

Biobased Chemistry and Technology Annual report 2015



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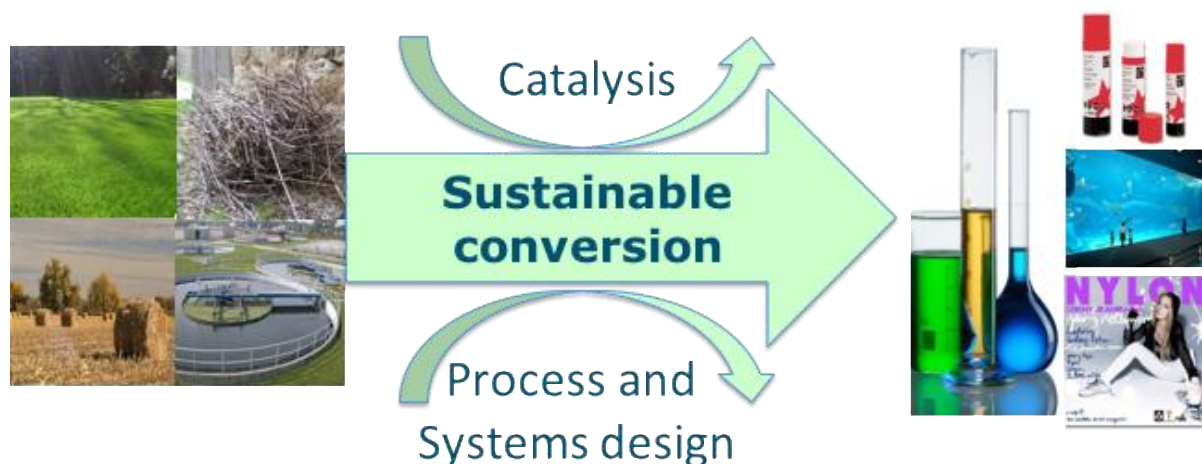
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Introduction

It is my pleasure to present to you the annual report 2015 of the Biobased Chemistry and Technology group. In 2015 we worked further on establishing our mission. We defined our mission as “BCT wants to develop sustainable conversion routes to aid in establishing a biobased economy”. To achieve that goal we defined two core research lines i.e catalysis and process and systems design.



The research lines are divided in three themes i.e conversion, technology and systems. In this report you can read some of the research highlights in these three fields. In the past year the group was subjected to peer review and we were happy to see that the review committee greatly appreciated the path which the group follows. Of course there are still challenges ahead. That is why we are also very happy that we received a.o. a research grant of the Dutch science foundation (partly co-financed by industry) in which our capabilities in conversion and process design are combined.

Biobased is also gaining in significance within education at WageningenUR. Projects are started to make a massive online open course (MOOC) on biobased sciences ranging from biomass production, conversion, refinery to economics, society and sustainability. Along the same line a procedure is started to set up a MSc curriculum on biobased sciences. The BCT group plays a crucial role in both.

For me this was an interesting and exiting year. I hope you feel the same after reading this report.

With kind regards

Prof. J.H. (Harry) Bitter
Chair holder Biobased Chemistry and Technology

Collaborations

The strategy of the BCT group is to develop fundamental insights in processes relevant for biobased conversions. Based on these fundamental insights we also want to suggest improvements in processes in the biobased field. Therefore collaborations with other groups within and outside Wageningen are established. Some of our collaborations are summarized in the table below.

At the end of 2015 discussions were started with other chemistry groups in Wageningen to establish the ‘Wageningen Institute of Chemistry’ (WIC). The WIC aims to promote and advance the chemistry research within Wageningen University.

Collaborating group in Wageningen	Topic
Environmental Technology (ETE)	Combining chemo and bio-electro-catalysis Modelling of water-energy-material nexus in industrial and urban environments
Bioprocess Engineering (BPE)	Modeling of algae systems
Wetsus	Waste water treatment and modeling
Organic chemistry (ORC)	Teaching and research proposals
Bionanotechnology (BioNT)	Combining catalysis and NMR in microreactors
Food and Biobased research (FBR)	Different research projects and acquisitions

The BCT group participates within Wageningen in the research schools VLAG and WIMEK and is part of the Netherlands Institute for Catalysis Research (NIOK) and the Institute for sustainable process technology (ISPT). In addition, the group participates in the Working Group on Drying (NWGD), the Dutch Process Control Initiative, the Dutch Institute for Systems and Control (DISC) and WETSUS.

The group collaborates intensively with other academic and industrial groups both within WageningenUR (DLO-FBR) and outside to address the multi-disciplinary character of the challenges (e.g., within EU projects, STW, BE-Basic, ISPT, Center for Biobased Economy (CBBE) and advisory boards such as the Biorenewables Business Platform).

Conversion Group

Staff: Dr. Elinor Scott, Dr. Piet Buwalda, Prof. Harry Bitter
PhD students and post-docs: Andrada But, Piet van der Zaal,
Luana Souza Macedo, Frits van der Klis, Roxani Chatzipanagiotou,
Xinhua Goerner-Hu, Gerben Wierda, Evie van der Wijst, Neus Blanch,
Tomas van Haasterecht
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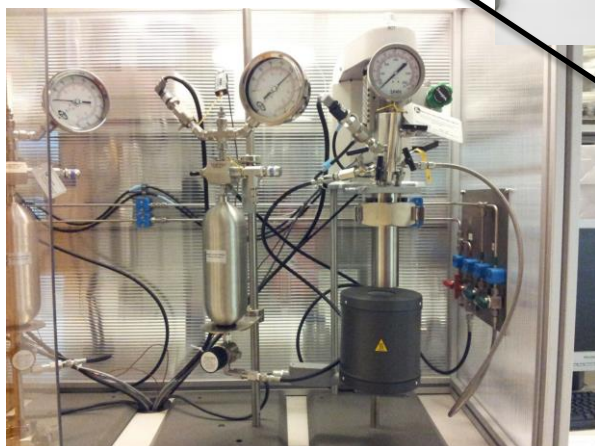
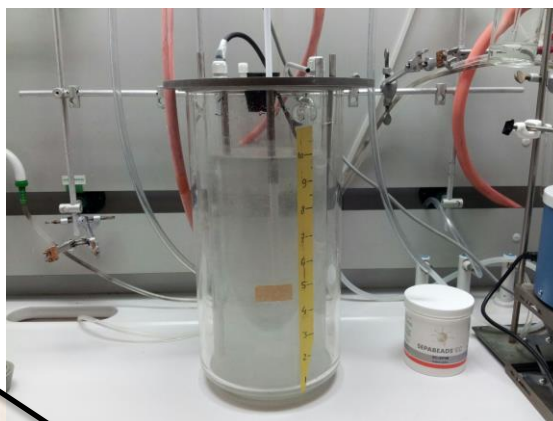


Background and goal

Environmental concerns, fluctuating oil prices and dwindling reserves are leading to the need for the production of biobased chemicals, materials and fuels. In order to achieve this new biomass pretreatments, (bio)chemical conversions and catalyst developments are required. As well as this biobased molecules offer opportunities for the production of novel and functional materials.

