separation of water and toluene was achieved at total flow rates as high as 80 mL/min, with potential to achieve even higher flow rates. The operability and flexibility of the membrane separator and a plate coalescer were compared experimentally as well as from a physical viewpoint. Surface tension-driven L–L separation was analyzed in general terms, critically evaluating different designs. It was shown that microporous membrane L–L separation can offer very large operating windows compared to other separation devices thanks to a high capillary pressure (Laplace pressure) combined with a large number of pores per unit area offering low pressure drop. The separation device can easily be operated by means of a back-pressure regulator ensuring flow-independent separation efficiency. Simple monitoring and control strategies as well as scaling-up/out approaches are proposed, concluding that membrane-based L–L separation may become a standard unit operation for continuous
pharmaceutical manufacturing.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, CHEC Research Centre, H. Lundbeck A/S
Authors: Cervera Padrell, A. E. (Intern), Morthensen, S. T. (Intern), Lewandowsk, D. J. (Intern), Skovby, T. (Ekstern), Kiil, S. (Intern), Gernaey, K. V. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.48 SJR 1.062 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.318 SNIP 1.029 CiteScore 2.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 0.99 CiteScore 2.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.13 SNIP 0.977 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.185 SNIP 1.12 CiteScore 2.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.212 SNIP 0.914 CiteScore 2.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.114 SNIP 0.97
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.046 SNIP 0.922
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.943 SNIP 0.901
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.012 SNIP 0.875
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.083 SNIP 0.882
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.847 SNIP 0.821
Scopus rating (2004): SJR 0.701 SNIP 0.787
Scopus rating (2003): SJR 0.421 SNIP 0.67
Scopus rating (2002): SJR 0.548 SNIP 0.869
**Design and operation of a filter reactor for continuous production of a selected pharmaceutical intermediate**

A novel filter reactor system for continuous production of selected pharmaceutical intermediates is presented and experimentally verified. The filter reactor system consists of a mixed flow reactor equipped with a bottom filter, to retain solid reactant particles, followed by a conventional plug flow reactor, where residual reactant is converted by titration. A chemical case study, production of the pharmaceutical intermediate allylcarbinol by a reaction between allylmagnesium chloride and 2-chloro-thioxanthone, in the presence of a side reaction is considered. The synthesis is conducted in tetrahydrofuran solvent. The use of the filter reactor design was explored by examining the transferability of a synthesis step in a present full-scale semi-batch pharmaceutical production into continuous processing. The main advantages of the new continuous minireactor system, compared to the conventional semi-batch operation, are reduced impurity formation and the use of much lower reactor volumes (factor of 1000 based on the laboratory reactor) and less solvent consumption (from 5.8 to 2.3L/kg reactant). Added challenges include handling of continuous solid powder feeding, stable pumping of reactive slurries, and a possibility of continuous control.

**General information**

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Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, H. Lundbeck A/S, Technical University of Denmark
Authors: Christensen, K. M. (Ekstern), Pedersen, M. J. (Intern), Dam-Johansen, K. (Intern), Holm, T. L. (Ekstern), Skovby, T. (Ekstern), Kil, S. (Intern)
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  Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
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  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 1.319 SNIP 1.708
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 1.293 SNIP 1.759
  Web of Science (2009): Indexed yes
  BFI (2008): BFI-level 2
  Scopus rating (2008): SJR 1.299 SNIP 1.6
  Web of Science (2008): Indexed yes
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  Web of Science (2007): Indexed yes
  Scopus rating (2006): SJR 1.308 SNIP 1.553
  Web of Science (2006): Indexed yes
  Scopus rating (2005): SJR 1.445 SNIP 1.801
  Scopus rating (2004): SJR 1.301 SNIP 1.858
  Web of Science (2004): Indexed yes
  Scopus rating (2003): SJR 1.7 SNIP 1.676
  Web of Science (2003): Indexed yes
  Scopus rating (2002): SJR 1.675 SNIP 1.279
  Web of Science (2002): Indexed yes
  Scopus rating (2001): SJR 1.706 SNIP 1.734
  Web of Science (2001): Indexed yes
  Scopus rating (2000): SJR 1.313 SNIP 1.307
  Web of Science (2000): Indexed yes
Formulation studies on stability of solid-state proteases for detergent applications

Enzymes are one of the most important components in the laundry detergents. They effectively contribute to the washing process by decreasing energy and water consumption, reducing environmental load of detergent products, leaving non-toxic water effluents and providing fabric care. Ensuring proper storage stability of enzyme granulates in the chemically hostile detergent matrix is a major challenge. It is believed that the main factors responsible for activity loss are humidity and H2O2 released from the bleaching agents.

In this study, the mechanism and inactivation kinetics of freeze-dried detergent protease, Savinase, were determined in a newly developed experimental setup, providing rapid assessment of solid-state enzyme stability under oxidizing conditions. The method was based on exposure of an enzyme column to known concentrations of H2O2 (g) and humidity in a thermally stabilized chamber. The kinetic studies revealed that the inactivation rate constant depends on the square of moisture adsorbed by the enzyme at corresponding temperature; and the inverse of the reaction rate constant is proportional to inverse of H2O2 concentration in the system. The peptide mapping studies showed that, the inactivation was caused by single-oxidation of the enzyme at Met222 residue. Formulation studies revealed that, having an anti-oxidative property, Na2S2O3 had a better activity-preservation effect compared to Na2CO3, retaining 80% and 60% residual activity, respectively. In addition, mixing the antioxidant homogeneously with the enzyme was found to provide a better protection than coating the salt as a separate layer due to crack formation and/or deliquescence of Na2S2O3 at high humidity.
Intumescent coatings under fast heating

Intumescent coatings are widely used to delay or minimise the destructive effects of fire. They are usually tested under conditions that simulate the relatively slow build-up of heat in a normal fire. Here, the effects of damage during a fire
Intumescent coatings under fast heating

Intumescentnye pokrytija shiroko ispol'zujutsja v stroitel'stve, tak kak oni mogut za-medlit' gorenie i umen'shit' ushherb, причиняемый огнем. Обычно при испытаниях эффективности таких покрытий симулируются условия медленного повышения температуры, как при обычном пожаре. В нашем исследовании рассмотрены последствия быстрого нагрева.

Intumescent coatings under fast heating

Intumescent coatings were studied.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Nørgaard, K. P. (Intern), Dam-Johansen, K. (Intern), Català, P. (Ekstern), Kiil, S. (Intern)
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Main Research Area: Technical/natural sciences
Investigation of Parameters Affecting Gypsum Dewatering Properties in a Wet Flue Gas Desulphurization Pilot Plant

Wet flue gas desulphurization (FGD) plants with forced oxidation, installed at coal and oil fired power plants for removal of SO$_2$(g), must produce gypsum of high quality. However, quality issues such as an excessive moisture content, due to poor gypsum dewatering properties, may occur from time to time. In this work, the particle size distribution, morphology, and filtration rate of wet FGD gypsum formed in a pilot-scale experimental setup, operated in forced oxidation mode, have been studied. The influence of holding tank residence time (10–408 h), solids content (30–169 g/L), and the presence of impurities (0.002 M Al$_2$F$_6$; 50 g quartz/L; 0.02 M Al$^{3+}$, and 0.040 M Mg$^{2+}$) were investigated. In addition, slurry from a full-scale wet FGD plant, experiencing formation of flat shaped crystals and poor gypsum dewatering properties, was transferred to the pilot plant to test if the plant would now start to produce low quality gypsum. The crystals formed in the pilot plant, on the basis of the full-scale slurry did, however, show acceptable filtration rates and crystal morphologies closer to the prismatic crystals from after pilot plant experiments with demineralized water. The gypsum slurry filtration rates were generally high, but a shorter residence time (10 h) and gypsum crystals experiencing breakage and/or attrition (408 h) showed slightly lower filtration rates. Both these experiments contained a higher fraction of fines, which may explain the slightly lower filtration rates. Crystals formed at a higher solids concentration and longer residence time (169 g/L and 120 h) showed a higher proportion of flat crystals, and the XRD pattern contained strong peaks at 31.1° (as the full-scale gypsum) and 29.1°, but no change in the filtration rate was obtained. It has not been possible in the pilot plant to form flat gypsum flakes with poor dewatering properties similar to those observed in full-scale plants.
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.047 SNIP 1.165
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.142 SNIP 1.267
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.105 SNIP 1.239
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.372 SNIP 1.41
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.342 SNIP 1.398
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ie3005435.pdf
Microcapsule-based self-healing anticorrosive coatings: Capsule size, coating formulation, and exposure testing

Self-healing coatings is a rapidly growing research area, where focus has mainly been on development of new approaches to the mechanism of self-healing. However, there is a growing need for investigation of practical issues related to formulation, application, and testing of true self-healing coatings. In this work, ways of reducing the size of poly(urea–formaldehyde) microcapsules, filled with linseed oil and intended for a microcapsule-based self-healing anticorrosive coating (above water exposure), are explored. The influence of microcapsules on epoxy coating performance is also studied. The actual self-healing effect was not part of this work. The synthesis parameters investigated are stirrer geometry, agitation rate, temperature, and stabilizer concentration. It was found that an increase in stirring rate, correct choice of temperature, and a high stabilizer concentration all caused a decrease in microcapsule size but were accompanied by excessive formation of nanoparticles. Thus, isolation of too large microcapsules has been performed by filtration utilizing a novel low-energy fluoropolymer-coated steel sieve. An estimation of the critical pigment (microcapsule) volume concentration (CPVC) was conducted using gloss measurements and a PVC ladder and found to be about 30 vol%. Due to the rather large capsules used (relative to the coating thickness), the low CPVC value can probably be ascribed to a fairly low packing efficiency in the coating, but this needs to be confirmed. Coating performance was evaluated using salt spray exposure and impact testing. Results of the impact testing showed that addition of microcapsules to a binder matrix did not compromise resistance of the coating to mechanical damage and led to formation of fewer and shorter cracks compared to a filler-containing coating. Flaking of the coating was also reduced. Results of the salt spray testing (3 weeks exposure) showed that with an increase of microcapsule content, in the interval 30–50 vol%, the extent of corrosion and potential coating delamination decreased and was identical to that of a full commercial anticorrosive coating.

General information
Model-based analysis of photoinitiated coating degradation under artificial exposure conditions

Coating degradation mechanisms of thermoset coatings exposed to ultraviolet radiation and humidity at constant temperature are investigated. The essential processes, photoinitiated oxidation reactions, intrafilm oxygen permeability, water absorption and diffusion, reduction of crosslink density, and development of a thin surface oxidation zone are quantified and a mathematical model for degrading coatings developed. Front-tracking techniques are used to determine the rate of movement of the oxidation and ablation fronts, the positions of which define the extension of the surface oxidation zone. Three previous and independent experimental investigations with two-component, densely crosslinked, epoxy–amine model coatings were selected for verification of the mathematical model. Simulations can match and explain transient mass loss and coating thickness reduction data and are in agreement with infrared measurements of carbonyl groups formed in the surface zone. The thickness of the stable surface oxidation zone, which is established after an initial ablation lag time, is estimated by the model to 0.5–2 μm in good agreement with previous measurements. Simulated concentration profiles of active groups, oxygen, and radicals in the stable surface oxidation zone are presented and analyzed. The mathematical model can be used for obtaining a quantitative insight into the degradation of thermoset coatings and has potential, after further development, to complete commercial coatings and dynamic exposure conditions, to become a supplementing tool for predicting in-service coating behavior based on accelerated laboratory measurements.

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Authors: Kiil, S. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.409 SNIP 0.614
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.45 SJR 0.421 SNIP 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.5 SJR 0.51 SNIP 1.062
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.46 SJR 0.534 SNIP 1.077
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.39 SJR 0.572 SNIP 1.364
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.24 SJR 0.517 SNIP 1.007
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Inline near-infrared (NIR) spectroscopy has been used to monitor a continuous synthesis of an active pharmaceutical ingredient (API) intermediate by a Grignard alkylation reaction. The reaction between a ketone substrate and allylmagnesium chloride may form significant impurities with excess feeding of the Grignard reagent beyond the stoichiometric ratio. On the other hand, limiting this reagent would imply a loss in yield. Therefore, accurate dosing of the two reactants is essential. A feedforward–feedback control loop was conceived in order to maintain the reaction as closely as possible to the stoichiometric ratio, leading the path to full process automation. The feedback control loop relies on NIR transmission measurements performed in a flow cell where, in contrast to labor-intensive offline HPLC analytical methods, the whole reaction product can be scanned in real time without sample dilution. A robust PLS (projection to latent structures) model was developed with a satisfactory standard error of prediction, providing quantification of the ketone substrate in solutions with a high variability of the major solution component - the alkoxide product. In addition, model performance supervision tools such as the spectral residuals or simple plots of pretreated spectra can assist in the identification of spectral outliers, which in this case could be related to Grignard reagent excess. If the sampling time of the NIR instrument is short enough, manipulating the inputs to the reactor may be used to obtain information about its dynamic behavior. This information is very useful for process control design, assessment of analytical tools and definition of sampling times. In this work, a systematic procedure for chemometric model building is followed, after which a discussion is made on some of the potential applications that can be found when exploiting the fast and rich information provided by NIR spectroscopy.
Self-Healing anticorrosive coatings

Self-healing anticorrosive coatings are multi-component so-called smart materials, which have been proposed as a way to long-lasting corrosion protection of steel structures. The presently most promising technology route is based on microcapsules, filled with active healing agents, and has been the focus of this work. The microcapsules consist of a solid polymeric shell and a liquid core material. When a microcrack, originating from internal stress or a physical damage, propagates through the coating, the microcapsules rupture and release healing agents, which flow to the fracture plane due to capillary forces. The healing agents then start to react, form a polymer network, and ‘glue’ the crack. The approach has been applied to development of an epoxy-based self-healing anticorrosive coating for above water heavy duty corrosion protection. Emphasis has been on investigation of practical issues associated with development and testing of this type of coating.

A laboratory investigation, to identify the most suitable method for production of mechanically stable (filled with industrially relevant core materials) and forming a free-flowing powder upon drying microcapsules, has been performed. Four different experimental procedures, available in the literature, have been used for encapsulation of six core materials, including epoxy resins, diluent, and linseed oil. Several challenges have been identified during the investigations. Main of them dealt with encapsulation of viscous healing agents and a necessity of a thorough adjustment of the synthesis procedures for a wider use with other than original core materials. Free-flowing powders of two types of microcapsules (filled with linseed oil and alkylglycidylether) have been produced and investigated for solvent stability, stability towards stirring and storage, as well as ease of capsule dispersion. A systematic laboratory study, for reduction of poly(urea-formaldehyde) microcapsule size, filled with linseed oil, has been performed. Several synthesis parameters were varied (temperature, stabilizer content, stirring rate, stirrer geometry) and mechanical means of separation were investigated. Capsules with a mean diameter less than 150 µm were obtained using a steel sieve coated with a fluoropolymer coating. These smaller capsules were used in further investigation as model capsules.

A range of microcapsule-containing coatings was formulated, applied to steel substrates, and subjected to salt spray exposure and reverse impact testing. Neither of the tests revealed any drawbacks from addition of microcapsules to an epoxy coating in a concentration up to 50 vol %. On the contrary, the results of the impact test has shown that addition of microcapsules reduces the intensity of crack formation (both in number and length) compared to filler-containing coatings and prevents the coating from flaking upon damage. Based on specular gloss measurements, a preliminary critical pigment (microcapsule) concentration (CPVC) value was estimated to about 30 vol %. The number is lower than anticipated and needs to be confirmed.

Finally, a 3-D model, based on Monte-Carlo simulations, has been developed for prediction of healing efficiency of a microcapsule-based anticorrosive coating. Two kinds of cracks were considered: cracks accommodated within the bulk coating and cracks starting from the coating surface. The model takes into account volume of the crack formed, crack geometry and linear dimensions, as well as diameter, volume concentration, and wall thickness of the microcapsules embedded in the coating. Simulations showed that diameter of microcapsules and crack geometry played an important role in the self-healing action of the coating, especially when low concentrations of capsules were used.
A systematic methodology for the design of continuous active pharmaceutical ingredient production processes

Continuous pharmaceutical manufacturing (CPM) has emerged as a powerful technology to obtain higher reaction yields and improved separation efficiencies, potentially leading to simplified process flowsheets, reduced total costs, lower environmental impacts, and safer and more flexible production. However, the change from batch-wise production towards continuous operation and the definition of flexible design spaces requires a high degree of process knowledge. Process Systems Engineering (PSE) offers multiple methods and tools which can assist in efficient knowledge acquisition, structuring and representation, as well as on how to employ this knowledge for process (re-)design. The aim of this paper is to introduce a methodology that systematically identifies already existing PSE methods and tools which can assist in the design of CPM processes. This methodology has been applied to a process for the production of an API developed by H. Lundbeck A/S, demonstrating the mentioned potential benefits that CPM can offer.

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Authors: Cervera Padrell, A. E. (Intern), Gani, R. (Intern), Kiil, S. (Intern), Skovby, T. (Ekstern), Gernaey, K. (Intern)
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A systematic methodology for the design of continuous active pharmaceutical ingredient production processes

Cinnamic Acid Derivatised Poly(Ethylene Glycol) as a Bioinspired UV-Adaptable Material

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Authors: [Authors listed]
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Fremstilling af UV-aktive polymerer

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Main Research Area: Technical/natural sciences

Investigation of the gypsum quality at three full-scale wet flue gas desulphurisation plants
In the present study the gypsum (CaSO4·2H2O) quality at three full-scale wet flue gas desulphurisation (FGD) plants and a pilot plant were examined and compared. Gypsum quality can be expressed in terms of moisture content (particle size and morphology dependent) and the concentration of residual limestone and other impurities. The particle size distributions (PSD) in the holding tanks of the investigated plants were similar, apart from a slightly higher fraction of small particles in the full-scale plants. These high levels of small particles could originate from nucleation, attrition or accumulation of fly ash and impurities from the sorbent. The crystal morphology obtained in the pilot plant was columnar with distinct crystal faces as opposed to the rounded shapes found at the full-scale plants. All the investigated full-scale plants consistently produced high quality gypsum (High purity, low moisture content and low impurity content). An episode concerning a sudden deterioration in the gypsum dewatering properties was furthermore investigated, and a change in crystal morphology, as well as an increased impurity content (aluminium, iron and fluoride), was detected.

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Kontinuerlig lægemiddelproduktion af små molekyler via organisk syntese

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Authors: Cervera Padrell, A. E. (Intern), Skovby, T. (Ekstern), Kiil, S. (Intern), Gernaey, K. (Intern)
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Mathematical modelling of simultaneous solvent evaporation and chemical curing in thermoset coatings: A parameter study

A mathematical model, describing the curing behaviour of a two-component, solvent-based, thermoset coating, is used to conduct a parameter study. The model includes curing reactions, solvent intra-film diffusion and evaporation, film gelation, vitrification, and crosslinking. A case study with a polyisocyanate and a polyol in an organic solvent, catalysed by an organotin compound, is selected for analysis. The transient effects on reactant conversion values and solid content of the film of the following parameters are studied: initial solvent concentration and film thickness, wind velocity, and bulk air concentration of solvent. Simulations of solvent evaporation are compared to experimental data from a previous investigation. As part of the parameter study, mechanisms of this complex coating system are discussed.

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Authors: Kiil, S. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3
Moving from batch towards continuous organic-chemical pharmaceutical production

Pharmaceutical ingredients have traditionally been produced in batches using multipurpose stirred vessels. Reactions and separations have typically been tailored to fit these units, facing multiple limitations when transferring synthetic routes from the laboratory to industrial scale. Scaling up thus resulted in many cases in low reaction yields and separation efficiencies. These limitations were however compensated by a relatively fast process implementation. For the pharmaceutical industry this meant that new drug products could be exclusively marketed for a longer time period, resulting in higher benefits than those that could be obtained with a highly optimized process requiring extra development time. Being the first to commercialize a product also meant a fundamental marketing
advantage, since healthcare professionals commonly related pharmaceutical products to the original trademark. Furthermore, once a pharmaceutical product was approved, changes to the original production process could only be achieved at the expense of revalidating the whole process in a worldwide market, which typically prevented pharmaceutical companies from optimizing already existing manufacturing processes.

Today, however, the pharmaceutical industry is facing a globalized market where national health institutions increasingly favor the prescription of low-cost generics, and it is more and more expensive to develop new pharmaceutical ingredients with the potential to become, for a few years, blockbusters. Fierce competition has therefore resulted in a need to reduce manufacturing costs and optimize the efficiency of production processes. In addition, ethical reasons and ever stricter legislations demand the development of sustainable processes with the lowest possible environmental footprint.

Continuous pharmaceutical manufacturing has been proposed as a way to facilitate process development and scale up, resulting in higher yields, improved quality, lower risks and reduced environmental impacts. Regulatory agencies, such as the FDA, have encouraged the transition towards novel technologies through increased process understanding.

Developing a process within a more flexible design space based on sound engineering judgment potentially allows process optimization once the product has already been approved. Micro- and mini-chemical systems have been envisaged as the optimal scale for pharmaceutical production, due to improved heat and mass transfer allowing safer operation in a larger design space. Scaling up to high throughputs could then be performed by replicating small-scale units as required.

However, significant uncertainties arise. For example, when should continuous processes be selected? Where are the highest benefits found? How can a continuous process be designed and implemented? Are continuous processes compatible with slow reactions? Do they allow problem free processing of solid particles? What is the cost needed to implement a continuous process?

This PhD thesis tries to answer some of those questions through the development of a systematic framework that takes advantage of continuous processing technologies and process systems engineering for the efficient design of continuous pharmaceutical processes. The framework consists of a step-by-step procedure that guides the user from drug discovery and the initial process development steps towards process implementation. Guidelines are suggested for the selection of the most suitable operating mode. Conceptual continuous processes can then be compared against traditional batch-wise processes in order to evaluate potential cost savings and/or lower environmental footprints.

The design framework has been applied to a process originally developed by H. Lundbeck A/S to produce zuclopenthixol, an active pharmaceutical ingredient. The synthetic process includes four reaction steps (alkylation by a Grignard reaction, hydrolysis of the alkoxide product, dehydration and hydroamination) with very different kinetics and thermodynamics, and several separation and solvent exchange steps. The implementation of continuous processes provided improved product quality without the need of some of the product isolation and purification steps, resulting in a significant simplification of the process. The process mass intensity (kg of raw materials used per kg of product obtained) could then be reduced to at least half the original value.

In this thesis, three of the unit operations included in the zuclopenthixol process were studied in detail. Specifically, the continuous alkylation reaction was achieved using a filter reactor coupled with a side-entry tubular reactor, using real-time in-line near-infrared (NIR) spectroscopy for monitoring the reaction and ensuring the right product quality. A subsequent hydrolysis of the alkoxide product was performed in continuous mode in a tubular reactor with segmented flow. The product of the hydrolysis reaction was fed to a hydrophobic membrane separator where the organic and aqueous phases were split. The organic phase was then dehydrated in continuous mode in a pressurized tubular reactor where the reaction rate of an otherwise slow reaction could be optimized by increasing the temperature above the normal boiling point of the solvent. These three unit operations could potentially be employed in similar reaction and separation steps, thus constituting ‘continuous-flow building blocks’ for the design of novel continuous pharmaceutical processes.
Performance of a Wet Flue Gas Desulfurization Pilot Plant under Oxy-Fuel Conditions

Oxy-fuel firing is a promising technology that should enable the capture and storage of anthropogenic CO2 emissions from large stationary sources such as power plants and heavy industry. However, this new technology has a high energy demand for air separation and CO2 compression and storage. Unresolved issues, such as determination of the optimal recycle location of flue gas, the flue gas cleaning steps required (SO2, NOx, and particles), and the impact of an oxy-fuel flue gas on the cleaning steps, also persist. The aim of this work was to study the performance of the wet flue gas desulfurization (FGD) process under operating conditions corresponding to oxy-fuel firing. The most important output parameters were the overall degree of desulfurization and the residual limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry. Pilot-scale experiments quantified that the introduction of a flue gas with 90 vol % CO2, at a holding tank pH 5.4, reduced the limestone dissolution rate significantly and thereby increased the residual, particulate limestone concentration in the gypsum slurry.
Main Research Area: Technical/natural sciences

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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
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Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.993 SNIP 1.241
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.046 SNIP 1.452
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.101 SNIP 1.266
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.191 SNIP 1.183
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.256 SNIP 1.346
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Scopus rating (2000): SJR 1.372 SNIP 1.41
Performance of a wet Flue Gas Desulphurisation Pilot Plant under Oxy-fuel Conditions

General information
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Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern)
Publication date: 2011

Synthesis of durable microcapsules for self-healing anticorrosive coatings: A comparison of selected methods

Self-healing materials have the ability to ‘repair’ themselves upon exposure to an external stimulus. In the field of coatings, extensive laboratory research has been conducted on these so-called smart materials in the last decade. In the present work, a self-healing concept for epoxy-based anticorrosive coatings, based on incorporation of microcapsules, filled with reactive agents, into the coating matrix, is investigated. Upon small damages to the coating, the reagents are released from the capsules and react, thereby forming a cross-linked network, which heals the crack. However, for the concept to work, microcapsules have to be strong enough to remain intact during storage and coating formulation and application. Furthermore, the capsules must remain stable for many years in the dry coating. Laboratory experiments, using four out of several encapsulation methods available in the literature, have been conducted to investigate the challenges associated with the synthesis of stable microcapsules. It was found that the nature of the core material strongly affects the microcapsule stability and performance. Furthermore, it was evident that experimental procedures developed for certain core materials were not suitable for encapsulation of other compounds without modifications. This is a severe limitation as not many of the encapsulation procedures have been developed for industrially relevant core materials such as epoxy resin. Results of experiments, aiming at finding optimal conditions for robust microcapsule production, are discussed.

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Authors: Nesterova, T. (Intern), Dam-Johansen, K. (Intern), Kiil, S. (Intern)
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Teaching chemical product design to engineering students: course contents and challenges

Chemical product design is not taught in the same way as traditional engineering courses like unit operations or transport phenomena. This paper gives an overview of the challenges that we, as teachers, have faced when teaching chemical product design to engineering students. Specific course contents and relevant teaching methods are discussed.

General information
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Authors: Skov, A. L. (Intern), Kiil, S. (Intern)
Publication date: 2011
The Effect of Substrate Topography on Coating Cathodic Delamination

This article describes the effect of steel substrate topography on coating cathodic delamination. The study showed that the surface preparation can be used to control and minimize the rate of cathodic delamination. The coating should have maximum wetting properties so that substrates with high peaks can be utilized.

General information

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Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Erik Weinell, C. (Intern), Sørensen, P. A. (Ekstern), Kiil, S. (Intern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.237 SNIP 0.343 CiteScore 0.11
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.207 SNIP 0.271 CiteScore 0.12
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.269 SNIP 0.547 CiteScore 0.15
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.273 SNIP 0.398 CiteScore 0.16
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 0.297 SNIP 0.528
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BFI (2009): BFI-level 1
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Scopus rating (2008): SJR 0.379 SNIP 0.244
Scopus rating (2007): SJR 0.15 SNIP 0.283
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UV-initierede "smart materials"

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Authors: Frankær, S. M. G. (Intern), Skov, A. L. (Intern), Kii, S. (Intern)
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Våd røggasafsvovling under oxy-fuel betingelser

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High-Performance Anticorrosive Coatings

General information
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Antifouling effect of hydrogen peroxide release from enzymatic marine coatings: Exposure testing under equatorial and Mediterranean conditions

Hydrogen peroxide (H₂O₂) may be considered an environmentally friendly antifouling alternative to common biocides such as Cu₂O and various organic compounds. In this work, the efficiency of antifouling coatings releasing hydrogen peroxide via enzyme-mediated conversion of starch, under Mediterraneanean and equatorial climatic conditions, is investigated. During seawater exposure of the coatings, starch is first converted to glucose by glucoamylase (rate-controlling step) and subsequently glucose is rapidly oxidised by hexose oxidase in a reaction producing hydrogen peroxide. The coatings formulated have been characterised in terms of common coating characteristics and immersed on rafts in seawater outside Singapore and Spain to monitor antifouling efficiency. The results have been compared to results previously reported from temperate waters in the North Sea outside The Netherlands. Using laboratory assays, the transient hydrogen peroxide release rate from the coatings at different temperatures has been measured. The investigations are used to evaluate the ocean performance of the antifouling coatings. Coatings can be formulated with starch/enzyme ‘pigments’ in considerable amounts and yet retain the mechanical properties required of an antifouling coating. However, the antifouling effect of the coatings immersed in seawater near Singapore and Spain, when inspected after 8 and 14 weeks, respectively, is insufficient. In comparison, previous studies under colder conditions showed an effect exceeding that of two commercial references over 67 days. The release rate of hydrogen peroxide from the coatings is shown to be greatly influenced by temperature, and therefore the results provided here suggest an antifouling effect that is highly dependent on the environment of the coating.
A passive apparatus for controlled-flux delivery of biocides: hydrogen peroxide as an example

A new test method has been developed to estimate the required release rate of hydrogen peroxide (H2O2) to prevent marine biofouling. The technique exploits a well-defined concentration gradient of biocide across a cellulose acetate membrane. A controlled flux of H2O2, an environmentally friendly biocide, was obtained. Larvae of the barnacle, Balanus improvisus, were subjected to known release rates of H2O2 from a surface, under laboratory conditions. It was found that the distribution of settled larvae was not significantly different from the controls when H2O2 fluxes of 5-8 μg cm(-2) day(-1) were applied. However, release rates of 40 μg cm(-2) day(-1) significantly displaced the distribution of settled larvae towards the area of the chamber farthest away from the membrane. Membrane tests in seawater (Jyllinge Harbour, Denmark) for over 16 weeks showed that release rates of H2O2 of approximately 2800 μg cm(-2) day(-1) deterred biofouling efficiently. A H2O2 release rate of about 224 μg cm(-2) day(-1) resulted in some slime formation, but it was less than that on the H2O2-free control. It appears that to obtain efficient resistance to biofouling in natural seawater requires much higher membrane release rates of H2O2 (factor of between 5 and 50) than laboratory membrane exposure assays using barnacle larvae.

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Authors: Olsen, S. M. (Intern), Pedersen, L. (Ekstern), Dam-Johansen, K. (Intern), Kiil, S. (Intern)
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Main Research Area: Technical/natural sciences
Cathodic delamination of seawater-immersed anticorrosive coatings: Mapping of parameters affecting the rate

Abstract: Cathodic delamination is one of the major modes of failure for organic coatings immersed in seawater and refers to the weakening or loss of adhesion between the coating and the substrate. The diminished adhesion is the result of electrochemical reactions occurring at the coating-steel interface, where solid iron is oxidized to ferrous ions and oxygen is reduced to hydroxyl ions. In this work, the effects of various parameters on cathodic delamination have been investigated.
The parameters are: permeability of the coating, concentration of dissolved oxygen and cations, polarization potential, type of binder, degree of curing, and pigment loading, shape and type. The results show that cathodic delamination increases with increasing concentration of cations up to the point where the concentration of dissolved oxygen becomes insufficient to maintain the corrosion rate. The rate of cathodic delamination is inversely proportional to the magnitude of polarization potential when ions can penetrate the coating, while cathodic polarization does not affect cathodic delamination when the ionic transport is restricted to the coating-steel interface. Increasing the pigment loading or partial replacement of spherical pigments with flake-shaped micaceous iron oxide or aluminium pigments reduces the rate of cathodic delamination. Finally, binders with an increasing amount of secondary hydroxyl groups in the polymer backbone reduce the rate of cathodic delamination while increasing the initial molar ratio of amide to epoxide increases cathodic delamination. (C) 2010 Elsevier B.V. All rights reserved.
Cathodic delamination: Quantification of ionic transport rates along coating-steel interfaces

So-called cathodic delamination is one of the major modes of failure for organic coatings immersed in electrolyte solutions (e.g. seawater). Cathodic delamination occurs as a result of the electrochemical reactions, which takes place on a corroding steel surface. This means that reactants must continuously be transported from the bulk solution to the cathodic areas. The transport of sodium ions from a defect in the coating to the cathodic areas is generally considered the rate-determining step for cathodic delamination because the transport of oxygen and water through the coating is sufficient for the corrosion processes. In this work, a novel practical method, which allows direct estimation of the apparent diffusion coefficient of sodium ions in the ultrathin aqueous layer at the coating-steel interface, is described. The apparent diffusion coefficients estimated are of similar magnitude as previously reported values and show an acceptable repeatability. The method was used to obtain the apparent diffusion coefficients of sodium ions in the coating-steel interface for three commercial inert-pigmented epoxy coatings. The delamination rates predicted using the apparent interfacial diffusion coefficients and Fick's second law, under the assumption of a transport controlled mechanism, show qualitative agreement with the observed delamination rates in 0.5 M sodium chloride. This confirms that the rate-determining step of cathodic delamination is the transport of sodium ions along the coating-steel interface. (C) 2009 Elsevier B.V. All rights reserved.
Cathodic delamination: Quantification of ionic transport rates along coating-steel interfaces

So-called cathodic delamination is one of the major modes of failure for organic coatings immersed in electrolyte solutions (e.g. seawater). Cathodic delamination occurs as a result of the electrochemical reactions, which takes place on a corroding steel surface. This means that reactants must continuously be transported from the bulk solution to the cathodic areas. The transport of sodium ions from a defect in the coating to the cathodic areas is generally considered the rate-determining step for cathodic delamination because the transport of oxygen and water through the coating is sufficient for the corrosion processes. In this work, a novel practical method, which allows direct estimation of the apparent diffusion coefficients of sodium ions in the ultrathin aqueous layer at the coating-steel interface, is described. The apparent diffusion coefficients estimated are of similar magnitude as previously reported values and show an acceptable repeatability. The method was used to obtain the apparent diffusion coefficients of sodium ions in the coating-steel interface for three commercial inert-pigmented epoxy coatings. The delamination rates predicted using the apparent interfacial diffusion coefficients and Fick's second law, under the assumption of a transport-controlled mechanism, show qualitative agreement with the observed delamination rates in 0.5 M sodium chloride. This confirms that the rate-determining step of cathodic delamination is the transport of sodium ions along the coating-steel interface.
Continuous Production of Pharmaceuticals

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, H. Lundbeck A/S
Authors: Christensen, K. M. (Ekstern), Pedersen, M. J. (Ekstern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Skovby, T. (Ekstern), Holm, T. L. (Ekstern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266154
Publication: Research › Conference abstract for conference – Annual report year: 2010

Design of Continuous Processes for Organic-Synthesis Based Production of Active Pharmaceutical Ingredients - a Methodology