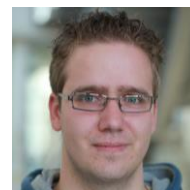
Main topics

- Application of homogeneous, heterogeneous and bio-catalysis in biobased reactions
- Developments of non-noble metal based catalysts
- Development of catalysts stable under conditions required for biomass conversion
- Novel functional materials from biomacromolecules
- Biomass pretreatment and cellulose conversion
- Biomass conversions using catalytic aqueous phase reforming



Selective catalytic transformations of non-edible carbohydrates

Name PhD: Frits van der Klis BSc.
Involved staff members: Prof. dr. J.H. Bitter;
Dr. D. S. van Es;
Dr. J. van Haveren
Project sponsor: TKI-programs, CatchBio, EU
SPLASH



Start/(expected) end date of project: October 2013 – October 2017

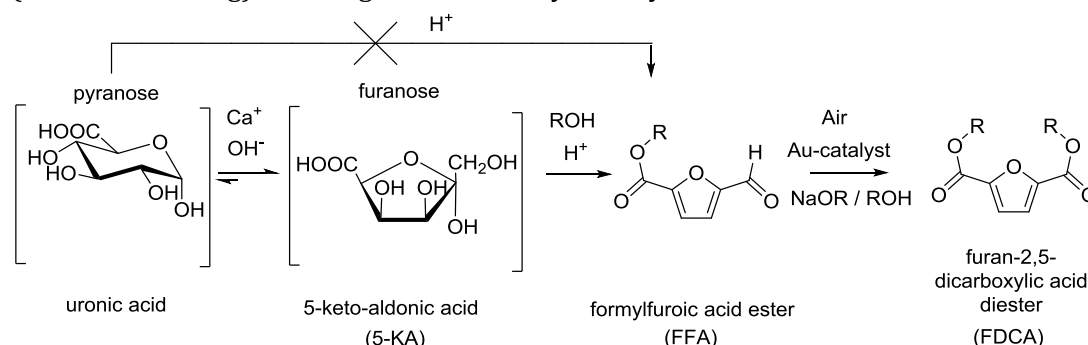
Background and goal of project

Carbohydrates are nature's main biomass constituent, and have already shown to be suitable starting materials for the production of a wide variety of bio-based chemicals. Many agro residues, such as sugar beet pulp, still contain valuable carbohydrates. The aim of my project is to selectively convert these non-edible carbohydrates into useful chemical building blocks.

Highlight of the past year

Furan-2,5-dicarboxylic acid (FDCA) is an interesting bio-based building block with applications ranging from polyesters and polyamides to plasticizers. In order to prevent the use of food-grade sugars for the production of FDCA, there is an increasing drive towards the use of non-food feedstocks. We developed a novel route to 2nd generation FDCA starting from uronic acids, which are abundantly present in agro residues like sugar beet pulp and citrus peels.

In aqueous solution uronic acids are mainly present in the pyranose form (6-membered ring), which prevents direct acid catalyzed cyclodehydration to 5-membered furans, giving undesired degradation instead. Our aim was to investigate if uronic acids can be selectively isomerized to their keto-isomers, which preferentially adopt a furanose form (5-membered ring), allowing for selective cyclodehydration to furans.



A base catalyzed isomerization of uronic acids gave the corresponding 5-keto-aldonic acids (5-KA) in high yield by selective precipitation of the Ca-salts. Subsequent acid catalyzed dehydration of 5-KA in alcoholic solvents gave formylfuroic acid (FFA) esters in good yield and high purity. Control experiments showed that FFA is not formed from the uronic acids, which shows the benefit of the isomerization step. Finally an oxidative esterification of FFA over supported Au-catalysts gave the desired FDCA esters, again in high yield and selectivity.

Type of student projects envisioned

Student projects all involve organic chemistry and/or catalysis orientated lab work, focused on the conversion of carbohydrates. Standard analysis during synthesis includes NMR, GC-MS, IR and HPLC. Catalysts will be analyzed by TEM, XRD, chemisorption and physisorption.

Aqueous phase reforming of bio-feedstocks

Name Postdoc: Neus Blanch Raga
Involved staff members: Harry Bitter
Project sponsor: Catchbio
Start/(expected) end date of project: 01/09/14-31/08/16



Background and goal of project

Biomass is a renewable feedstock which holds great potential to satisfy our future need for fuels and chemicals. Noble metal based catalysts have been investigated extensively, also for biomass based conversions because of their activity and stability. However, their availability is limited so there is a need for developing non-noble metal based catalysts such as Ni or Cu.

In this project I focus on the development of a non-noble metal based catalyst for the hydrothermal conversion of sugars to carboxylic acids.

Highlight of the past year

Last year we studied the hydrothermal conversion of C6 polyols (sorbitol) and sugars (glucose) with a Ni/AC catalyst (Fig. 1) in alkaline anaerobic conditions. It has been shown before that under these conditions Ni is stable. We investigated the role of the base comparing KOH and Ca(OH)₂.

Lactic acid was the main reaction product obtained in the liquid phase at 150°C in inert atmosphere for the two feedstocks when using KOH as a base. However, a wide range of other oxygenated products was also obtained to a lesser extent (such as glyceric acid, glycolic acid, formic acid or ethylene glycol).

The type of base played a key role on the selectivity (Fig.2). Ca(OH)₂ resulted in a higher LA yield compared to KOH. The presence of divalent cations enhances the selective formation of lactic acid during alkaline hydrolysis and decreases the total amount of other reaction products, because it affects the position where the C-C cleavage of the feed molecule (preferentially C3-C4 scission) occurs.

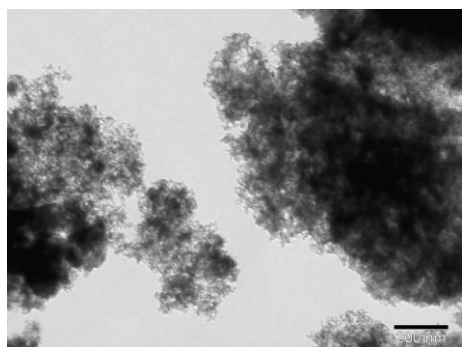


Fig.1: TEM image of the Ni/AC catalyst.

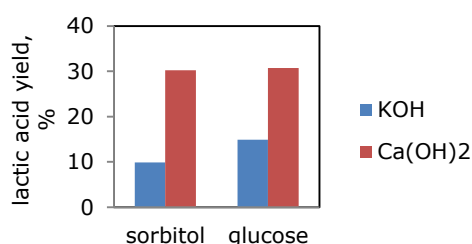


Fig.2: Lactic acid yield of C6 feedstocks with different bases (■ KOH, ■ Ca(OH)₂). Conditions: Autoclave, 25ml, 1 wt% feed Base/feed=2, 0.5g Ni/AC, 150°C, 15 hrs

Type of student projects envisioned

Some sub-projects for bachelor and master students are available at the moment. The projects are highly experimental, i.e. catalyst synthesis, characterization and testing. Therefore students need good lab skills. In addition there is one project available in which modelling (process design and sustainability analysis) plays a more important role.