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Cervera Padrell, A. E. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Kiil, S. (Intern), Skovby, T. (Ekstern)
Publication date: 2010

Development of epoxy-based self-healing anticorrosive coating

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Department of Biotechnology
Authors: Nesterova, T. (Intern), Pedersen, L. T. (Intern), Dam-Johansen, K. (Intern), Kiil, S. (Intern)
Number of pages: 2
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266148
Publication: Research › Conference abstract for conference – Annual report year: 2010

Mathematical modeling of simultaneous solvent evaporation and chemical curing in thermoset coating.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Publication date: 2010
Moving from batch toward continuous organic-chemical pharmaceutical production

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, CHEC Research Centre
Authors: Cervera Padrell, A. E. (Intern), Gernaey, K. (Intern), Gani, R. (Intern), Kiil, S. (Intern), Skovby, T. (Ekstern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 266261
Publication: Research › Poster – Annual report year: 2010

Quantification of simultaneous solvent evaporation and chemical curing in thermoset coatings
The mechanisms of simultaneous solvent evaporation and film formation in high-solids thermoset coatings are considered. The relevant phenomena, chemical reactions, solvent diffusion and evaporation, gelation, vitrification, network mobility restrictions, and crosslinking, are quantified and a mathematical model for a curing film is presented, which does not violate the local volume balance. For model verification, a previous investigation with a polyisocyanate and a polyol in methyl amyl ketone solvent, catalyzed by an organotin compound, was selected. In contrast to earlier modelling studies, simulations can match and explain detailed experimental data. For exemplification, simulations are used to analyse the influence of the various rate phenomena on the behavior of the solvent-based polyisocyanate/polyol film.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Coatings Technology and Research
Volume: 7
Issue number: 5
ISSN (Print): 1547-0091
Ratings:
BFI (2017): BFI-level 1
Reduction of cathodic delamination rates of anticorrosive coatings using free radical scavengers

Cathodic delamination is one of the major modes of failure for anticorrosive coatings subjected to a physical damage and immersed in seawater. The cause of cathodic delamination has been reported to be the result of a chemical attack at the coating-steel interface by free radicals and peroxides formed as intermediates in the cathodic reaction during the corrosion process. In this study, antioxidants (i.e., free radical scavengers and peroxide decomposers) have been incorporated into various generic types of coatings to investigate the effect of antioxidants on the rate of cathodic delamination of epoxy coatings on cold rolled steel. The addition of <5 wt% free radical scavengers to epoxy coatings improved the resistance toward cathodic delamination by up to 50% during seawater immersion, while peroxide decomposers had a limited effect. Testing using substrates prepared from stainless steel, copper, aluminum, galvanized steel, and brass also showed a reduction in the rate of cathodic delamination when the coating was modified with a free radical scavenger. The protective mechanism of free radical scavengers investigated for the primers are similar to that of antioxidants used for protection against photochemical degradation by UV-radiation of top coatings. Both substrate corrosion and degradation of a coating exposed to UV-radiation lead to the formation of free radicals as reactive intermediates.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Sørensen, P. A. (Intern), Weinell, C. E. (Ekstern), Dam-Johansen, K. (Intern), Kiil, S. (Intern)
Pages: 773-786
Publication date: 2010
Main Research Area: Technical/natural sciences
Replacement of traditional seawater-soluble pigments by starch and hydrolytic enzymes in polishing antifouling coatings

The use of starch and hydrolytic enzymes as replacement for traditional polishing pigments (e.g., Cu2O and ZnO) in antifouling coatings has been investigated. The enzymes facilitate a slow conversion of water-insoluble starch into water-soluble glucose, and dissolution of glucose causes the development of a leached (porous) layer in the wetted, outermost part of the coating. Subsequent water-binder interaction at the pore walls gives rise to polishing, in a manner similar to that of conventional antifouling coatings. Different starch types have been evaluated and classified as potential coating ingredients, and the impact of the addition of starch on the functional properties of the coating is described. Starches from rice, corn, and tapioca have been tested, and due to a smaller amount of water-soluble content and lesser tendency to agglomerate, corn starch is preferred. Leaching occurs in all the starch-enzyme coatings tested; however, polishing is only detected for two out of four binder systems investigated. Suitable polishing rates of 7-10 μm/month, based on the enzymatic starch-degradation, have been measured. Controls containing only starch (no enzyme) did not polish.

General information
State: Published
Solventafdampning, kemisk reaktion og netværksdannelse i en og samme maling

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Pages: 16-20
Stability of Enzymes in Granular Enzyme Products for Laundry Detergents

Enzymes have long been of interest to the detergent industry due to their ability to improve the cleaning efficiency of synthetic detergents, contribute to shortening washing times, and reduce energy and water consumption, provision of environmentally friendlier wash water effluents and fabric care. However, incorporating enzymes in detergent formulations gives rise to numerous practical problems due to their incompatibility with and stability against various detergent components. In powdered detergent formulations, these issues can be partly overcome by physically isolating the enzymes in separate particles. However, enzymes may lose a significant part of their activity over a time period of several weeks.

Possible causes of inactivation of enzymes in a granule may be related to the release of hydrogen peroxide from the bleaching chemicals in a moisture-containing atmosphere, humidity, autolysis of enzymes, high local pH in granule, oxygen, defects in granulate structure and the effect of other detergent components. However, the actual mechanism of inactivation is not known yet. It is believed that a combination of the factors mentioned above plays a role in the activity loss, and is the focus of this study.

The inactivation kinetics of technical grade enzyme powder was determined in a newly developed experimental setup, which was simple and effective and provided a better control over test conditions and fast sample generation. The method was based on the generation of hydrogen peroxide vapor and humidity by bubbling nitrogen gas through their corresponding solutions. An enzyme column, acting as a plug-flow reactor, was exposed to known concentrations of H$_2$O$_2$ (g) and humidity in a thermally stabilized chamber. Samples were analyzed for adsorptive behavior and residual enzyme activity.

Since the moisture is believed to play an important role in the stability of proteins, the monolayer hydration level of Savinase® was experimentally determined and theoretically calculated. Adsorbed moisture was found to have 3 a negative effect on enzyme activity. Below monolayer hydration level, the enzyme stability was significantly conserved, while at multilayer hydration level, especially when samples were exposed to 100% RH, the activity was reduced by 80% in a one week period. Since no auto-proteolytic activity and covalently-bound aggregate formation were detected, humidity possibly induced formation of unfavorable conformational changes, resulting in a decrease in enzyme’s catalytic efficiency.

Exposure to H$_2$O$_2$ (g) and humidity also resulted in significant H$_2$O$_2$ adsorption. The amount of adsorbed H$_2$O$_2$ did not depend on humidity in the gas stream, which implied that water and H$_2$O$_2$ were not competing for the same adsorption sites. In addition, the desorption studies revealed that while moisture was adsorbed by physisorption, H$_2$O$_2$ was adsorbed by either chemisorption or possibly involving formation of strong hydrogen bonds.

Inactivation of the solid-state enzyme was caused by the mutual effect of hydration and H$_2$O$_2$ (g) concentration. A simple mechanism for solid-state enzyme oxidation was proposed and the kinetic parameters in the resulting rate expression were derived. A good agreement between the derived equation and experimental data was obtained. The enzyme inactivation was found to depend on the square of moisture adsorbed by the enzyme at the corresponding temperature. The inverse of the reaction rate constant was also proportional to the inverse of H$_2$O$_2$ in the system.

Activity loss was expected to be caused by the oxidation of the enzyme by H$_2$O$_2$ vapor. The oxidative alterations on Savinase® were investigated by peptide mapping. Molecular mass examination of CNBr-cleaved fragments by MALDI TOF mass spectroscopy located the oxidation-labile residue. Due to its relatively accessible position on the exterior of the enzyme structure, only methionine 222 (Met 222) was oxidized; while other 2 Met residues, buried in the peptide backbone, remained unaffected. Being adjacent to the active site of Savinase®, Met 222 oxidation resulted in conformational and electrostatic shift in the catalytic site, causing a significant reduction of enzyme activity. The findings are in agreement with previously reported H$_2$O$_2$-induced oxidation studies of Savinase® in solutions.

Preliminary formulation studies were conducted and application of the designed setup on stability measurements of...
commercial granulates was illustrated. Addition of salts resulted in a considerable conservation of enzyme activity. Having an anti-oxidative property, sodium thiosulphate had a better activity-preservation effect compared to sodium carbonate. Due to a possible crack formation on granulate surface and/or deliquescence of sodium thiosulphate at high humidity showed that mixing the antioxidant homogeneously with the enzyme provided better protection than coating the salt as a separate layer. The effect of site-directed mutagenesis on Savinase® stability was illustrated and possible stability enhancing additives for enzyme granulates were proposed.

The present study is the first to report the solid-state inactivation kinetics and mechanism of Savinase®, subjected to controlled concentrations of $H_2O_2$ vapor and humidity. It provides practical information on solid-state stability measurements of biocatalysts in oxidative environments.
Anticorrosive coatings: a review

The main objective of this review is to describe some of the important topics related to the use of marine and protective coatings for anticorrosive purposes. In this context, "protective" refers to coatings for containers, offshore constructions, wind turbines, storage tanks, bridges, rail cars, and petrochemical plants while "marine" refers to coatings for ballast tanks, cargo holds and cargo tanks, decks, and engine rooms on ships. The review aims at providing a thorough picture of state-of-the-art in anticorrosive coatings systems. International and national legislation aiming at reducing the emission of volatile organic compounds (VOCs) have caused significant changes in the anticorrosive coating industry. The requirement for new VOC-compliant coating technologies means that coating manufacturers can no longer rely on the extensive track record of their time-served products to convince consumers of their suitability for use. An important aspect in the development of new VOC-compliant, high-performance anticorrosive coating systems is a thorough knowledge of the components in anticorrosive coatings, their interactions, their advantages and limitations, as well as a detailed knowledge on the failure modes of anticorrosive coatings. This review, which mainly deals with European experience and practice, includes a description of the different environments an anticorrosive coating system may encounter during service. In addition, examples of test methods and standards for determination of the performance and durability of anticorrosive coatings have been included. The different types of anticorrosive coatings are presented, and the most widely applied generic types of binders and pigments in anticorrosive coatings are listed and described. Furthermore, the protective mechanisms of barrier, sacrificial, and inhibitive coatings are outlined. In the past decades, several alternatives to organic solvent-borne coatings have reached the commercial market. This review also presents some of these technologies and discusses some of their advantages and limitations. Finally, some of the mechanisms leading to degradation and failure of organic coating systems are described, and the reported types of adhesion loss are discussed.

General information

State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Sørensen, P. A. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 135-176
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information

Journal: JCT Research
Volume: 6
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ISSN (Print): 1547-0091
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.409 SNIP 0.614
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.45 SJR 0.421 SNIP 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.5 SJR 0.51 SNIP 1.062
Cathodic delamination: Quantification of ionic transport rates along coating-steel interfaces

**General information**

State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Sørensen, P. A. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Weinell, C. (Ekstern)
Publication date: 2009

**Host publication information**

Title of host publication: Coatings Science Internation : Book of Abstracts
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 256364
Publication: Research › Article in proceedings – Annual report year: 2009

Design of controlled release systems for antifouling coatings

**General information**

State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Publication date: 2009
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 258245
Publication: Research › Paper – Annual report year: 2009
Inactivation of a solid-state detergent protease by hydrogen peroxide vapor and humidity

An experimental study on solid-state stability of a detergent protease (Savinase®) is reported. The inactivation kinetics of technical grade enzyme powder was determined as a function of gas phase H2O2 concentration and humidity by employing a quick assay running over few hours instead of several weeks as typical in industry. The results indicated that enzymes adsorbed significant amounts of moisture and H2O2 during exposure. The amount of adsorbed H2O2 did not depend on humidity in the gas stream, which implied that water and H2O2 were not competing for the same adsorption sites. Inactivation of the solid-state enzyme was caused by the mutual effect of increasing hydration and H2O2 (g) concentration. No auto-proteolytic activity or covalently bound aggregate formation was detected. A simple mechanism for solid-state enzyme oxidation was proposed and the kinetic parameters in the resulting rate expression of inactivation were derived. A good agreement between the derived equation and experimental data was obtained. The oxidative alterations on Savinase® were investigated by peptide mapping. Molecular mass examination of CNBr-cleaved fragments by MALDI-TOF mass spectroscopy located the oxidation-labile residue. Only one methionine (Met 222) was oxidized, while other residues remained unaffected. The study provides practical information on solid-state stability measurements of biocatalysts in oxidative environments.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Novozymes A/S
Authors: Biran, S. (Intern), Jensen, A. D. (Intern), Kiil, S. (Intern), Bach, P. (Ekstern), Simonsen, O. (Ekstern)
Pages: 73-79
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biotechnology
Volume: 141
Issue number: 1-2
ISSN (Print): 0168-1656
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.978 SNIP 0.937
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.987 CiteScore 2.87
Web of Science (2015): Indexed yes
Influence of substrate topography on cathodic delamination of anticorrosive coatings

The cathodic delamination of a commercial magnesium silicate and titanium dioxide pigmented epoxy coating on abrasive cleaned cold rolled steel has been investigated. The rate of delamination was found to depend on interfacial transport from the artificial defect to the delamination front and thereby the substrate topography, whereas the coating thickness had little influence. The presence of a significant potential gradient between the anode and the cathode and the dependency of the delamination rate on the tortuosity of the steel surface suggests that cathodic delamination is controlled by migration of cations from the defect to the delamination front. This means that abrasive blasting, to some extent, can be applied to control and minimize the observed rate of cathodic delamination. The lifetime of the species causing disbondment suggested that sodium hydroxide or potassium hydroxide and not peroxide species or radicals are the causative agents at
free corrosion potential (i.e. without impressed current).

**General information**

State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Sørensen, P. A. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 142-149
Publication date: 2009
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Progress in Organic Coatings
Volume: 64
Issue number: 2-3
ISSN (Print): 0300-9440
Ratings:

- **BFI (2017): BFI-level 1**
- **Web of Science (2017): Indexed Yes**
- **BFI (2016): BFI-level 1**
- Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3
- **BFI (2015): BFI-level 1**
- Scopus rating (2015): SJR 0.849 SNIP 1.39 CiteScore 2.84
- **Web of Science (2015): Indexed yes**
- **BFI (2014): BFI-level 1**
- Scopus rating (2014): SJR 0.992 SNIP 1.566 CiteScore 2.8
- **Web of Science (2014): Indexed yes**
- **BFI (2013): BFI-level 1**
- Scopus rating (2013): SJR 1.03 SNIP 1.663 CiteScore 2.58
- **ISI indexed (2013): ISI indexed yes**
- **Web of Science (2013): Indexed yes**
- **BFI (2012): BFI-level 1**
- Scopus rating (2012): SJR 1.043 SNIP 1.862 CiteScore 2.39
- **ISI indexed (2012): ISI indexed yes**
- **Web of Science (2012): Indexed yes**
- **BFI (2011): BFI-level 1**
- Scopus rating (2011): SJR 0.884 SNIP 1.606 CiteScore 2.34
- **ISI indexed (2011): ISI indexed yes**
- **Web of Science (2011): Indexed yes**
- **BFI (2010): BFI-level 1**
- Scopus rating (2010): SJR 0.983 SNIP 1.537
- **Web of Science (2010): Indexed yes**
- **BFI (2009): BFI-level 1**
- Scopus rating (2009): SJR 0.867 SNIP 1.333
- **Web of Science (2009): Indexed yes**
- **BFI (2008): BFI-level 1**
- Scopus rating (2008): SJR 0.829 SNIP 1.298
- Scopus rating (2007): SJR 1.088 SNIP 1.362
- **Web of Science (2007): Indexed yes**
- Scopus rating (2006): SJR 1.243 SNIP 1.598
- **Web of Science (2006): Indexed yes**
- Scopus rating (2005): SJR 0.928 SNIP 1.168
- **Web of Science (2005): Indexed yes**
- Scopus rating (2004): SJR 0.692 SNIP 1.121
- **Web of Science (2004): Indexed yes**
- Scopus rating (2003): SJR 0.604 SNIP 1.497
- **Scopus rating (2002): SJR 1.037 SNIP 1.312**
Inorganic precursor peroxides for antifouling coatings

Modern antifouling coatings are generally based on cuprous oxide (Cu2O) and organic biocides as active ingredients. Cu2O is prone to bioaccumulation, and should therefore be replaced by more environmentally benign compounds when technically possible. However, cuprous oxide does not only provide antifouling properties, it is also a vital ingredient for the antifouling coating to obtain its polishing and leaching mechanism. In this paper, peroxides of strontium, calcium, magnesium, and zinc are tested as pigments in antifouling coatings. The peroxides react with seawater to create hydrogen peroxide and highly seawater-soluble ions of the metal. The goals have been to establish the antifouling potency of an antifouling coating that releases hydrogen peroxide as biocide, and to investigate the potential use of peroxides as water-soluble polishing and leaching pigments. The investigations have shown that it is possible to identify particulates that, when applied as pigments in antifouling coatings, will provide polishing and leaching rates comparable to those of Cu2O-based coatings. Furthermore, the combination of polishing and hydrogen peroxide leaching by a coating based on zinc peroxide in a suitable binder matrix provides antifouling properties exceeding those of a similar coating based entirely on zinc oxide.
Modelling the design and optimization of chemically active marine antifouling coatings, advances in marine antifouling coatings and technologies

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Yebra, D. (Ekstern)
Publication date: 2009

Publication information
Publisher: British Welding Research Association
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 258246
Publication: Research - peer-review › Book – Annual report year: 2009

Moving From Batch towards Continuous Organic-Chemical Pharmaceutical Production

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Computer Aided Process Engineering Center
Authors: Cervera Padrell, A. E. (Intern), Skovby, T. (Ekstern), Kiil, S. (Intern), Gani, R. (Intern), Gernaey, K. (Intern)
Publication date: 2009

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 252815
Publication: Research › Sound/Visual production (digital) – Annual report year: 2009

Quantification of gypsum crystal nucleation, growth, and breakage rates in a wet flue gas desulfurization pilot plant

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern)
Pages: 2746-2753
Publication date: 2009
Main Research Area: Technical/natural sciences
Spray Drying of Suspensions for Pharma and Bio Products: Drying Kinetics and Morphology
An experimental investigation of the spray drying behavior of droplets containing excipients and carrier materials used in the pharmaceutical and biotechnological industries has been conducted. Specifically, rice starch suspensions with different amounts of TiO₂, maltodextrin, dextrin, NaCl and Na₂SO₄ are dried. The drying rate is measured, and the morphology formation is mapped to obtain a more fundamental understanding of the drying process, which is very useful when designing product formulations. In the pilot spray dryer, droplet generation is based on the JetCutter technology and die droplets are dried under well-defined temperature and flow conditions. The droplets are sampled during drying to determine the drying rate, and the dried particles are collected for morphology analysis. The results show that reducing the water activity in a suspension of insolubles by adding various amounts of inorganic salts or carbohydrates causes an increase in the droplet temperature during spray drying resulting in a rather constant the drying rate. Further, the results show that small alterations in the droplet composition may significantly change the final particle morphology. The observed morphologies are discussed in detail.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Niro A/S, Novozymes A/S
Authors: Sloth, J. (Ekstern), Jørgensen, K. (Ekstern), Bach, P. (Ekstern), Jensen, A. D. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern)
Pages: 3657-3664
Publication date: 2009
Main Research Area: Technical/natural sciences

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Journal: Industrial & Engineering Chemistry Research
Volume: 48
Issue number: 7
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Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.066 SNIP 1.338 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.086 SNIP 1.24 CiteScore 2.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Crystallisation of Gypsum and Prevention of Foaming in Wet Flue Gas Desulphurisation (FGD) Plants

The aim of this project is to investigate two operational problems, which have been experienced during wet flue gas desulphurisation (FGD) operation, i.e. poor gypsum dewatering properties and foaming. The results of this work can be used for the optimization of wet FGD-plants in terms of reliability of operation and consistency of the gypsum quality obtained. This work may furthermore be of interest to other industrial systems in which foaming or gypsum crystallisation may take place. FGD is an industrial process, which removes sulphur dioxide (SO2) from flue gases generated by fossil fuel combustion at power plants and other heavy industries, thereby abating the detrimental effects known as “acid rain”. The majority of the 680 FGD-plants installed at power plants worldwide in 1999 (2.41×105 MWe) were using the wet FGD-technology. This process absorbs ~ 99 % of the SO2 by an alkaline slurry, where it is oxidised to sulphate (SO42-) and crystallised as gypsum (CaSO4·2H2O) - a commercial product. The crystallisation process and the operating conditions under which it takes place, will determine the particle size distribution (PSD), the crystal morphology and thereby the dewatering properties. Experiments in a falling film wet FGD pilot plant have shown a strong non-linear behaviour (in a ln(n(l))) vs. l plot) at the lower end of the particle size range, compared to the well-known linear “mixed suspension mixed product removal (MSMPR)” model. A transient population balance model, fitted to experimental breakage data, was able to model an increase in the fraction of small particles, but not to the extent observed for the experimental steady state PSD. A three-parameter, size-dependent growth model, previously used in the literature to describe sodium sulphate decahydrate (Na2SO4·10H2O) and potassium aluminium sulphate (KAl(SO4)2·12H2O) crystallisation, was able to describe the experimental data, indicating a surface integration controlled growth mechanism. The PSD at three full-scale wet FGD-plants were comparable to the gypsum produced in the pilot plant. However, the crystals had fewer distinct crystals faces and more rounded tuber resembling shapes. An episode with a deterioration in gypsum dewatering properties at unit 3 of Amager Power Plant was linked to a change in crystal morphology, possibly due to adsorption of growth retarding aluminium fluoride compounds at specific crystal faces. Excessive foaming within wet FGD-plants has been associated with a range of operational problems as well as an increased degree of SO2 absorption. Foaming agents include surfactants, macromolecules (such as polymers or proteins), and finely dispersed solids. The foaming ability of particles, electrolytes and buffers, present in a wet FGD-plant, has been investigated by laboratory scale Bikerman experiments. Adipic acid, as well as a combination of small particles and an electrolyte, have been demonstrated to generate weak transient foams. Pilot plant experiments showed an increased absorption efficiency of SO2 using a foaming solution of calcium chloride (CaCl2) with small quartz particles, compared to pure non-foaming tap water.
Lipase catalyzed glycerolysis processing is of industrial interest since it can be carried out at ambient temperatures and atmospheric pressures. Previously, glycerolysis conducted in a column packed with immobilized lipase were highly potential to ensure a high MAG formation in a short time. In spite of optimal reaction conditions a complex heterogeneous reactant mixture with a glycerol in oil emulsion occurs. Hence, the movement of material from phase to phase as well as through the catalyst pores becomes important since it can influence the performance of the immobilized enzyme reactor. To examine which basic features that need to be considered to obtain an industrially beneficial procedure continuous and
easily operated glycerolysis was studied in different lipase packed columns. Immobilized Candida antarctica lipase B was used to catalyze the glycerolysis reaction between glycerol and sunflower oil dissolved in a binary tert-butanol:tert-pentanol medium. Practical design-related issues such as required reaction time, enzyme capacity, expansion of the enzyme during wetting, and the effect of different column length-to-diameter ratios, fluid velocities and particle sizes of the enzymes were evaluated.

General information
State: Published
Organisations: Food Production Engineering, Department of Systems Biology, CHEC Research Centre, Department of Chemical and Biochemical Engineering, Danisco AS
Authors: Damstrup, M. (Intern), Jensen, A. D. (Intern), Kiil, S. (Intern), Sparsø, F. V. (Ekstern), Xu, X. (Intern)
Publication date: 2008

Evaluation method for the drying performance of enzyme containing formulations
A method is presented for fast and cheap evaluation of the performance of enzyme containing formulations in terms of preserving the highest enzyme activity during spray drying. The method is based on modeling the kinetics of the thermal inactivation reaction which occurs during the drying process. Relevant kinetic parameters are determined from differential scanning calorimeter (DSC) experiments and the model is used to simulate the severity of the inactivation reaction for temperatures and moisture levels relevant for spray drying. After conducting experiments and subsequent simulations for a number of different formulations it may be deduced which formulation performs best. This is illustrated by a formulation design study where 4 different enzyme containing formulations are evaluated. The method is validated by comparison to pilot scale spray dryer experiments.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Sloth, J. (Intern), Bach, P. (Ekstern), Jensen, A. D. (Intern), Kiil, S. (Intern)
Pages: 121-129
Publication date: 2008

Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.15
Foaming in Wet Flue Gas Desulfurization Plants. The Influence of Particles, Electrolytes, and Buffers

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern), Sønder, K. B. (Ekstern)
Pages: 3239-3246
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Volume: 47
Issue number: 9
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes

formulation design, downstream processing, enzyme production, differential scanning calorimetry, enzyme deactivation, kinetic parameters

DOIs:
10.1016/j.bej.2007.11.024
Source: orbit
Source-ID: 221466
Publication: Research - peer-review › Journal article – Annual report year: 2008
Skumproblemer i industrielle processer

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern), Sønder, K. B. (Ekstern)
Pages: 10-12
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 12
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
Adhesion between coating layers based on epoxy and silicone

The adhesion between a silicon tie-coat and epoxy primers, used in marine coating systems, has been studied in this work. Six epoxy coatings (with varying chain lengths of the epoxy resins), some of which have shown problems with adhesion to the tie-coat during service life, have been considered. The experimental investigation includes measurements of the surface tension of the tie-coat and the critical surface tensions of the epoxies, topographic investigation of the surfaces of cured epoxy coatings via atomic force microscopy (AFM), and pull-off tests for investigating the strength of adhesion to the silicon/epoxy systems. Calculations for determining the roughness factor of the six epoxy coatings (based on the AFM topographies) and the theoretical work of adhesion have been carried out. The coating surfaces are also characterized based on the van Oss-Good theory. Previous studies on the modulus of elasticity of the polymers involved have also been considered. It was found that adhesion problems might be due to inadequate wetting, the significantly different topographies, and differences in the mechanical strengths of the epoxies. Acid-base interactions calculated from the van Oss-Good theory were found useful in explaining the enhanced adhesion for some epoxy/silicone surfaces.
Applicability of a fiber-supported catalyst on a buchwald-hartwig Amination reaction

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Christensen, H. (Ekstern), Kiil, S. (Intern), Dam-Johansen, K. (Intern)
Pages: 956-965
Publication date: 2007
Characterization of pigment-leached antifouling coatings using BET surface area measurements and mercury porosimetry

In this work BET surface area measurements and mercury porosimetry are used to characterize leached layers formed when seawater-soluble pigments (Cu2O and ZnO) dissolve during accelerated leaching of simple antifouling coatings. Measurements on single-pigment coatings show that an increasing fraction of Cu2O or ZnO pigment particles becomes unavailable for dissolution when the concentration of the pigment decreases in the coating and the interparticle distance in the binder matrix becomes larger. Experimental data for a coating initially containing a mixture of Cu2O and TiO2 pigments suggest that a substantial fraction of the smaller and inert TiO2 particles may be lost from the coating upon dissolution of the larger Cu2O particles. This inert particle translocation effect is important to take into account when interpreting polishing and leaching data and when developing mathematical models of antifouling coating behaviour because the active binder surface area and porosity of the leached layer are substantially increased. A similar effect was not observed for a coating with a mixture of ZnO and TiO2 pigments. The two experimental methods are expected to be useful for practical analysis of leaching of seawater-soluble components from commercial antifouling coatings.
Design and Development of Biological, Chemical, Food and Pharmaceutical Products

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, The Danish Polymer Centre
Authors: Wesselingh, J. (Ekstern), Kiil, S. (Intern), Vigild, M. E. (Intern)
Publication date: 2007

Publication information
Publisher: John Wiley and Sons, Ltd.
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 208335
Publication: Research - peer-review › Journal article – Annual report year: 2007

Enzyme-based Antifouling Coatings

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Olsen, S. M. (Intern), Pedersen, L. (Ekstern), Kiil, S. (Intern), Laursen, M. (Ekstern), Dam-Johansen, K. (Intern)
Publication date: 2007

Publication information
Publisher: John Wiley and Sons, Ltd.
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 211041
Publication: Research - peer-review › Book – Annual report year: 2007
Enzyme-based antifouling coatings: a review

A systematic overview is presented of the literature that reports the antifouling (AF) protection of underwater structures via the action of enzymes. The overall aim of this review is to assess the state of the art of enzymatic AF technology, and to highlight the obstacles that have to be overcome for successful development of enzymatic AF coatings. The approaches described in the literature are divided into direct and indirect enzymatic AF, depending on the intended action of the enzymes. Direct antifouling is used when the enzymes themselves are active antifoulants. Indirect antifouling refers to the use of enzymes to release an active biocide with AF activity. For direct AF, several patents have been granted, and a commercial product has been launched. However, the achievement of an efficient broad-spectrum AF coating based on a single or a few enzymes has not yet been achieved. An indirect AF coating is not yet available commercially. The technology is mainly limited by the instability of substrate supply, whether the substrates are found in the surrounding seawater or in the coating itself. Legislative issues regarding which part(s) of an enzyme system should be regarded as biocidal for product registration purposes are also considered. The above question currently remains unanswered for technologies utilising indirect enzymatic AF.

General information

State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Electromagnetic Systems, Department of Electrical Engineering
Authors: Olsen, S. M. (Intern), Pedersen, L. T. (Intern), Laursen, M. (Ekstern), Kiil, S. (Intern), Dam-Johansen, K. (Intern)
Pages: 369-383
Publication date: 2007
Main Research Area: Technical/natural sciences

Publication information

Journal: Biofouling
Volume: 23
Issue number: 5
ISSN (Print): 0892-7014
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 0.989 SNIP 1.103 CiteScore 3.31
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.232 SNIP 1.138 CiteScore 3.23
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.291 SNIP 1.459 CiteScore 3.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.223 SNIP 1.262 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.027 SNIP 1.131 CiteScore 3.08
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.144 SNIP 1.403 CiteScore 3.2
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.937 SNIP 0.736
Web of Science (2010): Indexed yes
Enzyme Degradation during Spray Drying

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Sloth, J. (Intern), Bach, P. (Ekstern), Kiil, S. (Intern), Jensen, A. D. (Intern)
Publication date: 2007

Host publication information
Title of host publication: Book of Abstracts
Main Research Area: Technical/natural sciences
Conference: European Congress of Chemical Engineering - 6, Copenhagen, Denmark, 16/09/2007 - 16/09/2007
Source: orbit
Source-ID: 211021
Publication: Research - peer-review › Article in proceedings – Annual report year: 2007

Gypsum crystal degradation in wet Flue Gas Desulphurisation (FGD) Plants

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern)
Publication date: 2007
Event: Abstract from European Congress of Chemical Engineering - 6, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 209005
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2007

Marine Fouling and Antifouling, a Literature Survey

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Olsen, S. M. (Intern), Kiil, S. (Intern), Pedersen, L. T. (Ekstern)
Continuous and easily operated glycerolysis was studied in different lipase-packed columns to evaluate the most potential process set-ups for industrial monoacylglycerol (MAG) production. Practical design-related issues such as enzyme-filling degree, required reaction time, mass transfer investigations, and capacity and stability of the enzyme were evaluated. A commercially available immobilized Candida antarctica lipase B was used to catalyze the glycerolysis reaction between glycerol and sunflower oil dissolved in a binary tert-butanol:tert-pentanol medium. Considering easy handling of the enzyme and measured expansion when wetted with a reaction mixture, a filling degree of 52 vol % dry enzymes particles per column volume seemed appropriate. Twenty minutes was required to reach equilibrium conditions with a MAG content of 50-55 wt %. Only insignificant indications of mass transfer limitations were observed. Hence, the commercial lipase seemed adequate to use in its available particle size distribution ranging from 300 to 900 μm. A column length-to-diameter ratio of less than 25 did not interfere with the transfer of the fluid mixture through the column. Under the tested conditions, the enzyme could be active for approximately 92 days before enzyme renewal was needed. This corresponds to a very high enzyme capacity with approximately 2000 L pure MAG produced per kg enzyme.
Teaching and Learning in Chemical Product Engineering - an Evolving par of the Chemical Engineering Curriculum

Over the last decade Chemical Product Engineering has evolved as part of the Chemical Engineering Curriculum at several universities in Europe and America. At the DTU Chemical Product Engineering was introduced in 2000. This presentation will report on the experiences gained from teaching classes and preparing a text book on the subject. [1] Chemical Product Engineering is solidly based on chemical technical and engineering knowledge. Furthermore, the subject naturally calls for a holistic approach to teaching and learning and introduces elements which target transferable and professional engineering skills. Such skills are important in Chemical Product Engineering when dealing with open-ended problems, creative problem solutions, operating in a team working environment and exercising project management. In our course we emphasise team activities, formative feedback to the students as well as helping the individual to become more assertive and understanding of personal assets. These teaching elements included in Chemical Product Engineering represent a series of general issues in Chemical Engineering Education, which must be discussed as the education is going to adapt to the changes of the surrounding world and a globalized society. In this presentation we will put Chemical Product Engineering into perspective with the EFCE recommendations on Chemical Engineering Education [2] and also relate curriculum discussions with the CDIO Initiative for producing the next generation of engineers. [3] [1] Design and Develop Bio, Chemical, Food and Pharma Products, to be published, Wiley & Sons, 2007. [2] Chemical Engineering Research and Design 83(A11), 1331 – 1334, 2005. [3] World Transactions on Engineering and Technology Education 2(1), 49-52, 2003.
Mathematical Modelling and Experimental Investigation of Full-scale Gypsum Producing Wet Flue Gas Desulphurisation

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Nygaard, H. (Intern), Johnsson, J. E. (Intern), Kill, S. (Intern), Dam-Johansen, K. (Intern)
Number of pages: 128
Publication date: Feb 2006
Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 186353
Publication: Research › Ph.D. thesis – Annual report year: 2006

Accelerated Optimisation of Chemically-Active of Paint Products

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Yebra, D. (Ekstern), Kill, S. (Intern), Weinell, C. (Ekstern), Dam-Johansen, K. (Intern)
Publication date: 2006
Event: Abstract from 13th International Conference on Marine Corrosion and Fouling, Rio de Janeiro, Brazil.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195807
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2006

Antifouling Paint Containing Enzymes as Active Antifoulant

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Olsen, S. (Ekstern), Kill, S. (Intern), Thorslund, L. (Ekstern), Laursen, M. (Ekstern), Dam-Johansen, K. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195791
Publication: Research › Conference abstract for conference – Annual report year: 2006
Dissolution rate measurements of sea water soluble pigments for antifouling paints: ZnO

The dissolution of soluble pigments from both tin-based and tin-free chemically active antifouling (AF) paints is a key process influencing their polishing and biocide leaching rates. In this context, a low time- and resources-consuming method capable of screening the pigment behaviour in the search for the most promising materials or mixtures is of great interest. A preliminary attempt to develop such a method is presented in this paper based on the widely used ZnO pigments.