Biocatalytic Formation of Industrial Nitriles from Biomass

Name PhD: Andrada But

Involved staff members: Elinor Scott, Johan Sanders

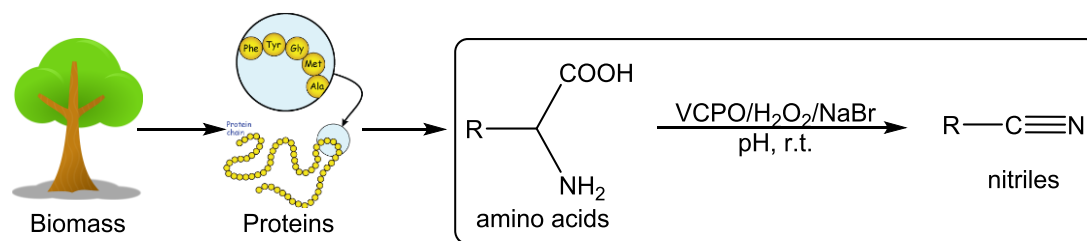
Project sponsor: Wageningen University

Start/(expected) end date of project: 11.06.2012-10.06.2016



Background and goal of project

Introduction of functionality into hydrocarbons to produce functional chemicals is energy intensive. This is especially true for nitrogen containing chemicals where ammonia is used. Research is focusing on the transformation of amino acids from protein-rich waste streams into bulk chemicals, one example is glutamic acid (Glu) – a versatile starting material for the syntheses of N-succinonitrile and acrylonitrile *via* 3-cyanopropanoic acid (CPA). CPA can be chemically produced using NaBr and excess NaOCl, however, salt formation and the need to cool the reaction have undesirable economic and ecological effects. A more viable conversion of Glu to CPA is *via* enzymatic oxidative decarboxylation using HOBr produced by vanadium chloroperoxidase (VCPO) from H₂O₂ and NaBr.



Highlight of the past year

In the first part of the year, the role of halides and their concentration was explored on amino acids with different functionalities and the consequences of this on conversion and selectivity.

It was found that the conversion and selectivity can be modified as a function of NaBr concentration but not as a function of halide type. Based on this the influence of the side chain length and functionality were studied. It was found that there is an optimum length – 5 carbons – where most amino acids gave very high selectivity. Moreover, the functionality present on the side chain that give the best results towards the nitrile formation is the carboxylic functionality. It was hypothesized that subtle interactions between the acidic amino acids and the halide salt change the conformation of amino acid in solution.

Influence of different parameters on conversion and selectivity of amino acids towards nitriles							
Halide (X ⁻)		Br ⁻ concentration		Side chain			
				Functionality		Length	
F ⁻	0	low	+/-	-COOH	++	4	0/-
Cl ⁻	0	high	+	-OH	+	5	++
Br ⁻	+	very high	-	-CH ₃	0	6	+

'0' = no effect, '-' to '++' = negative to highly positive effect.

Type of student projects envisioned

The typical work within this project involves lab experiments (enzymatic reactions) and analytical studies (spectrometry, HPLC, others).

IsoMalto/Malto-Polysaccharides: novel polysaccharides from starch

Name PhD: PH van der Zaal MSc
Involved staff members: dr. PL Buwalda, prof. dr. JH Bitter
Project sponsor: TKI/AVEBE
Start/(expected) end date: 01-10-2013/01-10-2017



Background and goal of project

Starch is a natural polysaccharide that makes up a large part of the human diet. The compound itself is biodegradable and is used in a wide variety of applications. Due to its relatively low price and its high availability starch is an attractive substrate for (enzymatic) modification. The discovery of the GtfB enzyme (4,6- α -glucanotransferase) opens up a new way to modify starch. This enzyme is able to alter the intrinsic properties of starch by cleaving α -1,4 glycosidic linkages and introducing α -1,6 glycosidic linkages into the polysaccharide.



The products of this enzymatic modification are named IsoMalto/Malto-Polysaccharides (IMMPs). IMMPs can be considered as a new generation of polysaccharides with added functionality for products in and outside the food industry, such as: food fibers, nutraceuticals, texturizers, replacement of synthetic polymers, biomedical materials and many other possible applications.

Highlight of the past year

Last year we found evidence of a high molecular weight fraction in the produced IMMPs. This year we were able to fractionate the high molecular weight fraction from the IMMPs on a preparative scale. This fractionation with Size Exclusion Chromatography, based on their hydrodynamic volume, paves the way for in depth structural analysis. Each obtained fraction will be thoroughly analyzed on linkage content with ^1H NMR (Nuclear Magnetic Resonance) and methylation analysis.

The aim of this project is to make the IMMPs, to map the properties, and to design optimal products for further applications.

Opportunities for thesis projects

- ❖ In depth chemical analysis of novel polysaccharides, including; molecular weight, ratio of α -1,4: α -1,6 linkages and directed (enzymatic) modification.
- ❖ Physical analysis of novel polysaccharides, including; viscosity, elasticity, gel strength, glass transition point and directed (enzymatic) modification.

Information: piet.vanderzaal@wur.nl; piet.buwalda@wur.nl

Transition metal carbides and phosphides for the production of alkanes from fatty acids

Name PhD: Luana Souza Macedo

Involved staff members: Prof. Dr. J.H. Bitter (WUR), Prof. Dr. V. Teixeira da Silva (UFRJ)

Project sponsor: WUR – sandwich project

Start/(expected) end date of project: 01-03-2014/01-10-2016



Background and goal of project

Lately much attention has been given to the conversion of biomass into biofuel to decrease the crude oil dependency of countries and because of the sustainability of biomass. Vegetable oils have many similarities to fossil diesel however they present higher oxygen content, what induces corrosion of diesel engines. To overcome this problem, deoxygenation is needed to remove the oxygen atoms from vegetable oils.

The most used catalysts for deoxygenation reactions are based on noble metals. However, due to their limited availability, replacement by other good available metals is desirable. Transition metal carbides and phosphides have similar catalytic properties as noble metals and hold therefore great potential. The main goal of this project is investigate the role of the support, using different carbons, on the catalytic performance of metal-carbides (W_2C and Mo_2C) and phosphides (Ni_2P) for the deoxygenation of fatty acids.

Highlight of the past year

Ni_2P was synthesized on different carbon based supports i.e., activated carbon (AC), carbon covered alumina (CCA) and carbon nanofibers (CNF) and tested for deoxygenation of oleic acid at 350 °C and 30 bar of H_2 in a continuous flow trickle bed reactor. All catalysts presented high conversion (> 90% under our conditions), however different product distributions (Figure 1) were obtained. The C17/C18 ratio increased in the order $Ni_2P/AC < Ni_2P/CNF < Ni_2P/CCA$, which means that more C18 was obtained as product over Ni_2P/AC compared to Ni_2P/CCA . This difference can be attributed to the strength of the active site as visualized by CO binding strength (Figure 2) and to the density of the active sites. Active sites of Ni_2P/CCA are stronger and are speculated to be responsible for the production of the higher C17/C18 ratio. Besides, AC presents the highest surface area among the supports, leading to the lowest density of Ni sites and the lowest products C17/C18 ratio. We hypothesize that the selectivity of C17 and C18 in deoxygenation of oleic acid over Ni_2P catalyst is influenced by an electronic effect caused by the support and by the density of Ni sites.