While highly pure, nano-polished, monocrystalline ZnO substrates yielded very low dissolution rates in the order of $17.3 \pm 3.7 \mu g \text{Zn}^{2+} \text{cm}^{-2} \text{day}^{-1}$, pellets prepared by compacting and sintering technical grade ZnO pigments dissolved about three times faster according to inductively-coupled plasma mass spectrometry (ICP-MS) measurements. The rougher and more porous surface exposed, together with the larger number of defects in the lattice structure, are hypothesised to be responsible for the faster sea water attack of the pellets compared to the ZnO crystals. In any case, the ZnO dissolution rates reported in this paper are markedly lower than those associated with the sea water dissolution of cuprous oxide (Cu2O) particles which are also used in AF paints. Experimental performance testing of model antifouling paints formulated with ZnO and/or Cu2O demonstrates that the binder/pigment interaction should not be disregarded if the leaching of sea water soluble pigments from paint systems is to be determined. (C) 2006 Elsevier B.V. All rights reserved.
Drying of latex films and coatings: Reconsidering the fundamental mechanisms

The two existing theories describing drying of latex films or coatings are reconsidered. Subsequently, a novel mathematical drying model is presented, the simulations of which can match and explain experimental drying rate data of two previous investigations with latex films. In contrast to previous model studies, but in agreement with observations, simulations suggest that during the falling rate period of the drying process of a latex film, a porous skin of partly coalesced latex particles is indeed formed, which limits transport of water vapour from the receding air-liquid interphase to the surface of the film. The value of the effective diffusion coefficient of water vapour in the dry and partly coalesced layer (7 x 10(-7) m(2)/s at 19-24 degrees C), the adjustable parameter of the model for the falling rate period, was found to be independent of initial wet film thickness (89-1322 mu m), latex particle size (500-600 nm), initial polymer volume concentration (19-47 vol.%), and molecular weight of latex polymer (not quantified). Simulations also demonstrate that the transition from a constant to a falling drying rate in all cases takes place when the polymer volume concentration of the latex film is equal to that of hexagonal closest packed monodisperse spheres (74 vol.%). Consequently, the model has predictive properties and model inputs are only needed on the specific experimental (or field) conditions of interest. The effects on drying time of variations in relative humidity, wet film thickness, initial polymer volume concentration, and air flow velocity are simulated and analysed using the new model. (c) 2006 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Pages: 236-250
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Progress in Organic Coatings
Volume: 57
Issue number: 3
ISSN (Print): 0300-9440
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.849 SNIP 1.39 CiteScore 2.84
Effect of Solvents on the Product Distribution and Reaction Rate of a Buchwald-Hartwig Amination Reaction

The Buchwald-Hartwig amination reaction between p-bromotoluene and piperazine in the presence of the homogeneous catalytic system Pd(dba)$_2$/(+/-)BINAP and the base NaO-t-Bu was investigated in two different classes of solvents: aprotic, nonpolar and aprotic, polar. The reaction was carried out using microwaves as the heating source, and it was found that the product distribution was strongly dependent on the class of the solvent. Based on the experimental results the selectivity towards the desired monosubstituted aryl piperazine was calculated, and it was found that the most appropriate solvent for the Buchwald-Hartwig amination reaction under the conditions applied was m-xylene.
Effects of marine microbial biofilms on the biocide release rate from antifouling paints – A model-based analysis

The antifouling (AF) paint model of Kiil et al. [S. Kiil, C.E. Weinell, M.S. Pedersen, K. Dam-Johansen, Analysis of self-polishing antifouling paints using rotary experiments and mathematical modelling, Ind. Eng. Chem. Res. 40 (2001) 3906-3920] and the simplified biofilm growth model of Gujer and Warmer [W. Gujer, O. Warmer, Modeling mixed population biofilms, in: W.G. Characklis, K.C. Marshall (Eds.), Biofilms, Wiley-Interscience, New York, 1990] are used to provide a reaction engineering-based insight to the effects of marine microbial slimes on biocide leaching and, to a minor extent, polishing behaviour of AF paints. It is concluded that the perturbation of the local sea water conditions (e.g. pH), as a consequence of the metabolic activity of the biofilm should not affect the net biocide leaching and binder reaction rates significantly. This results from the thin and poorly active biofilms which presumably grow onto the highly effective modern AF paints. According to simulations, the experimental decrease in the biocide leaching rate caused by biofilm growth must be mainly attributed to adsorption of the biocide by the exopolymeric substances secreted by the microorganisms. The effects of biofilms on the leaching of any generic active compound (e.g. natural antifoulants) are discussed in relation to their potential release mechanisms. The largest influence of biofilms is predicted for those active compounds that are released by a diffusion-controlled mechanism (typically tin-free algaecides). (c) 2006 Elsevier B.V. All rights reserved.
Efficient monoacylglycerol processing by enzymatic glycerolysis in organic media: -Evaluation of immobilized Candida antarctica lipase B behavior

General information
State: Published
Organisations: Food Production Engineering, Department of Systems Biology, CHEC Research Centre, Department of Chemical and Biochemical Engineering, Danisco AS
Authors: Damstrup, M. (Intern), Kiil, S. (Intern), Jensen, A. (Intern), Sparsø, F. V. (Ekstern), Xu, X. (Intern)
Publication date: 2006
Event: Poster session presented at 97th AOCS Annual Meeting & Expo, St. Louis, MO, United States.
Main Research Area: Technical/natural sciences
Source-ID: 191266
Publication: Research – peer-review › Journal article – Annual report year: 2006

Enzymes in Antifouling Coatings, a review

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Olsen, S. (Ekstern), Kiil, S. (Intern), Thorslund, L. (Ekstern), Laursen, M. (Ekstern), Dam-Johansen, K. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source-ID: 191345
Publication: Research › Poster – Annual report year: 2006

Evaluation of Binary Solvent Mixtures for Efficient Monoacylglycerol Production by Continuous Enzymatic Glycerolysis
Formation of Enzyme Containing Granules by Spray Drying

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Sloth, J. (Intern), Kiil, S. (Intern), Jensen, A. D. (Intern), Bach, P. (Ekstern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195787
Publication: Research › Conference abstract for conference – Annual report year: 2006

Gypsum Crystallisation in Wet Flue Gas Desulphurisation (FGD)

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, B. B. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195808
Publication: Research › Poster – Annual report year: 2006

Målinger i absorptionskolonnen på Asnæsværket

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Hansen, J. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern), Dam-Johansen, K. (Intern), Nygaard, H. G. (Ekstern)
Pages: 10-14
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 4
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Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Mathematical Modeling of Tin-Free Chemically-Active Antifouling Paint Behavior

Mathematical modeling has been used to characterize and validate the working mechanisms of tin-free, chemically-active antifouling (AF) paints. The model-based analysis of performance data from lab-scale rotary experiments has shown significant differences between antifouling technologies as regards the biocide leaching and the surface polishing processes. Hence, the modeling framework developed in this work is built so as to describe any generic, chemically-active AF paint through model parameters, the values of which can be obtained or adjusted from relatively fast measurements. The detailed quantitative information on reacting AF paint systems obtained can be used for accelerated product optimization purposes, thus facilitating the transition to cleaner antifouling technologies using, for example, fast-degrading natural or synthetic bioactive components. (c) 2006 American Institute of Chemical Engineers.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, The Hempel Foundation Coatings Science and Technology Centre (CoaST), Hempel AS
Authors: Yebra, D. M. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 1926-1940
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: A I Ch E Journal
Volume: 52
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.034 SNIP 1.268 CiteScore 3.11
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.085 SNIP 1.417 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.07 SNIP 1.332 CiteScore 2.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Model based analysis of the drying of a single solution droplet in an ultrasonic levitator

A model for the drying of a single solution droplet into a solid, dense particle is presented and simulations are made to achieve a more fundamental understanding of the single droplet drying process relevant in connection with spray drying processes. Model predictions of drying behaviour are compared to data for the drying of aqueous solutions of maltodextrin DE 15 and trehalose from experiments conducted using an ultrasonic levitator. Model predictions are in good agreement with the experimental data, indicating that the model describes the most important physical phenomena of the process.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, GEA Niro A/S, Freidrich-Alexander-University of Erlangen-Nürnberg
Novel Non-Aqueous Acrylic Nanodispersions in Controlled-Release Self-Polishing Antifouling Paints

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Publication date: 2006
Event: Abstract from 13th International Conference on Marine Corrosion and Fouling, Rio de Janeiro, Brazil.
Main Research Area: Technical/natural sciences
Source-ID: 188777
Publication information
Journal: Research - peer-review › Journal article – Annual report year: 2006

Parametric Study of Tin-Free Antifouling Model Paint Behavior Using Rotary Experiments

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Yebra, D. M. (Ekstern), Kiil, S. (Intern), Erik Weinell, C. (Intern), Dam-Johansen, K. (Intern)
Pages: 1636-1649
Publication date: 2006
Main Research Area: Technical/natural sciences
Publication information
Journal: Industrial & Engineering Chemistry Research
Volume: 45
ISSN (Print): 0888-5885
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Presence and effects of marine microbial biofilms on biocide-based antifouling paints

Marine microorganisms are capable of successfully colonizing toxic surfaces through the formation of biofilm structures. In this article, most of the literature reporting the presence of marine biofilms on chemically-active antifouling paints is briefly reviewed. Of special concern is the influence of the dense extracellular polymeric substances (EPS) matrix on the release
rate of the compounds involved in antifouling paint performance (i.e. active compounds and controlled-release binder molecules). A deeper understanding of these phenomena is of interest for both environmental legislators and paint formulators.

**General information**
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Hempel A/S
Authors: Yebra, D. M. (Ekstern), Kiil, S. (Intern), Erik Weinell, C. (Intern), Dam-Johansen, K. (Intern)
Pages: 33-41
Publication date: 2006
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Biofouling
Volume: 22
Issue number: 1
ISSN (Print): 0892-7014

**Ratings:**
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 0.989 SNIP 1.103 CiteScore 3.31
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.232 SNIP 1.138 CiteScore 3.23
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.291 SNIP 1.459 CiteScore 3.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.223 SNIP 1.262 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.027 SNIP 1.131 CiteScore 3.08
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.144 SNIP 1.403 CiteScore 3.2
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.937 SNIP 0.736
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.325 SNIP 1.909
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.821 SNIP 0.64
Scopus rating (2007): SJR 0.876 SNIP 1.456
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.907 SNIP 1.145
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.689 SNIP 0.653
Scopus rating (2004): SJR 0.72 SNIP 0.962
Scopus rating (2003): SJR 0.557 SNIP 1.329
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.614 SNIP 0.735
Scopus rating (2001): SJR 0.519 SNIP 0.627
Scopus rating (2000): SJR 0.623 SNIP 1.171
Scopus rating (1999): SJR 0.681 SNIP 1.149

Original language: English
Production of Heat Sensitive Monoacylglycerols by Enzymatic Glycerolysis in Tert-pentanol: Process Optimization by Response Surface Methodology

The aim of this study was to optimize production of MAG by lipase-catalyzed glycerolysis in a tert-pentanol system. Twenty-nine batch reactions consisting of glycerol, sunflower oil, tert-pentanol, and commercially available lipase (Novozym®435) were carried out, with four process parameters being varied: Enzyme load, reaction time, substrate ratio of glycerol to oil, and solvent amount. Response surface methodology was applied to optimize the reaction system based on the experimental data achieved. MAG, DAG, and TAG contents, measured after a selected reaction time, were used as model responses. Well-fitting quadratic models were obtained for MAG, DAG, and TAG contents as a function of the process parameters with determination coefficients (R²) of 0.89, 0.88, and 0.92, respectively. Of the main effects examined, only enzyme load and reaction time significantly influenced MAG, DAG, and TAG contents. Both enzyme amount and reaction time showed a surprisingly nonlinear relationship between factors (process parameters) and responses, indicating a local maximum. The substrate ratio of glycerol to oil did not significantly affect the MAG and TAG contents; however, it had a significant influence on DAG content. Contour plots were used to evaluate the optimal conditions for the complex interactions between the reaction parameters and responses. The optimal conditions established for MAG yield were: enzyme load, 18% (w/w of oil); glycerol/oil ratio, 7:1 (mol/mol); solvent amount, 500% (vol/wt of oil); and reaction time, 115 min. Under these conditions, a MAG content of 76% (w/w of lipid phase) was predicted. Verification experiments under optimized reaction conditions were conducted, and the results agreed well with the range of predictions.

General information
State: Published
Organisations: Food Production Engineering, Department of Systems Biology, CHEC Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Danisco AS
Authors: Damstrup, M. L. (Intern), Jensen, T. (Ekstern), Sparsø, F. V. (Ekstern), Kiil, S. Z. (Intern), Jensen, A. D. (Intern), Xu, X. (Intern)
Pages: 27-33
Publication date: 2006
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the American Oil Chemists' Society
Volume: 83
Issue number: 1
ISSN (Print): 0003-021X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.696 SNIP 0.905 CiteScore 1.64
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.682 SNIP 0.997 CiteScore 1.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.767 SNIP 1.043 CiteScore 1.68
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.809 SNIP 1.074 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.871 SNIP 1.236 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.833 SNIP 1.292 CiteScore 1.98
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.763 SNIP 1.056
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.863 SNIP 1.183
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 0.667 SNIP 1.037
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.663 SNIP 0.891
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.658 SNIP 0.851
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.706 SNIP 0.973
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.73 SNIP 0.993
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.761 SNIP 1.145
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.977 SNIP 1.172
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.911 SNIP 1.245
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.735 SNIP 1.126
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.918 SNIP 1.278

Original language: English
Candida antarctica lipase, Glycerolysis, Monoacylglycerols, Response surface methodology (RSM), Sunflower oil, Tert-pentanol

DOIs:
10.1007/s11746-006-1171-5
Source: orbit
Source-ID: 197294
Publication: Research - peer-review › Journal article – Annual report year: 2006

Scale Up of Pharmaceutical Production of Organic Chemical Compounds

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Christensen, H. (Ekstern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Nielsen, O. (Ekstern), Sommer, M. (Ekstern)
Publication date: 2006
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 195790
Publication: Research › Conference abstract for conference – Annual report year: 2006

Spraytørring ved fremstilling af enzymholdige partikler

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Determination of inactivation mechanism of enzymes in laundry detergents

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Biran, S. (Intern), Jensen, A. D. (Intern), Kiil, S. (Intern), Bach, P. (Ekstern), Simonsen, O. (Ekstern)
Pages: S96-S96
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biotechnology
Volume: 118
ISSN (Print): 0168-1656
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.978 SNIP 0.937
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.068 SNIP 0.987 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.113 SNIP 1.144 CiteScore 2.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.173 SNIP 1.188 CiteScore 3.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.255 SNIP 1.312 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.157 SNIP 1.064 CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Enzymatisk produktion af monoglycerider

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Damstrup, M. (Ekstern), Jensen, A. (Intern), Kiil, S. Z. (Intern), Sparsø, F. (Ekstern), Xu, X. (Ekstern)
Pages: 27-30
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Dansk Kemi
Volume: 86
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 186377
Publication: Research › Journal article – Annual report year: 2005

Enzymatisk produktion af monoglycerider
Experimental investigation of the degradation rate of adipic acid in wet flue gas desulphurisation plants

Biofouling on ship hulls is prevented by the use of antifouling (A/F) paints. Typically, sea water soluble rosin or rosin-derivatives are used as the primary means of adjusting the polishing rate of the current chemically active self-polishing paint systems to a suitable value. Previous studies have shown that mathematical coating models based on a fundamental knowledge of the underlying mechanisms of A/F paints is a promising tool for accelerated product testing at different operational conditions of a sailing ship or a paint rotor. Such models can also be used for generation of ideas aiming at product optimisation and innovation (e.g. incorporation of natural active agents). This study seeks to attain scientifically founded knowledge of the reaction mechanisms and the rate of reaction with sea water of a Zn-carboxylate of a synthetic rosin compound. The kinetic expression attained can be used as input to mathematical models describing the behaviour of rosin-containing tin-free A/F paints. The experimental procedures developed can be easily implemented by marine paint companies for the screening of novel controlled-release binder materials for A/F paints. As a first step, it is demonstrated that the degradation of this Zn-containing rosin-derivative by sea water plays a key role in the polishing mechanism of paints formulated with such a resin. Then, the relevant literature available on the sea water behaviour of rosin and rosin-based binders is reviewed. Subsequently, two experimental procedures for the reaction rate estimation of the selected rosin-derived resin are presented; one is based on a gravimetric approach while the other uses flame atomic absorption spectroscopy (FAAS) to determine the total Zn2+ released by the resin. Both methods yield well-defined reaction conditions and sufficiently high accuracies. The latter is important because very low steady state reaction rates (about 0.70 +/- 0.26 mu g Zn(2+)cm(-2)day(-1) at 25 degrees C and pH 8.2) are measured. Steady state reaction rates of Cu2+- and Mg2+-derivatives are also determined and discussed. The experimental procedures developed are used to investigate the influence of NaCl concentration (12-52 g/l), pH (7.8-8.5) and sea water temperature (10-35 degrees C) on the rate of reaction of the Zn-carboxylate. Within that range of sea water conditions, the following kinetic expression is found to describe the steady state Zn2+ release rate resulting from the reaction of the Zn-carboxylate with sea water:
where the natural logarithm of the pre-exponential factor, In (A), is 18.0 +/- 2.5 (the unit of A being the same as k(1)), the activation energy, E-a, is 18.5 +/- 6.0 kJ/mol and the reaction order with respect to the hydroxide ion concentration, a, is 0.86 +/- 0.42. L-znR is the estimated solubility product of the ZnR resin which has a value of 3.1 x 10(-12) (mol/l)(-3) (about 6 mg Zn2+/l in equilibrium). The low value of the activation energy is believed to result from the complex reaction mechanisms hypothesised rather than pointing at a certain diffusion control in the reaction rate experiments. The reverse reaction is found not to affect the hydrolysis rate within the pores, of antifouling paints significantly. It is concluded, from the reaction mechanism proposed, that the observed partial exchange of Zn2+ for Cu2+ in the resin structure during paint dispersion and immersion results in a lower reaction rate compared to the pure ZnR. Cu-carboxylate has a reaction rate of about 5.8 +/- 1.0 mu g CuR cm(-2) day(-1) at 25 degrees C and pH 8.2. The presence of Mg and Na compounds (probably Mg- and Na-resinate) in the solid paint film has also been detected, and will influence the reaction rate by modifying the ZnR exposed surface area. (c) 2005 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Meseguer Yebra, D. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 256-275
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Progress in Organic Coatings
Volume: 53
Issue number: 4
ISSN (Print): 0300-9440
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.849 SNIP 1.39 CiteScore 2.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.992 SNIP 1.566 CiteScore 2.8
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.03 SNIP 1.663 CiteScore 2.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.043 SNIP 1.862 CiteScore 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.884 SNIP 1.606 CiteScore 2.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.983 SNIP 1.537
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.867 SNIP 1.333
Solvent Optimization for Efficient Enzymatic Monoacylglycerol Production Based on a Glycerolysis Reaction

This study was aimed at screening solvent systems of varying polarities to identify suitable solvents for efficient and practical enzymatic glycerolysis. Several pure solvents and solvent mixtures were screened in a batch reaction system consisting of glycerol, sunflower oil, and Novozymo (R) 435 lipase. Out of 13 solvents tested, tert-butanol and tert-pentanol were the only pure solvents suitable for a fast glycerolysis reaction with an acceptably high formation of MAG. In these systems, MAG contents of 68-82% were achieved within a few hours. Mixtures of tert-butanol/hexane, tert-pentanol/hexane, and tert-butanol/tert-pentanol in varying ratios also gave high MAG contents (58-78%). The tertiary alcohols tert-butanol and tert-pentanol, or mixtures of one of them with hexane, seemed to be the best choice among the solvents tested with respect to reaction efficiency, practical industrial applications, and steric hydroxyl group hindrance, which suppresses the ester formation with FA.

General information
State: Published
Organisations: Food Production Engineering, Department of Systems Biology, CHEC Research Centre, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Danisco AS
Authors: Damstrup, M. (Intern), Jensen, T. (Ekstern), Sparsø, F. V. (Ekstern), Kiil, S. (Intern), Jensen, A. (Intern), Xu, X. (Intern)
Pages: 559-564
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: J A O C S
Volume: 82
Issue number: 8
ISSN (Print): 0003-021X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.696 SNIP 0.905 CiteScore 1.64
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.682 SNIP 0.997 CiteScore 1.66
Web of Science (2015): Indexed yes
Candida antarctica lipase, Glycerolysis, Monoacylglycerols, Organic solvents, Sunflower oil, Tertiary alcohols

DOIs:
10.1007/s11746-005-1109-y
Source: orbit
Source-ID: 184229
Publication: Research - peer-review › Journal article – Annual report year: 2005

Antifouling technology-past, present and future steps towards efficient and environmentally friendly antifouling coatings

The imminent ban of environmentally harmful tributyltin (TBT)-based paint products has been the cause of a major change in the antifouling paint industry. In the past decade, several tin-free products have reached the commercial market, and claimed their effectiveness as regards the prevention of marine biofouling on ships in an environmentally friendly manner. The main objective of this review is to describe these products in as much detail as possible based on the knowledge available in the open literature. This knowledge has been supplemented by means of performance data provided, upon request, by some of the paint-producing companies. An exhaustive review of the historical development of antifouling systems and a detailed characterisation of sea water are also included. The need for studies on the behaviour of
chemically active paints under different sea water conditions is emphasised. In addition, the most common booster biocides used to replace TBT-containing compounds are listed and described. It must be stressed that there is still a lack of knowledge of their potential environmental side effects.

The current interest in providing innovative antifouling technologies based on an improved understanding of the biological principles of the biofouling process is also considered in this review. From the analysis of the factors affecting the biofouling process, the interference with the settlement and attachment mechanisms is the most promising environmentally benign option. This can be accomplished in two main ways: imitation of the natural antifouling processes and modification of the characteristics of the substrate. The former mostly focuses on the study of the large amount of secondary metabolites secreted by many different marine organisms to control the fouling on their surfaces. The many obstacles that need to be overcome for the success of this research are analysed. The potential development of broad-spectrum efficient coatings based on natural antifoulants is far from commercialisation. However, exploitation of a weakening of biofouling adhesion by means of the non-stick and fouling-release concepts is at a rather advanced stage of development. The main advantages and drawbacks of these systems are presented along with a brief introduction to their scientific basis. Finally, other alternatives, which may eventually give rise to an efficient and environmentally benign antifouling system, are outlined. (C) 2003 Elsevier B.V. All rights reserved.

**General information**

State: Published  
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering  
Authors: Yebra, D. M. (Intern), Kiil, S. (Intern), Dam-Johansen, K. (Intern)  
Pages: 75-104  
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Main Research Area: Technical/natural sciences

**Publication information**

Journal: Progress in Organic Coatings  
Volume: 50  
Issue number: 2  
ISSN (Print): 0300-9440  
Ratings:  
BFI (2017): BFI-level 1  
Web of Science (2017): Indexed Yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.89 SJR 0.852 SNIP 1.3  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.849 SNIP 1.39 CiteScore 2.84  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.992 SNIP 1.566 CiteScore 2.8  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.03 SNIP 1.663 CiteScore 2.58  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.043 SNIP 1.862 CiteScore 2.39  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.884 SNIP 1.606 CiteScore 2.34  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.983 SNIP 1.537  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 0.867 SNIP 1.333  
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.829 SNIP 1.298
Scopus rating (2007): SJR 1.088 SNIP 1.362
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.243 SNIP 1.598
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.928 SNIP 1.168
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.692 SNIP 1.121
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.604 SNIP 1.497
Scopus rating (2002): SJR 1.037 SNIP 1.312
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.619 SNIP 0.92
Scopus rating (2000): SJR 0.857 SNIP 1.132
Scopus rating (1999): SJR 0.723 SNIP 1.167
Original language: English
chemical product design, biofouling, antifouling paint, tin-free, biocides, fouling-release
DOIs:
10.1016/j.porgcoat.2003.06.001
Source: orbit
Source-ID: 116866
Publication: Research - peer-review › Review – Annual report year: 2004

Forskningscentret CHEC

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Pages: 1-5
Publication date: 2004
Main Research Area: Technical/natural sciences

Publication information
Journal: Forskning i Bioenergi
Volume: 1
Issue number: 5
ISSN (Print): 1604-6331
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Original language: Danish
Source: orbit
Source-ID: 154163
Publication: Research › Journal article – Annual report year: 2004

Full-scale measurements of SO2 gas phase concentrations and slurry compositions in a wet flue gas desulphurisation spray absorber

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Pages: 1151-1164
Publication date: 2004
Main Research Area: Technical/natural sciences
Chemical Product Design - A new multidisciplinary teaching and research activity at Institut for Kemiteknik

General information
State: Published
Organisations: CERE – Center for Energy Ressources Engineering, Department of Chemical and Biochemical Engineering, CHEC Research Centre, Computer Aided Process Engineering Center
Authors: Kontogeorgis, G. (Intern), Kiil, S. (Intern), Abildskov, J. (Intern), Johannessen, T. (Intern), Dam-Johansen, K. (Intern)
Publication date: 2003

Host publication information
Title of host publication: Proceedings of the European Congress of Chemical Engineering
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 41347
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Chemical product engineering of antifouling paints using mathematical modeling

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Authors: Kiil, S. (Intern)
Publication date: 2003

Host publication information
Title of host publication: 7th International Conference on Chemical Engineering, Granada
Main Research Area: Technical/natural sciences
Conference: 7th International Conference on Chemical Engineering, Granada, Spain, 01/01/2003
Source: orbit
Source-ID: 41242
Publication: Research › Conference abstract in proceedings – Annual report year: 2003

Controlled drug delivery from swellable hydroxypropylmethylcellulose matrices: model-based analysis of observed radial front movements

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Dam-Johansen, K. (Intern)
Pages: 1-21
Publication date: 2003
Main Research Area: Technical/natural sciences
Estimation of Polishing and Leaching Behaviour of Antifouling Paints Using Mathematical Modelling: a Literature Review

The development of chemically active antifouling paints has traditionally been based on an empirical approach. Optimisation and evaluation of novel and existing products are frequently conducted by means of, for example, systematic paint rotary tests in the laboratory or at sea sites. In this review, the usefulness of combining rotary experiments with the development of detailed mathematical models of paint behaviour will be discussed with reference to the relevant literature. Mathematical models can generally be used in the design of suitable release systems for various active components such as proteins or biocides, as well as for the estimation of release rates from different compositions of paints under various seawater conditions. Insoluble matrix, soluble matrix and self-polishing paints will be considered. Simulations from recent publications that show the effects of dynamic changes in seawater on paint behaviour will be presented. Examples of potential uses of paint models for accelerated polishing and leaching tests and screening of novel paint components will also be discussed. Directions of future modelling work are suggested.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern), Pedersen, M. S. (Ekstern), Codolar, S. A. (Ekstern)
Pages: 37-43
Publication date: 2003
Main Research Area: Technical/natural sciences

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Journal: Biofouling
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Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 0.989 SNIP 1.103 CiteScore 3.31
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.232 SNIP 1.138 CiteScore 3.23
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.291 SNIP 1.459 CiteScore 3.81
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.223 SNIP 1.262 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.027 SNIP 1.131 CiteScore 3.08
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.144 SNIP 1.403 CiteScore 3.2
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.937 SNIP 0.736
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.325 SNIP 1.909
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.821 SNIP 0.64
Scopus rating (2007): SJR 0.876 SNIP 1.456
Web of Science (2007): Indexed yes
Experimental investigation of a pilot-scale jet bubbling reactor for wet flue gas desulphurisation

In the present work, an experimental parameter study was conducted in a pilot-scale jet bubbling reactor for wet flue gas desulphurisation (FGD). The pilot plant is downscaled from a limestone-based, gypsum producing full-scale wet FGD plant. Important process parameters, such as slurry pH, inlet flue gas concentration of SO2, reactor temperature, and slurry concentration of Cl- have been varied. The degree of desulphurisation, residual limestone content of the gypsum, liquid phase concentrations, and solids content of the slurry were measured during the experimental series.

The SO2 removal efficiency increased from 66.1% to 71.5% when the reactor slurry pH was changed from 3.5 to 5.5. Addition of Cl(in the form of CaCl2 . 2H(2)O) to the slurry (25 g Cl-/l) increased the degree of desulphurisation to above 99%, due to the onset of extensive foaming, which substantially increased the gas-liquid contact area. An increase in the inlet flue gas SO2 concentration from 502 to 991 ppmv led to a decrease in the SO2 removal efficiency from 80.1% to 69.4%. A temperature increase from 296 to 323 K caused a reduction in the degree of desulphurisation from 69.4% to 68.1%, but this result is almost within the experimental uncertainty. The residual limestone level in the gypsum formed increased with increasing values of reactor slurry pH, inlet flue gas SO2 concentration, and slurry concentration of Cl-. (C) 2003 Elsevier Ltd. All rights reserved.
Experimental Study of Drag Resistance using a Laboratory Scale Rotary Set-Up

This work covers an experimental study of the drag resistance of different painted surfaces and simulated large-scale irregularities, viz. dry spraying, weld seams, barnacle fouling and paint remains. A laboratory scale rotary set-up was used to determine the drag resistance, and the surface roughness of the samples was determined by means of two different stylus-based methods, one having a 1.6 mm ball stylus (giving the macro-roughness) and the other having a needle type stylus (giving the micro-roughness). It is demonstrated that, in the case of ideal painted surfaces (low macro-roughness), the micro-roughness is much more important than the macro-roughness. On the other hand, the study also indicates that larger scale irregularities have a much greater influence on the drag resistance compared to measurements of the paint system alone.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Dynamic simulations of a self-polishing antifouling paint exposed to seawater

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern), Pedersen, M. S. (Ekstern), Codolar, S. A. (Ekstern)
Pages: 45-54
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Coating Technology
Volume: 74
Issue number: 929
Original language: English
Source: orbit
Source-ID: 40882
Publication: Research - peer-review › Journal article – Annual report year: 2002

Erratum: Dynamic simulations of a self-polishing antifouling paint exposed to seawater

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Kiil, S. (Intern), Dam-Johansen, K. (Intern), Codolar, S. A. (Ekstern), Pedersen, M. S. (Ekstern), Erik Weinell, C. (Intern)
Number of pages: 3
Pages: 89-91
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Main Research Area: Technical/natural sciences

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Journal: Journal of Coatings Technology and Research
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Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.409 SNIP 0.614
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.45 SJR 0.421 SNIP 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.5 SJR 0.51 SNIP 1.062
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.46 SJR 0.534 SNIP 1.077
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.39 SJR 0.572 SNIP 1.364
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.24 SJR 0.517 SNIP 1.007
ISI indexed (2011): ISI indexed no
Mathematical modelling of a self-polishing antifouling paint exposed to seawater: A parameter study

A Fundamental mathematical model for a self-polishing antifouling paint was used to conduct a parameter study. The aims were to show how a mathematical model can reduce the amount of experimental work needed to estimate the behaviour of self-polishing antifouling paints at different conditions, and to suggest ways of controlling biocide release rates. A case study with an antifouling paint based on the well-known tributyltin self-polishing copolymer system showed that the rate of paint polishing was influenced, to various degrees, by the following parameters: seawater pH and concentration of NaCl, pigment particle size, pigment volume concentration of the paint, the rate of pigment dissolution, and the pore size distribution of the leached layer. The modelling approach can be applied to any type of self-polishing antifouling paint provided that kinetic, solubility and diffusivity data are available for the pertinent rate-influencing steps.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Pedersen, M. S. (Ekstern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 45-52
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Research & Design
Volume: 80
Issue number: 0
ISSN (Print): 0263-8762
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.813 SNIP 1.303 CiteScore 2.79
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 1.449 CiteScore 2.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.027 SNIP 1.692 CiteScore 2.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.957 SNIP 1.668 CiteScore 2.56
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.933 SNIP 1.614 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Seawater-Soluble Pigments and Their Potential Use in Self-Polishing Antifouling Paints: Simulation-based Screening Tool

This work concerns the on-going development of efficient and environmentally friendly antifouling paints for biofouling control on large ocean-going ships. It is illustrated how a detailed mathematical model for a self-polishing antifouling paint exposed to seawater can be used as a product engineering tool to obtain a quick estimate of the paint behaviour that a given seawater-soluble pigment will provide. In the present context, “pigment” refers to relevant particulate solids of organic-, inorganic-, or biological nature. Simulations performed at 15 and 30\degree C suggest that pigment solubility and seawater diffusivity of dissolved pigment species have a significant influence on the polishing and leaching behaviour of a typical self-polishing paint system. The pigment size distribution, on the other hand, only has a minor influence on the paint-seawater interaction. Simulations also indicate that only compounds which are effective against biofouling at very low seawater concentrations are useful as active antifouling paint ingredients. The need for model verification and exploration of practical issues, subsequent a given pigment has been found of interest, is discussed. The model approach is of relevance in the search for novel antifouling paints and for the development of accelerated test methods. (C) 2002 Elsevier Science B.V. All rights reserved.
Simulation studies of the influence of HCl absorption on the performance of a wet flue gas desulphurisation pilot plant

The mathematical model of Kiil et al., (Ind. Eng, Chem. Res. 37 (1998) 2792) for a wet flue gas desulphurisation (FGD) pilot plant was extended to include the simultaneous absorption of HCl. In contrast to earlier models for wet FGD plants, the inclusion of population balance equations for the limestone particles enabled a quantitative description of the influence of HCl absorption on essential process parameters such as the degree of desulphurisation and the residual limestone level of the gypsum produced.