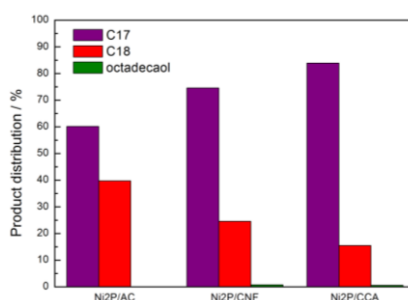


Figure 1. Product distribution for catalysts Ni_2P/AC , Ni_2P/CNF and Ni_2P/CCA in oleic acid HDO at 350 °C

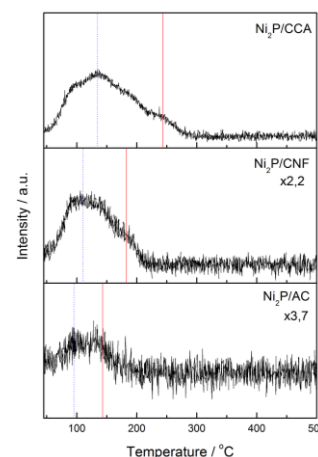


Figure 2. CO TPD profile for catalysts Ni_2P/AC , Ni_2P/CNF

Type of student projects envisioned

Lab work with use of some

characterizations techniques to understand and make results clearer, e.g. transmission electron microscopy.

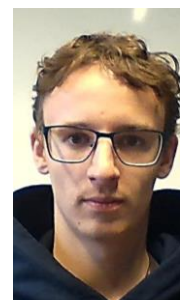
Real time monitoring of reactions with micro NMR spectroscopy

Name PhD: Gerben Wierda

Involved staff members: Prof. dr. Harry Bitter, Prof. dr. Aldrik Velders, Dr. Elinor Scott

Project sponsor: Graduate school VLAG

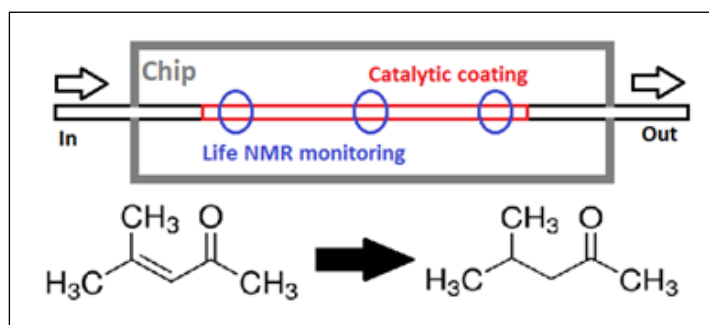
Start / (expected) end date of project: September 2015 – September 2019



Background and goal of project

Inside a plug flow reactor concentrations of products and reactants change as function of the position along the reactor due to conversion. In my project I will study the chemical composition of a reaction mixture as function of position in the reactor by using NMR spectroscopy. Insights in how the conditions influence catalyst performance inside the reactor are anticipated.

The project started in September 2015. During the first month fused silica tubes were coated with $\text{AlO}(\text{OH})$ on which nanosized Pt particles were deposited. As first show case we aim for the liquid phase hydrogenation of mesityl oxide (MO) to methyl isobutyl ketone (MIBK, see scheme). In a later stage a solid base catalyst will be added to make the mesityl oxide by the self-condensation (and dehydration) of acetone.



Highlight of the past year

The project just started

Type of student projects envisioned

As the project is yet in the laboratory coating phase current thesis work would entail laboratory work on the catalytic coating in the capillary tubing and subsequent analysis of the formed coatings.

Biobased chemicals from polyhydroxybutyrate

Name PhD: Jurjen Spekreijse

Involved staff members: Elinor Scott, Harry Bitter

Project sponsor: STW

Start/end date of project: 8-2011/8-2015



Background and goal of project

Carbon from agro industrial waste streams can be isolated and valorized as the biobased plastic polyhydroxybutyrate (PHB). However, the properties of PHB make it a challenging material to process. In this project we aim to convert PHB to known chemicals that already have an existing infrastructure. This way we can replace the fossil based chemicals by biobased drop-in chemicals. The target chemicals for this project are methyl acrylate and propylene, which can be obtained in two steps (Figure 1).

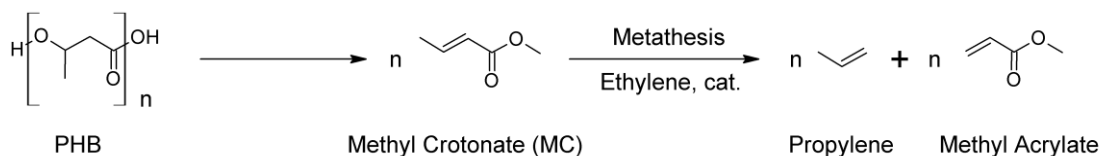


Figure 1. The conversion of PHB to propylene and methyl acrylate.

Highlight of the past year

In order to improve the feasibility of the metathesis step in the conversion of PHB to propylene and methyl acrylate, we immobilized the homogeneous metathesis catalyst in a metal organic framework (MOF). MIL-101-NH₂(Al) was chosen as MOF due its suitable cavity and pore sizes. However, during the mechanochemical immobilization procedure the structure of the MOF is partially modified to the thermodynamic product MIL53-NH₂(Al). Even with the structural change of the MOF, we obtained an active immobilized catalyst in a MOF using mechanochemical methods.

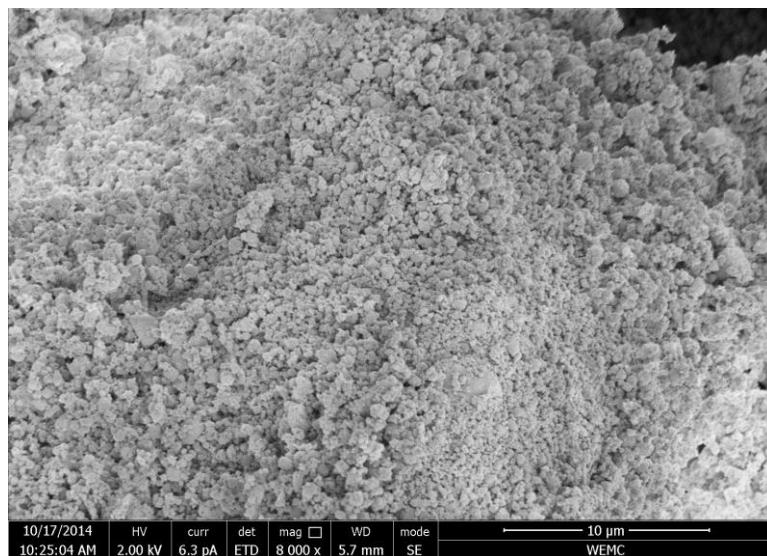


Figure 2. Scanning Electron Microscopy picture of the catalyst immobilized in a MOF.

Type of student projects envisioned

Not applicable due to end of project.

Combining *Chemo-* and *Bio-* electro-catalytic synthesis of chemicals

Name PhD: Konstantina Roxani Chatzipanagiotou, MSc
 Involved staff members: prof. dr. Harry Bitter (BCT),
 prof. dr. ir. Cees Buisman (ETE), dr. ir. David Strik (ETE)
 Start/(expected) end date of project: March 2015/March 2019



Background and goal of project

Carbon dioxide (CO₂) is the primary contributor to climate change, and there is globally ongoing effort to reduce CO₂ emissions. CO₂ can be converted to valuable products using various methods, for example with chemical or biological conversion. A novel mechanism is microbial electro-synthesis (MES), in which electrochemically active microbes use renewable electricity to convert CO₂ in organic molecules, such as fuels (Figure 1).

MES is considered more efficient and sustainable than photosynthetic bio-fuel production, but still faces challenges that limit its application, related to the poor transfer of electrons from the

cathode electrode to the microbes, the narrow product spectrum and low product separation efficiency. The objective of this project is to overcome these limitations, by combining electro-chemical and bio-electro-chemical conversion of CO₂.

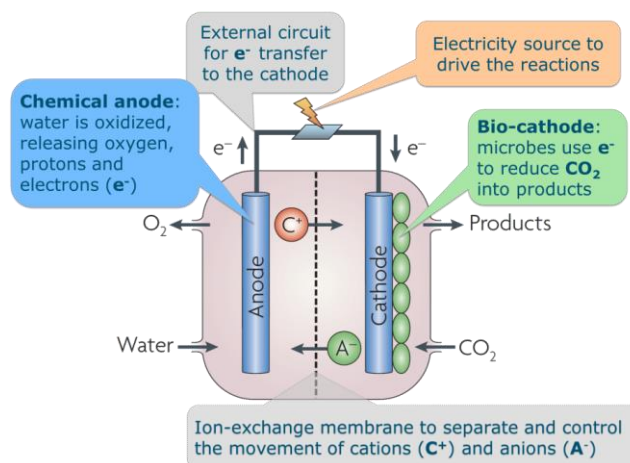
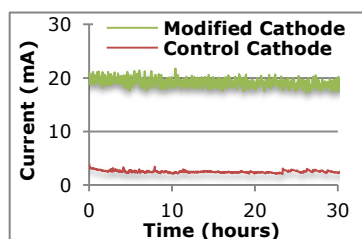
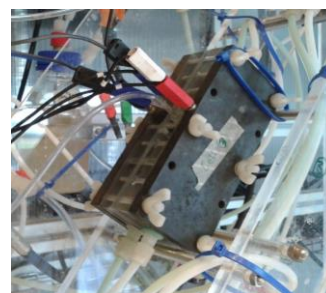


Figure 1. Above: The MES cell schematic (modified, Rabaey and Rozendal, 2010).

Right: Experimental set-up used for the electrochemical tests.



flow of electrons over time (i.e. current), one of the limiting factors of MES, increases significantly when a modified cathode is used, compared to control tests. Currently, the effect of electro-catalysts in biological systems is investigated, in experimental reactors as shown in Figure 1.

Figure 2: Current increases by more than 650% when electro-catalysts are added to the cathode.

Type of student projects envisioned

Research topics can involve both modeling and laboratory methodology. Modeling of the individual and combined catalytic processes could enhance the understanding of this complex reactor. New cathodes with different preparation methods, catalysts, and support materials will be investigated, using chemical, spectroscopic, and surface characterization techniques. Long-term bio-electro-chemical experiments will be performed to investigate the effect of environmental and biological factors.

Processing of feathers to proteins – from fundamental insight to application

Name PhD/Postdoc: Xinhua Goerner-Hu

Involved staff members: Dr. Elinor Scott, Prof. dr. Harry Bitter

Project sponsor: SARIA A/S GmbH & Co. KG

Start/(expected) end date of project: 01.06.2015-18.03.2019



Background and goal of project

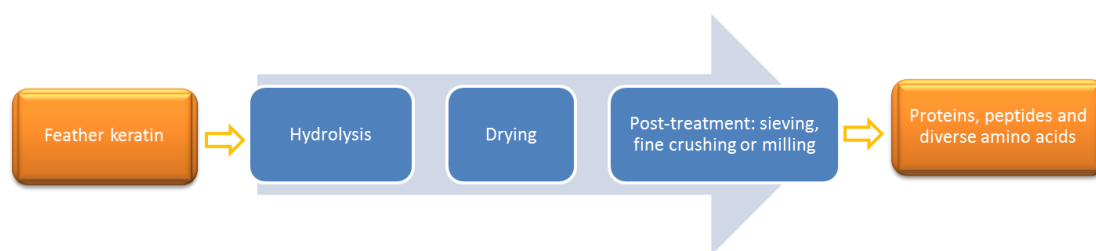
Annually more than 1 million tons of feathers are produced as by-product from European poultry slaughterhouses. The amount of feather as by-product rises steadily with increasing poultry consumption. On the other hand, the increasing consumption of meat products requires more livestock and therefore also increasing amounts of protein rich feed is needed.

Feathers contain 85% - 90% keratin. Keratin is a structure protein which contains proteins needed by animals but it cannot be digested directly. Therefore hydrolysis of keratin is needed to make it digestible. In that process the disulphide bonds in the keratin are broken and amide bonds are broken to form more digestible smaller proteins, peptides and amino acids.

Processed feather proteins are used as feed ingredient for pet food, aqua diets and feed for fur animals. Eight essential amino acids in feather protein meal (ARG, ILE, LEU, PHE, THR, VAL TRP and CYS) are present in higher amounts than in fish meal. However, due to the unbalanced amino acid composition of feather, e.g. lack of three other essential amino acids, LYS, MET and HIS, feather meal is only part of complementary feed composition.

The conventional industrial feather protein processing method is thermal pressure hydrolysis. However, during the heating in that process the nutritional value of the feather proteins decreases significantly.

The aim of the project is to study the feather hydrolysis deeply and to obtain high nutritional value of feather proteins under industrially implementable production conditions.



Technology

Theme leader: A.J.B. van Boxtel



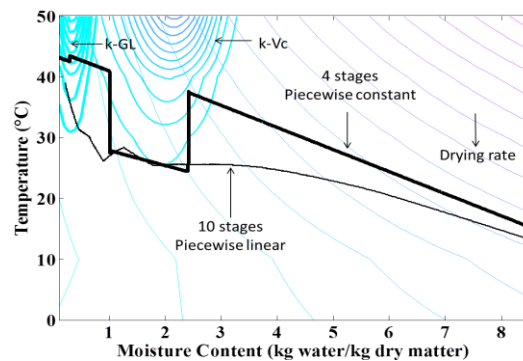
Background and goal of this theme

Creating a biobased economy needs sustainable solutions for biomass conversion and separation. Knowledge on mechanisms of conversion and separation, and how to control these mechanisms is essential. We combine experimental with modelling work to elucidate complex interactions in biomass conversion and to drive them in the aimed direction.