Simulations showed that the presence of 100 ppmv HCl in the flue gas reduced the degree of desulphurisation from 85 to 84% and increased the residual limestone level of the gypsum from 2.1 to 2.4 wt%. It was found that these undesired effects from HCl absorption could be counteracted by adding adipic acid to the slurry in a concentration of about 1 mM. The influence of holding tank pH and the inlet flue gas concentration of SO2 on the degree of desulphurisation and the residual limestone level was found to be almost the same irrespective of HCl was present (100 ppmv) in the flue gas or not. The results presented are of importance in the analysis of the performance of wet FGD plants installed at power plants firing coals of varying Cl contents. (C) 2002 Elsevier Science Ltd. All rights reserved.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Nygaard, H. (Intern), Johnsson, J. E. (Intern)
Pages: 347-354
Publication date: 2002
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 57
Issue number: 3
ISSN (Print): 0009-2509
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Use of spray dry absorption product in wet flue gas desulphurisation plants: pilot-scale experiments

**General information**
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Zheng, Y. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern), Zhong, Q. (Ekstern)
Pages: 1899-1905
Publication date: 2002
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Fuel
Volume: 81
Issue number: 15
Original language: English
Source-ID: 40858
Publication: Research - peer-review • Journal article – Annual report year: 2002

Analysis of Self-Polishing Antifouling Paints Using Rotary Experiments and Mathematical Modeling

**General information**
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Stanley, M. (Ekstern), Dam-Johansen, K. (Intern), Erik Weinell, C. (Intern)
Pages: 3906-3920
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Industrial & Engineering Chemistry Research
Volume: 40
Issue number: 18
ISSN (Print): 0888-5885
Ratings:
Chemical Product Engineering - A Cross-centre Activity at Institut for Kemiteknik

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering, Center for Phase Equilibria and Separation Processes, Computer Aided Process Engineering Center, The Aerosol Laboratory
Publication date: 2001
Event: Abstract from Conference on Refocusing Chemical Engineering, Barga, Italy.
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 59685
Publication: Research › Conference abstract for conference – Annual report year: 2001

Optimisation of a wet FGD pilot plant using fine limestone and organic acids

The effects of adding an organic acid or using a limestone with a fine particle size distribution (PSD) have been examined in a wet flue gas desulphurisation (FGD) pilot plant. Optimisation of the plant with respect to the degree of desulphurisation and the residual limestone content of the gypsum has been the aim of the work. In contrast to earlier
investigations with organic acids, all essential process parameters (i.e. gas phase concentration profiles of SO(2), slurry pH profiles, and residual limestone in the gypsum) were considered. Slurry concentrations of adipic acid in the range of 0-7 mM were employed. The overall degree of desulphurisation in the plant increased from 83% at 0 mM to 90% at 3 mM and the residual limestone level was reduced from 4.6 to 1.4 wt%. Increasing the slurry concentration of adipic acid above 3 mM gave only a slightly higher degree of desulphurisation. The wet FGD model of Kill et al. (Ind. Eng. Chem. Res., 37 (1998) 2792) was extended to include buffer systems and verified against experimental data. Subsequently, the model was used as a tool to identify the optimal organic acid dissociation constants (as pK(a) values) and concentration levels at different operating conditions. At a holding tank pH of 5.5 and a temperature of 50 degreesC, simulations with Bryozo limestone and a monoprotic buffer suggested that the optimum pK(a) value is between 4.5-5.5 and 5.5-6.5 with respect to the degree of desulphurisation and the residual limestone level, respectively. Adipic acid has pK(a) values close to these ranges (pK(1) = 4.40 and pK(2) = 5.41 at 50 degreesC). Changing limestone type (in the absence of organic acids) to one with a lower average particle size (i.e. from 20 to 4 mum) increased the overall measured degree of desulphurisation from 83 to 87% and reduced the residual limestone level from 4.6 to 1.3 wt%. Increasing the holding tank pH level from 5.5 to 5.8 affected the degree of desulphurisation and the residual limestone level only slightly. At holding tank pH levels between 5.88 and 5.90, a high degree of desulphurisation was observed, but the residual limestone content in the gypsum increased to somewhere between 19 and 30 wt%, making this pH range unsuitable for use in a full-scale plant. The investigations have shown that both the addition of organic acids and the use of a limestone with a fine PSD can be used to optimise wet FGD plants. (C) 2001 Elsevier Science Ltd. All rights reserved.

General information
State: Published
Organisations: CHEC Research Centre, Department of Chemical and Biochemical Engineering
Authors: Frandsen, J. (Intern), Kiil, S. (Intern), Johnsson, J. E. (Intern)
Pages: 3275-3287
Publication date: 2001
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 56
Issue number: 10
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Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Sulfur Chemistry in Combustion II: Flue Gas Desulfurization

General information
State: Published
Organisations: Department of Applied Chemistry
Authors: Johnsson, J. E. (Intern), Kiil, S. (Intern)
Pages: 283-301
Publication date: 2000

Host publication information
Title of host publication: Pollutants From Combustion - Formation and Impact on Atmospheric Chemistry, C. Vovelle (ed.)
Publisher: NATO ASI Series, Kluwer Academic Publisher
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 173908
Publication: Research - peer-review › Article in proceedings – Annual report year: 2000

Forsøgskørsel på Amagerværket

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Amagerværket
Authors: Bruun, M. (Ekstern), Kiil, S. (Intern), Johnsson, J. E. (Intern)
Publication date: 1999

Publication information
Original language: Danish
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 175400
Lecture Notes on Liquid-Solid Reactions of Ship Bottom Paints Exposed to Seawater

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Number of pages: 17
Publication date: 1999

Publication information
Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
Used in DTU course 36223 Industrial Reaction Engineering
Source: orbit
Source-ID: 173824
Publication: Research - peer-review › Book – Annual report year: 1999

Literature Survey on Tin-based Selfpolishing Antifouling: Paints: Mechanisms and Modelling

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Number of pages: 65
Publication date: 1999

Publication information
Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
CHEC report 9903. Confidential
Source: orbit
Source-ID: 173825
Publication: Research - peer-review › Report – Annual report year: 1999

Modelling of Limestone Dissolution in Wet FGD Systems

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Applied Chemistry
Authors: Kiil, S. (Intern), Johnsson, J. E. (Intern), Dam-Johansen, K. (Intern)
Pages: 1-10
Publication date: 1999
Conference: Chemistry in Power Plants, Essen, 01/01/1999
Main Research Area: Technical/natural sciences

Publication information
Journal: Conference Proceedings for Power Plant Chemistry 1999
Volume: 1
Original language: English

Bibliographical note
CHEC paper 9924
Source: orbit
Source-ID: 173374
Publication: Research - peer-review › Journal article – Annual report year: 1999
Modelling of Limestone Dissolution in Wet FGD Systems: The Importance of an Accurate Particle Size Distribution

In wet flue gas desulphurisation (FGD) plants, the most common sorbent is limestone. Over the past 25 years, many attempts to model the transient dissolution of limestone particles in aqueous solutions have been performed, due to the importance for the development of reliable FGD simulation tools. In this work, a critical examination of the models was conducted. The survey revealed that the models rely on the use of adjustable parameters in order to match experimental data. To investigate this, a simple particle model was set up. Model predictions were compared to experimental data for three different Danish limestone types with very different particle size distributions (PSDs). All limestones were of a high purity. Model predictions were found to be qualitatively in good agreement with experimental data without any use of adjustable parameters. Deviations between measurements and simulations were attributed primarily to the PSD measurements of the limestone particles, which were used as model inputs. The PSDs, measured using a laser diffraction-based Malvern analyser, were probably not representative of the limestone samples because agglomeration phenomena took place when the particles were suspended in a liquid solution. The measured PSDs were sensitive to the addition of a dispersing agent, the dispersion time, and the presence of ultrasound. It was found that the different PSDs influenced the simulated rate of dissolution significantly (i.e. from below to above the measured dissolution rate). The results of this work show that a representative PSD is essential in order to model the rate of dissolution of limestone particles accurately.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Applied Chemistry
Authors: Kiil, S. (Intern), Johnsson, J. E. (Intern), Dam-Johansen, K. (Intern)
Pages: 26-30
Publication date: 1999
Main Research Area: Technical/natural sciences

Publication information
Journal: PowerPlant Chemistry
Volume: 1
Issue number: 5
ISSN (Print): 1438-5325
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ISI indexed (2013): ISI indexed no
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Original language: English
Source: orbit
Source-ID: 173372
Publication: Research - peer-review › Journal article – Annual report year: 1999

Experimental and Theoretical Investigations of Wet Flue Gas Desulphurisation
This thesis describes experimental and theoretical investigations of wet flue gas desulphurisation (FGD). A review of the current knowledge of the various rate determining steps in wet FGD plants is presented. The experimental work covers laboratory studies as well as pilot- and full-scale experiments. In the theoretical part of the work, the laboratory and pilot plant observations are investigated using mathematical modelling. The mechanism underlying the rate of dissolution of finely grinded limestone particles was examined in a laboratory batch apparatus using acid titration. Three Danish limestones of different origin were tested. A transient, mass transport controlled, mathematical model was developed to describe the dissolution process. Model predictions were found to be qualitatively in good agreement with experimental data. Deviations between measurements and simulations were attributed primarily to the particle size distribution (PSD) measurements of the limestone particles, which were used as model inputs. The measured PSD was probably not representative of a given limestone sample because of agglomeration phenomena taking place in the disperser, preventing a stable and accurate measurement. Other factors, such as convective mass transfer, porosity and porosity changes, and perhaps surface reaction, may also influence the rate of dissolution. However, those effects could not, due to the uncertainty of the PSD, be confirmed. Empirical correlations for the dimensionless mass transfer coefficients in a pilot plant (falling- film column) were determined. The correlations are valid at gas phase Reynolds numbers from 7500 to 18,300 and liquid phase Reynolds numbers from 4000 to 12,000, conditions of industrial relevance. The presence of inert particles in the liquid phase was found to decrease the rate of gas phase mass transport with up to 15 %, though the effect could not be correlated. A detailed model for a wet FGD pilot plant, based on the falling film principle, was developed. All important rate determining steps, absorption of SO2, oxidation of HSO3-, dissolution of limestone, and crystallisation of gypsum were included. Model predictions were compared to experimental data such as gas phase concentration profiles of SO2, slurry pH profiles, solids contents of the slurry, liquid phase concentrations, and residual limestone in the gypsum. Simulations were found to match experimental data for the two Danish limestone types (Faxe Bryozo and a chalk, Mikrovit) investigated. Gas phase mass transport was found to be the dominating rate determining step, though the liquid phase mass transport resistance could not be neglected. Simulations and experimental data both showed the same degree of desulphurisation and absorber pH profile for the two limestone types using a holding tank pH of 5.5, but the residual limestone in the gypsum was significantly lower for the chalk. Furthermore, simulations showed that between 10 and 30 % of the limestone dissolves in the absorber depending on the process conditions. A typical holding tank pH of 5-
5.5 (also used in full-scale wet FGD packed towers) was found to be a reasonable compromise between residual limestone in the gypsum and the degree of desulphurisation. Simulations were only slightly sensitive to the temperature in the interval 313 - 333 K, pertinent for full-scale wet FGD packed towers. The possibility of co-firing straw and coal was investigated in a full-scale power plant. No effects on the overall performance of the wet FGD plant were observed, though laboratory experiments with fine dust and fly ash from the full-scale experiments showed a decrease in limestone reactivity. However, the test period was only about one week, probably not allowing the FGD plant to reach steady state operation. Pilot-scale experiments were initiated to investigate the possibility of oxidising dry scrubber by-products (TASP) to gypsum in wet FGD plants. The investigations showed that it was possible to oxidise the TASP at concentrations of up to 300 g/litre (feed tank basis). The residual Ca(OH)₂ in the TASP could be exploited for desulphurisation resulting in a reduced limestone consumption and an increased removal rate of SO₂. The simultaneous presence of Al³⁺ and F⁻ did not, as reported in the literature, inhibit the rate of dissolution. The results of this work demonstrate that mathematical modelling can be a powerful tool in the process of obtaining a detailed understanding of the complex interactions between chemical reactions and mass transport phenomena in wet FGD plants.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Number of pages: 115
Publication date: 1998

**Publication information**

Place of publication: Vedbæk
Publisher: Tekst & Tryk A/S
ISBN (Print): 87-90142-30-6
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 170267
Publication: Research - peer-review › Book – Annual report year: 1998

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**Experimental Investigation and Modelling of a Wet Flue Gas Desulphurisation Pilot Plant**

A detailed model for a wet flue gas desulphurisation (FGD) pilot plant, based on the packed tower concept, has been developed. All important rate determining steps, absorption of SO₂, oxidation of HSO₃⁻, dissolution of limestone, and crystallisation of gypsum were included. Population balance equations, governing the description of particle size distributions of limestone in the plant, were derived. Model predictions were compared to experimental data such as gas phase concentration profiles of SO₂, slurry pH-profiles, solids content of the slurry, liquid phase concentrations, and residual limestone in the gypsum. Simulations were found to match experimental data for the two limestone types investigated. A parameter study of the model was conducted with the purpose of validating assumptions and extracting information on wet FGD systems. The modelling tools developed may be applicable to other wet FGD plants.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Michelsen, M. L. (Intern), Dam-Johansen, K. (Intern)
Pages: 2792-2806
Publication date: 1998
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Industrial & Engineering Chemistry Research
Volume: 37
Issue number: 7
ISSN (Print): 0888-5885
Ratings:
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
- Web of Science (2015): Indexed yes
Mass transfer in wetted-wall columns: correlations at high Reynolds numbers

The rate of gas-and liquid-phase mass transport in a pilot-scale wetted-wall column with an inner diameter of 3.26 cm and a length of 5 m was investigated. Empirical correlations for the physical liquid-phase mass transfer coefficient \( k(L)(O) \) and the gas-phase mass transfer coefficient \( k(G) \) were determined. In dimensionless form, the correlations are given by

\[
Sh(L) = 0.01613 \cdot Re \cdot G^{0.664} \cdot Re \cdot L^{0.426} \cdot Sc \cdot L^{0.5}
\]

\[
Sh(G) = 0.00031 \cdot Re \cdot G^{1.05} \cdot Re \cdot L^{0.207} \cdot Sc \cdot G^{0.5}
\]
and are valid at gas-phase Reynolds numbers from 7500 to 18,300 and liquid-phase Reynolds numbers from 4000 to 12,000, conditions of industrial relevance. To our knowledge, no correlations for Sh(G) have been reported in the literature which are valid at such high Reynolds numbers. The wetted-wall column was equipped with six intermediate measuring positions for gas and two for liquid samples, giving rise to a high accuracy of the obtained correlations. Our data showed that Sh(L) and Sh(G) both depend on Re-G and Re-L due to changes in the interfacial area at the high Reynolds numbers employed. The presence of inert particles in the liquid-phase may influence the rate of mass transport, and experimental work was initiated to study the effect on k(G). A decrease in k(G) of up to 15% was seen at solid concentrations ranging from 0 to 30 wt%, though the observed effect could not be correlated. (C) 1997 Published by Elsevier Science Ltd.
Solution of adsorption problems involving steep moving profiles

The moving finite element collocation method proposed by Kiil et al. (1995) for solution of problems with steep gradients is further developed to solve transient problems arising in the field of adsorption. The technique is applied to a model of adsorption in solids with bidisperse pore structures. Numerical solutions were found to match the analytical solution when it exists (i.e. when the adsorption isotherm is linear). Results of this application study show that the method is simple yet sufficiently accurate for use in adsorption problems with steep moving gradients, where global collocation methods fail or require a prohibitive number of collocation points. The technique is general in nature and may also be applied to a large variety of multiphase transient heat or mass transfer problems involving steep gradients.

General information

State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Queensland
Authors: Kiil, S. (Intern), Bhatia, S. K. (Ekstern)
Pages: 893-896
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information

Journal: Computers & Chemical Engineering
Volume: 22
Issue number: 7-8
ISSN (Print): 0098-1354
Ratings:
  BFI (2017): BFI-level 2
  Web of Science (2017): Indexed Yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 3.39 SJR 1.008 SNIP 1.607
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 1.122 SNIP 1.724 CiteScore 3.04
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.184 SNIP 1.738 CiteScore 3.22
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 1.223 SNIP 1.776 CiteScore 3.06
Wet Flue Gas Desulphurisation and New Fuels

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern), Dam-Johansen, K. (Intern), Michelsen, M. L. (Intern)
Number of pages: 115
Publication date: 1998

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 165837
Publication: Research - peer-review › Journal article – Annual report year: 1998
Modelling of wet FGD Pilot Plant

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering
Authors: Kiil, S. (Intern)
Number of pages: 25
Publication date: 1997

Publication information
Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
Internal report (not official CHEC report)
Source: orbit
Source-ID: 174287
Publication: Research - peer-review › Report – Annual report year: 1997

Full-scale co-firing of straw and coal

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, SK Power
Authors: Pedersen, L. S. (Ekstern), Michelsen, H. P. (Intern), Kiil, S. (Intern), Hansen, L. A. (Intern), Dam-Johansen, K. (Intern), Kildsig, F. (Ekstern), Christensen, J. (Ekstern), Jespersen, P. (Ekstern)
Pages: 1584-1590
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel
Volume: 75
Issue number: 13
Original language: English
Source: orbit
Source-ID: 165622
Publication: Research - peer-review › Journal article – Annual report year: 1996

Modelling of catalytic oxidation of NH3 and reduction of NO on limestone during sulphur capture
A theoretical study of the complex transient system of simultaneous sulphur capture and catalytic reactions of N-containing compounds taking place on a single limestone particle is conducted. The numerical technique developed previously by the authors (Kiil et al. 1994) based on collocation on moving finite elements is used to solve the model equations. To our knowledge, this is the first serious attempt to model such transient systems in detail. The particle is divided into moving zones, described by the reaction between limestone and SO2, and each zone is assigned a certain catalytic activity with respect to each species involved. An existing particle model, the Grain-Micrograin Model, which simulates sulphur capture on limestone under oxidizing conditions is considered in the modelling. Simulation results in good qualitative agreement with experimental data are obtained here for the catalytic chemistry of NH3 during simultaneous sulphur capture on a Stevns Chalk particle. The reduction of NO by NH3 over CaSO4 (which is the product of the reaction between SO2, O2 and limestone) was found to be important because this reaction could explain the change in selectivity with increased solid conversion observed experimentally. Simulations also suggested that it may be advantageous with respect to the emission of NO to use small instead of big limestone particles for desulphurisation in fluidised bed combustors due to the ways different sized particles capture SO2.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Queensland
Authors: Kiil, S. (Intern), Bhatia, S. K. (Ekstern), Dam-Johansen, K. (Intern)
Pages: 587-601
Publication date: 1996
Main Research Area: Technical/natural sciences

Publication information
Solution of transient problems with steep gradients: novel front-tracking strategy

A finite element collocation method is formulated for heat and mass transfer problems involving a steep moving profile of the dependant variable. An efficient, parametrically convergent front-tracking procedure is developed based on a balance on a moving front, and the technique is applied and tested for the case of a gas-solid noncatalytic reaction in a porous solid at high Thiele modulus. Accurate and convergent steep profiles are obtained here for Thiele modulus larger than 50 for the case of slab as well as spherical geometry and found to match the analytical solution when it exists (such as for slab geometry).