Using Process Systems Engineering tools, the performance of complete production systems is predicted and optimized. Hereby we search for solutions which meet both production performance and sustainability (LCA).

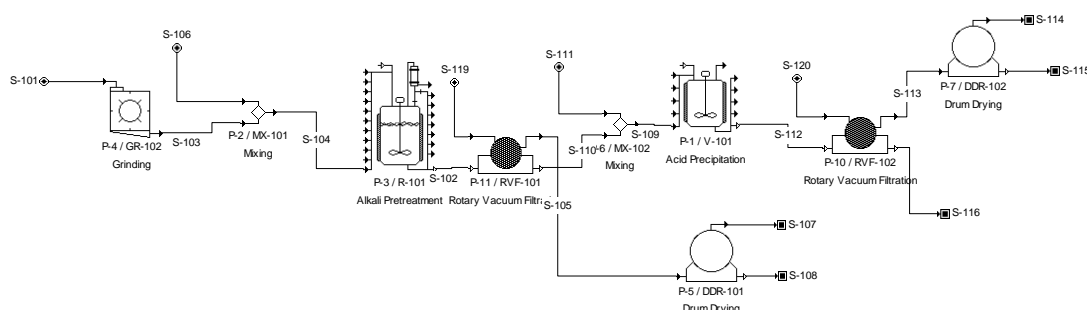
Main topics

- Mechanisms and models for preprocessing of biomass
- Reactor and production chain design for catalytic conversion of polysaccharides
- Component (protein, carbohydrate etc.) recovery from waste streams using new techniques
- Integrated sustainable biorefineries (algae, lignocellulosic biomass, milk-to-powder, duckweed cultivation)
- Life Cycle Analysis (LCA) combined with process design
- Sustainable processing in the region (system analysis and control)
- Control of individual and integrated processing steps in biorefineries
- Energy efficient processing (for example drying of biomass, vegetables)



These thesis subjects are related to the research work of Sanne Moejes, Chen, Zhang, Farnoosh Fasaei, Ellen Slegers, Rachel van Ooteghem, Emmanuel Amankwah and to the other two main BCT main themes. In this work we have a strong cooperation with AlgaePARC, DLO-FBR and TNO.

In 2015 a project proposal on new process principles for the production of anionic polysaccharides was granted. This project is combined with another BCT project which concerns the catalytic conversion.



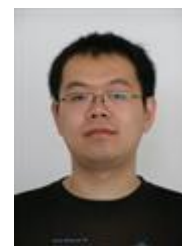
Biorefinery of leafy biomass using green tea residue as a model material

Name PhD: Chen Zhang

Involved staff members: Marieke Bruins & Johan Sanders

Project sponsor: STW

End date of project: 2016-1-1



Background and goal of project

With the rapidly growing world population and improving living standards, “Twice the food production at half the ecological footprint” is the goal for 2050. In fact, a boost in food demand is mainly required in developing countries, where the farmlands are limited and/or of poor quality. Rather than improving crop-production yield, developing biorefinery technology for unused biomass, such as leaves, in developing countries may be the key to fulfil the food demand.

The aim of this study is to develop new processes and applications to optimally utilize all components of leafy biomass in the feed and/or food industry using green tea residues (GTR) as a starting material, which can further apply to other leafy biomass.

Highlight of the past year

An integrated process was designed for the biorefinery of GTR, which can be used as an example for other leafy biomass. As shown in the Fig.1, this integrated process produced pectin and protein simultaneously at high yield. Approximately 85% of pectin and 90% of protein can be obtained, whereas other components can be combusted for energy. Instead of using NaOH, KOH was used for extraction. The generated potassium salts can be used as fertilizer, which improves the sustainability of the whole process. A profit of 105\$ is expected for processing 1 ton GTR by this integrated process.

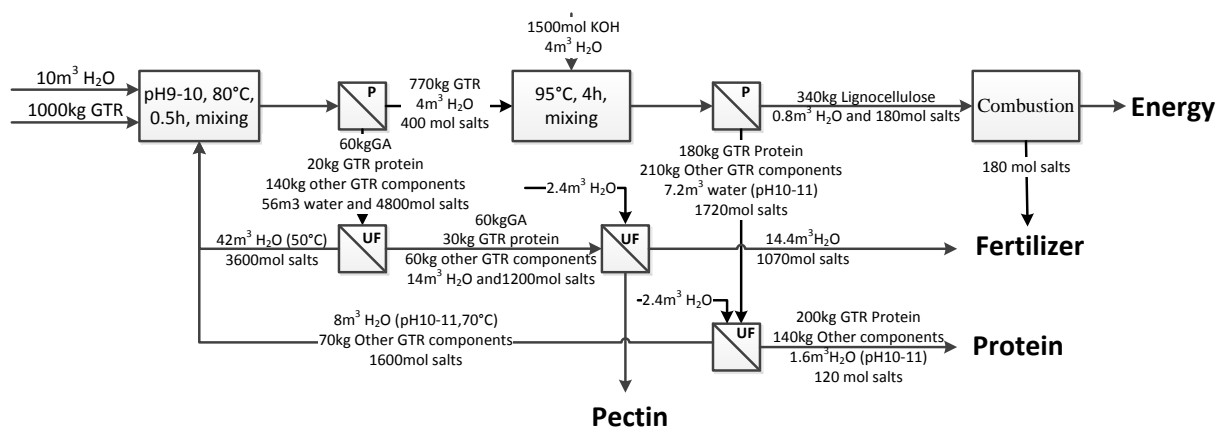


Fig.1 Integrated process of weak alkaline pectin extraction with KOH protein extraction using potassium salts as fertilizer. P: Press; UF: Ultra-filtration.

Economics and technology of biorefinery for animal feed sources

Name PhD: Marja Teekens (extern)

Involved staff members: Johan Sanders, Marieke Bruins

Project sponsor: Ministry of Economic Affairs (CBBE/ CAH Vilentum Dronten)

Start/end date of project: 01-02-2013 till 2016



Background and goal of project

Due to the growing demands for biomass, caused by an increasing world population and utilisation of biobased building blocks in industry, biomass has to be used more efficiently. Processing biomass into multifunctional components can contribute to this increasing demand.

The goal of the project is first to illustrate *if* and *how* biorefinery simultaneously delivers a high quality feed product and biobased products. As a second aim, the project tries to determine why economically and technologically feasible biorefinery initiatives are not grown into a technological innovation system yet.

Highlight of the past year

Biorefinery of grass and maize makes regional produced protein available for livestock. The impact of grass and maize refinery units on profit, nutrients, soil organic matter and land use, are simulated for pig and dairy farms in an intensively used agricultural region in the Netherlands, through a modeling approach. A precondition was maintaining animal productivity. Several scenario's on land use and P-excretion were simulated. The outcomes were compared to the existing agricultural system. The model shows that import of concentrates can be decreased to negligible amounts, for pigs as well as for cattle. Total economic profit in the region does not falter and even increases a little. At the same time the local P-cycle is more circular, total land use decreases, and soil organic matter increases a little.