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, University of Queensland
Authors: Kiil, S. (Intern), Bhatia, S. K. (Ekstern), Dam-Johansen, K. (Intern)
Pages: 2793-2799
Publication date: 1995
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Engineering Science
Volume: 50
Issue number: 17
ISSN (Print): 0009-2509
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.05 SJR 1.037 SNIP 1.442
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.038 SNIP 1.606 CiteScore 2.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.115 SNIP 1.642 CiteScore 2.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.157 SNIP 1.866 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.189 SNIP 1.847 CiteScore 2.77
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.205 SNIP 1.685 CiteScore 2.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.319 SNIP 1.708
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.293 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.299 SNIP 1.6
Projects:

UV degradation and interlayer adhesion loss
Department of Chemical and Biochemical Engineering
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Wang, Ting (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Coatings for high pressure and high temperature
Department of Chemical and Biochemical Engineering
Period: 15/08/2017 → 14/08/2020
Number of participants: 4
Phd Student:
Ferrero, Gianni (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Novel testing methods for intumescent coating
Department of Chemical and Biochemical Engineering
Period: 15/10/2016 → 14/10/2019
Number of participants: 3
Phd Student:
Zeng, Ying (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Understanding Sulphuric Acid Accumulation in Lube oil in Diesel Engines
Department of Chemical and Biochemical Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 4
Phd Student:
Lejre, Kasper Hartvig (Intern)
Supervisor:
Fosbøl, Philip Loldrup (Intern)
Glarborg, Peter (Intern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Low friction non-fouling coatings for high fuel efficiency at reduced speed
Department of Chemical and Biochemical Engineering
Period: 01/08/2015 → 31/07/2018
Number of participants: 4
Phd Student:
Wang, Xueting (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Tullberg, Marcus (Ekstern)
Main Supervisor:
Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Sulcor - Securing Corrosion Free Conditions
Department of Chemical and Biochemical Engineering
Period: 01/07/2015 → 30/06/2018
Number of participants: 5
Phd Student: Nielsen, Henrik Lund (Intern)
Supervisor: Glarborg, Peter (Intern)
Kiil, Søren (Intern)
Thomsen, Kaj (Intern)
Main Supervisor: Fosbøl, Philip Loldrup (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Anti-stick coatings in the cement and mineral industries**
Department of Chemical and Biochemical Engineering
Period: 01/03/2015 → 31/08/2016
Number of participants: 4
Phd Student: Mørk, Kasper Skov (Intern)
Supervisor: Dam-Johansen, Kim (Intern)
Sivebæk, Ion Marius (Intern)
Main Supervisor: Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

**Continuous crystallization and filtration of Ective Pharmaceutical Ingredients and Intermediates for pharmaceutical production**
Department of Chemical and Biochemical Engineering
Period: 15/09/2014 → 14/09/2017
Number of participants: 5
Phd Student: Capellades Mendez, Gerard (Intern)
Supervisor: Christensen, Troels V. (Ekstern)
Dam-Johansen, Kim (Intern)
Mealy, Michael J. (Ekstern)
Main Supervisor: Kiil, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

**Protective Coatings in the Cement and Mineral Industry**
Department of Chemical and Biochemical Engineering
Period: 15/08/2014 → 02/10/2017
Number of participants: 3
Phd Student: Møller, Victor Buhl (Intern)
**Continuous crystallization and filtration in production of pharmaceuticals**

Department of Chemical and Biochemical Engineering  
**Period:** 15/12/2013 → 07/02/2014  
**Number of participants:** 3  
**PhD Student:** Visan, Aura (Ekstern)  
**Supervisor:** Dam-Johansen, Kim (Intern)  
**Main Supervisor:** Kiil, Søren (Intern)  
**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Samfinansierede - Virksomhed  
**Project:** PhD

**Design of hydrophilic polymers for activated non-fouling coatings**

Department of Chemical and Biochemical Engineering  
**Period:** 01/12/2013 → 15/03/2017  
**Number of participants:** 8  
**PhD Student:** Noguer, Albert Camós (Intern)  
**Supervisor:** Dam-Johansen, Kim (Intern)  
**Hvilsted, Søren (Intern)**  
**Olsen, Stefan Møller (Intern)**  
**Main Supervisor:** Kiil, Søren (Intern)  
**Examiner:** Szabo, Peter (Intern)  
**Bressy, Christine (Ekstern)**  
**Martínez, Eduardo Andrés (Ekstern)**  
**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Eksternt finansieret virksomhed  
**Project:** PhD

**Fuel Efficiency and Fouling Control Coatings in Maritime Transport**

Department of Chemical and Biochemical Engineering  
**Period:** 01/12/2011 → 30/09/2015  
**Number of participants:** 8  
**PhD Student:** Lindholdt, Asger (Intern)
Wind Turbine Blade Coatings with Anti-Erosion Properties

Department of Chemical and Biochemical Engineering
Period: 01/09/2011 → 26/11/2014
Number of participants: 7
PhD Student:
Zhang, Shizhong (Intern)

Supervisor:
Dam-Johansen, Kim (Intern)
Sørensen, Per Aggerholm (Intern)

Main Supervisor:
Kiil, Søren (Intern)

Examiner:
Szabo, Peter (Intern)
Stack, Margaret (Ekstern)
Sylvestor Nielsen, Kim (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Development of new materials for dielectric electroactive polymers as actuators and generators

Department of Chemical and Biochemical Engineering
Period: 15/08/2011 → 26/11/2014
Number of participants: 7
PhD Student:
Madsen, Frederikke Bahrt (Intern)

Supervisor:
Daugaard, Anders Egede (Intern)
Hvilsted, Søren (Intern)

Main Supervisor:
Skov, Anne Ladegaard (Intern)

Examiner:
Kiil, Søren (Intern)
Brook, Michael Adrian (Ekstern)
Graz, Ingrid Maria (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD
Design of continuous reactor systems for API production
Department of Chemical and Biochemical Engineering
Period: 01/08/2011 → 17/12/2014
Number of participants: 7
Phd Student: Pedersen, Michael Jønch (Intern)
Supervisor: Kiil, Søren (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor: Dam-Johansen, Kim (Intern)
Examiner: Gernaey, Krist V. (Intern)
Kappe, Oliver (Ekstern)
Petersen, Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Mathematical Modelling of vegetable oil crystallisation
Department of Chemical and Biochemical Engineering
Period: 01/05/2011 → 27/08/2014
Number of participants: 7
Phd Student: Hjorth, Jeppe Lindegaard (Intern)
Supervisor: Dam-Johansen, Kim (Intern)
Leth-Miller, Rasmus (Intern)
Main Supervisor: Kiil, Søren (Intern)
Examiner: Abildskov, Jens (Intern)
Flöter, Eckhard (Ekstern)
Schafer, Olivier (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Diversity screening for novel enzymes degrading synthetic polymers
Department of Chemical and Biochemical Engineering
Period: 01/02/2011 → 26/11/2014
Number of participants: 7
Phd Student: Lezyk, Mateusz Jakub (Intern)
Supervisor: Badia, Antoni Sánchez (Ekstern)
Kiil, Søren (Intern)
Main Supervisor: Mikkelsen, Jørn Dalgaard (Intern)
Examiner: Eliasson Lantz, Anna (Intern)
Derks, Patrick M.F. (Ekstern)
Visser, Jacob (Jaap) (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

**Design and testing of robust and efficient fire-retardant coatings**
Department of Chemical and Biochemical Engineering
Period: 01/01/2011 → 28/05/2014
Number of participants: 6
Phd Student: Nørgaard, Kristian Petersen (Intern)
Supervisor: Dam-Johansen, Kim (Intern)
Main Supervisor: Kiil, Søren (Intern)
Examiner: Jappe Frandsen, Flemming (Intern)
Deters, David C. (Ekstern)
Giovanni, Camino (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

**Analysis and Quantification of Foaming Phenomena in Wet Flue Gas Desulphurization Plants**
Department of Chemical and Biochemical Engineering
Period: 01/06/2010 → 03/02/2014
Number of participants: 6
Phd Student: Qin, Siqiang (Intern)
Supervisor: Hansen, Brian Brun (Intern)
Main Supervisor: Kiil, Søren (Intern)
Examiner: Jappe Frandsen, Flemming (Intern)
Fogh, Folmer (Ekstern)
Karlsson, Hans T. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Processes for Low CO2 Emissions**
Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 18/12/2013
Number of participants: 8
Phd Student: Pathi, Sharat Kumar (Intern)
Supervisor: Hjuler, Klaus (Ekstern)
Illerup, Jytte Boll (Intern)
Lin, Weigang (Intern)
Main Supervisor: 
Dam-Johansen, Kim (Intern)
Examiner: 
Kiil, Søren (Intern)
Jensen, Lars Skaarup (Intern)
Murillo, Ramón (Ekstern)

Examiner: 
Kiil, Søren (Intern)
Jensen, Lars Skaarup (Intern)
Murillo, Ramón (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Separation of Chiral Active Pharmaceutical Ingredients: A First Step Towards Continuous Preferential Crystallization in the Pharmaceutical Industry

Department of Chemical and Biochemical Engineering
Period: 01/01/2010 → 24/06/2013
Number of participants: 7
Phd Student:
Chaaban, Joussef Hussein (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Christensen, Troels V. (Ekstern)
Kalman Nagy, Zoltan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Stimuli-Adaptable Materials

Department of Chemical and Biochemical Engineering
Period: 01/05/2009 → 21/05/2013
Number of participants: 7
Phd Student:
Frankær, Sarah Maria Grundahl (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Kiil, Søren (Intern)
Main Supervisor:
Skov, Anne Ladegaard (Intern)
Examiner:
Hvilsted, Søren (Intern)
Hansen, Kristoffer Karsten (Intern)
Hietala, Sami (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Self-Healing anticorrosive coatings

Department of Chemical and Biochemical Engineering
Moving from batch towards continuous organic-chemical pharmaceutical production

Department of Chemical and Biochemical Engineering
Period: 01/08/2008 → 08/02/2012
Number of participants: 8
Phd Student:
Cervera Padrell, Albert Emili (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Kiil, Søren (Intern)
Skovby, Tommy (Ekstern)
Main Supervisor:
Gernaey, Krist V. (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Aelterman, Wim (Ekstern)
Hartman, Ryan L. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

High-Performance Anticorrosive Coatings

Department of Chemical and Biochemical Engineering
Period: 01/02/2007 → 04/06/2010
Number of participants: 7
Phd Student:
Sørensen, Per Aggerholm (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Jappe Frandsen, Flemming (Intern)
Gelling, Victoria J. (Ekstern)
Sørensen, Ole Borring (Ekstern)

Financing sources
Controlled Release of Environmentally Friendly Antifouling Agents from Marine Coatings

Department of Chemical and Biochemical Engineering
Period: 01/11/2005 → 01/04/2009
Number of participants: 7
PhD Student: Olsen, Stefan Møller (Intern)
Supervisor: Dam-Johansen, Kim (Intern)
Pedersen, Lars Thorslund (Intern)
Main Supervisor: Kil, Søren (Intern)
Examiner: Woodley, John (Intern)
Swain, Geoffrey W. (Ekstern)
Erik Weinell, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Gypsum Crystallisation and Foaming Prevention in Wet Flue Gas Desulphurization (FGD) Plants

Department of Chemical and Biochemical Engineering
Period: 01/03/2005 → 27/10/2008
Number of participants: 6
PhD Student: Hansen, Brian Brun (Intern)
Supervisor: Johnsson, Jan Erik (Intern)
Main Supervisor: Kil, Søren (Intern)
Examiner: Wedel, Stig (Intern)
Karlstsson, Hans T. (Ekstern)
Kristensen, Nicholas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Influence of Formulation in Formation of Enzyme Granules by Sparay Drying

Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 28/01/2007
Number of participants: 7
PhD Student: Sloth, Jakob (Intern)
Supervisor: Bach, Poul (Ekstern)
Jensen, Anker Degn (Intern)
Main Supervisor: Kil, Søren (Intern)
Examiner:
Woodley, John (Intern)
Hansen, Tomas T. (Ekstern)
Seville, Jonathan P. K. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Produktion af lægemidler
Department of Chemical and Biochemical Engineering
Period: 01/09/2004 → 25/02/2008
Number of participants: 7
Phd Student:
Christensen, Henrik (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Nielsen, Ole (Ekstern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Gernaey, Krist V. (Intern)
Buchwald, Stephen L. (Ekstern)
Dancer, Robert J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Emission fra cement produktion
Department of Chemical and Biochemical Engineering
Period: 01/02/2004 → 30/04/2007
Number of participants: 7
Phd Student:
Hu, Guilin (Intern)
Supervisor:
Hansen, Jens Peter (Intern)
Wedel, Stig (Intern)
Main Supervisor:
Dam-Johansen, Kim (Intern)
Examiner:
Kiil, Søren (Intern)
Hupa, Mikko (Ekstern)
Jensen, Lars Skaarup (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Process Development for the Enzymatic Production of Partial Acylglycerol
National Food Institute
Period: 01/11/2003 → 27/10/2008
Number of participants: 9
Phd Student:
Damstrup, Marianne (Intern)
Stability of Enzymes in Granular Enzyme Products for Laundry Detergents

Department of Chemical and Biochemical Engineering
Period: 01/09/2003 → 01/09/2010
Number of participants: 8
Phd Student:
Biran, Suzan (Intern)
Supervisor:
Bach, Poul (Ekstern)
Kiil, Søren (Intern)
Simonsen, Ole (Ekstern)
Main Supervisor:
Jensen, Anker Degn (Intern)
Examiner:
Mikkelsen, Jørn Dalgaard (Intern)
Cedervall, Tommy (Ekstern)
Hansen, Tomas T. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Efficient and environmentally friendly antifouling paints

Department of Chemical and Biochemical Engineering
Period: 01/05/2002 → 30/09/2005
Number of participants: 7
Phd Student:
Meseguer Yebra, Diego (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Erik Weinell, Claus (Intern)
Main Supervisor:
Kiil, Søren (Intern)
Examiner:
Villadsen, John (Intern)
Codolar, Santiago Arias (Ekstern)
Finansieringskilder
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Modellering af gipsproducerede røggasafsvovlingsanlæg
Department of Chemical and Biochemical Engineering
Period: 01/10/1999 → ...
Number of participants: 9
PhD Student:
Nygaard, Helle Gottschalk (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Fogh, Folmer (Ekstern)
Jensen, Jørgen Nørklit (Ekstern)
Kiil, Søren (Intern)
Main Supervisor:
Johnsson, Jan Erik (Intern)
Examiner:
Wedel, Stig (Intern)
Jensen, Flemming (Ekstern)
Karlsson, Hans T. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Alternative metoder til energieffektive stofadskillelser
Department of Chemical and Biochemical Engineering
Period: 01/06/1999 → 21/12/2003
Number of participants: 6
PhD Student:
Eden, Mario Richard (Intern)
Supervisor:
Gani, Rafiqul (Intern)
Main Supervisor:
Jørgensen, Sten Bay (Intern)
Examiner:
Kiil, Søren (Intern)
Cordiner, Joan (Ekstern)
Kraslawski, Andrzej (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Våd Røggasafsvovling
Technical University of Denmark
Number of participants: 4
PhD Student:
Kiil, Søren (Intern)
Supervisor:
CHEC
CHEC is an acronym for the fundamental and applied research programme on Combustion and Harmful Emission Control. CHEC’s main areas of expertise are industrial high-temperature processes, formation and removal of pollutants, particulate solids (characterisation, reactivity and dynamics). Within these areas the objectives are to educate scientists and engineers, to gain new fundamental information on the subjects, to assist industry and public authorities in the selection, development, design and operation of processes in order to improve efficiencies and in order to avoid or minimise harmful emissions, to catalyse international cooperation between Danish companies and Danish and foreign research organisations.

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Danish Maritime Institute
Danish Gas Technology Centre A/S
GasResearch Institute
Danish Technological Institute
Elsam A/S
Elkraft A.m.b.A.
ELTRA I/S
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National Risk Management Research Laboratory
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Nagoya University
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VVT Chemical Technology
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