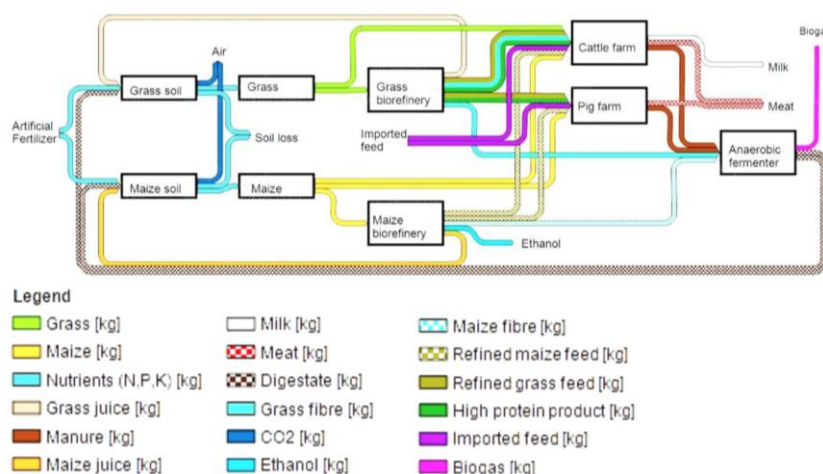


Figure 1: Schematic overview of the modelled agricultural system, showing processes and flows between them. Kilograms are based on dry matter. (Source: Forthcoming publication Teekens et al.)

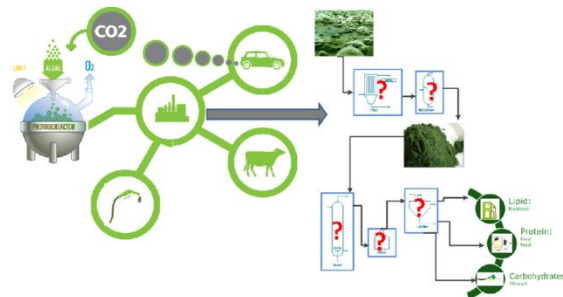
System Analysis of Algae Biorefinery

Name PhD: Farnoosh Fasaei

Involved staff members: Ton van Boxtel, Harry Bitter

Project sponsor: AlgaePARC Biorefinery

Start/(expected) end date of project: 01-09-2013/01-09-2017



Background and goal of project

The biobased economy is emerging due to undeniable fact of a limited amount of conventional resources of energy and food. Recently, biobased products from microalgae gained increased attention in the field of biobased economy and biotechnology. Microalgae feedstock is promising as a potential substitute for fossil and animal based sources of energy and food. To commercialize the algal biomass as an agricultural commodity, the production costs should be decreased while the yield is increased. Algae biorefinery refers to the conversion of algae biomass into a range of valuable biobased products and energy.

Highlight of the past year

During last year the library of the simulation models for feasible unit operations has been updated. In each model the characteristic of the flow streams like flow rate, algae concentration and internal processes and also relations inside each unit have been included in order to quantify accurate energy consumption and yield production. By linking energy and mass balance based models for each unit operation together, the performance of different process chains (scenarios) can be quantified. Production of lipids, proteins and carbohydrates and energy requirement are being addressed via different process design plots.

One of the main aims was to develop and demonstrate a simulation environment for the prediction of the performance of a planned algae biorefinery chain with respect to economics. To fulfil the mentioned demand a user interface for easy application of models is developed. The graphical interface takes advantage of the computer's graphics capabilities to make an interactive program for which it is not necessary to learn complex command languages(MATLAB).

Scenarios for possible and potential algae biorefinery are defined with respect to physical and chemical constrains in the processing chains. A product tree is created to have more insight about the potential of each designed process chain.

Possible thesis project

Recovery and recycle of by streams in algae biorefinery

Chemical potential of algae biorefinery by keeping the functionality of three groups of products lipids, proteins and carbohydrates

Economic and cost estimation of different algae biorefinery plants (upscaling)

Sensitivity analysis of algae biorefinery

LCA analysis of algae biorefinery

Redesign and optimization of the milk powder production chain

Name PhD: Sanne Moejes

Involved staff members: Ton van Boxtel

Project sponsor: EU FP7 project

Start/(expected) end date of project: 12-2013 till 11-2017



Background and goal of project

The food sector is responsible for large energy consumptions, mainly caused by the use of thermal processes. Milk powder production involves many thermal processes, making it highly energy consuming. The past decades the current production process is optimized to a high extend. The EU goals, however, demand for a further improvement of environmental impact. Redesigning the milk powder production chain is necessary to make a next step forward in energy reduction as well as environmental impact. Introduction of new technologies will be the key. Optimization of single process units will have an influence on up- and downstream process units. Therefore it is important to take the whole production chain into account. The goal is to design an optimization routine which takes energy and water consumption, LCA aspects, and economical aspects into account, resulting in a sustainable milk powder production chain.

Highlight of the past year

After describing and modeling the state-of-the-art in milk powder production in the first year, we continued in the second year with the innovative technologies. This information resulted in a review manuscript describing the need for development of new technologies and their potential. Figure 3 shows the possible energy reduction when replacing current concentrating and drying process by new ones. Important is the surplus heat created by using monodisperse drying with air recycling after dehumidification by either zeolites or a membrane contactor. By applying pinch technology to identify the possibilities for heat recovery and subsequent optimization of the operational conditions it was proved that the surplus heat reused in the system. With these results the energy consumption in milk powder production can at least be halved. Results were presented at the EFFoST conference in Athens.

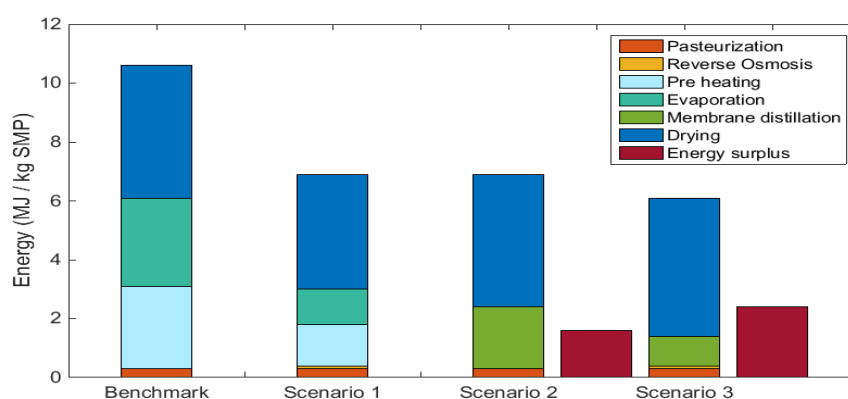


Figure 3. Energy requirements for milk powder production via different scenarios. Benchmark is the current situation. Scenario 1 uses RO, evaporation and multi stage drying. Scenario 2 uses membrane distillation and monodisperse drying with a membrane contactor. Scenario 3 uses membrane distillation and monodisperse drying with a zeolite.

Type of student projects envisioned

Modeling will be the core of student projects. Examples could be development of in depth mechanism models of the innovative technologies, or more broth chain analysis. Main focus is on energy and sustainability evaluation in general, which involves both environmental and economic aspects.

Modelling and Control for a Sustainable Future

Name staff member: dr. R.J.C. (Rachel) van Ooteghem MSc.



Background and goal of project

Working with various thesis students from different backgrounds and studies made me realize that, as diverse as their subjects may be, modelling (and sometimes control) plays an essential role to come to a new design of a process. The goal of this design is always to make it better, more environment friendly, more sustainable. Often the task is to close the cycle in a smarter way, by introducing new possibilities for feed, or gaining energy from sun, wind or other sources.

Some thesis projects from previous years include:

Dynamic modelling of duckweed growth

Micro algal production combined with anaerobic manure digesting

Modelling of biogas production process in an anaerobic digester

Local sustainable hydrogen production, collaboration between farm and tank station

Investigating the production of anhydrous ammonia on the farm

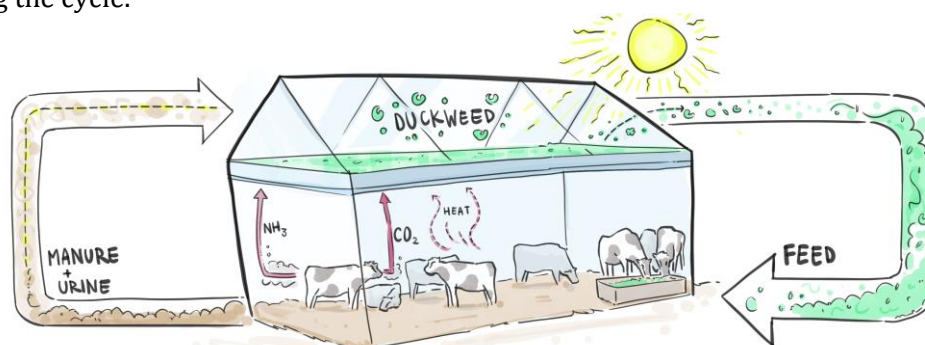
Mechanistic modelling of pig growth to investigate the possibilities to feed pigs individually

Algae cultivation in vertical plate reactors, researching the decay of diffuse light

Highlight of the past year

In 2015 Niek van den Top won the Shell Bachelor Prize in 2015 for his work on the ECOFERM farm, a closed-cycle farm for rosé calves where duckweed production is combined with growing calves.

The concept of the ECOFERM farm is to use the body heat of the calves and their urine and manure to grow duckweed. The duckweed is then used as feed for the calves, thus closing the cycle.



Type of student projects envisioned

Student projects include modelling scientific models based on first principles (e.g. energy and mass balances, equations from physics), programming and computing expected results. If possible, these models will be validated with data which is measured on location, or on self-made setups.

Sustainable biorefinery design

Name Postdoc: Ellen Slegers

Involved staff members: Ton van Boxtel

Project sponsor: EU FP7 MIRACLES, AlgaePARC Biorefinery

Start/(expected) end date of project: 2013 - 2017



Background and goal of project

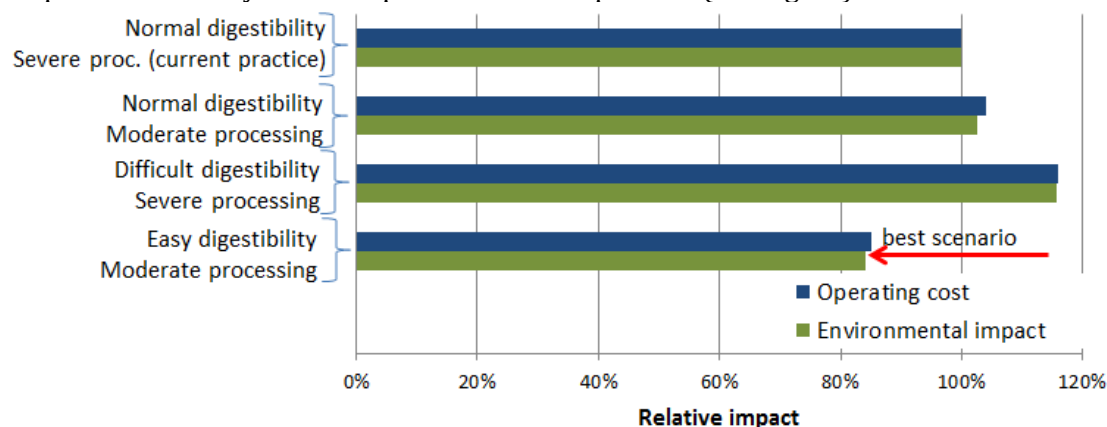
I study the design of sustainable biorefinery chains. Technical models are developed to simulate the technical feasibility and performance of process designs, using engineering rules and laboratory data. These results are the basis for assessing the environmental sustainability. Two main research challenges are:

- How does environmental sustainability compete with the technical and economic performance?
- How to include sustainability during process design?

Highlights of the past year

In the paper 'The potential of optimised process design to advance LCA performance of algae systems' we discussed how process simulations can advance LCA results. We propose to perform process simulations to evaluate various production and design scenarios, and to link these to LCA.

In another study, the effect of biological properties of maize stover on the processing efficiency, economic and environmental impacts was assessed. The maize stover was grouped based on its digestibility, i.e. normal (current practice), difficult, and easy (breeding for biorefinery). The processing efficiency into sugars was determined for each of these groups. This was done for severe and moderate processing conditions. For the current maize only severe processing results in acceptable product yields. The results show that maize stover with easy digestibility has the best overall performance. This performance can be achieved with moderate processing. The combination of easy digestibility and moderate processing results in reducing the overall environmental impacts and cost by 15% compared to current practice (see Figure).



Relative environmental impact and operating cost for four maize scenarios. Proc. = processing.

Type of student projects envisioned

- sustainability analysis (mostly LCA). Typical case studies: algae, coffee cherries, potato, wheat, sugar beet, maize.
- development of sustainability assessment methods
- integrating LCA with early process design
- scenario modelling of biorefineries
- biomass storage (lab work linked to model development)
- logistic modelling of algae biorefinery chains.

Sustainable process design; other subjects

Theme leader: A.J.B. van Boxtel, R.J.C. van Ooteghem

Involved PhD's and post-docs: E.A.Y Amankwah, C. Gomez, P. Perez, student projects.

Project sponsors: WUR-sandwich PhD-fund, KNUST Ghana, Universidad Nacional de Colombia, University of Santiago de Compostela, AlgaePARC, ECOFERM.

Background and goal of project

The theme sustainable process design includes also a project on solar adsorption drying and some developing projects. In these projects we develop new ideas that enhance sustainability in processing. The project are performed in cooperation with third parties like universities and non-profit organizations.

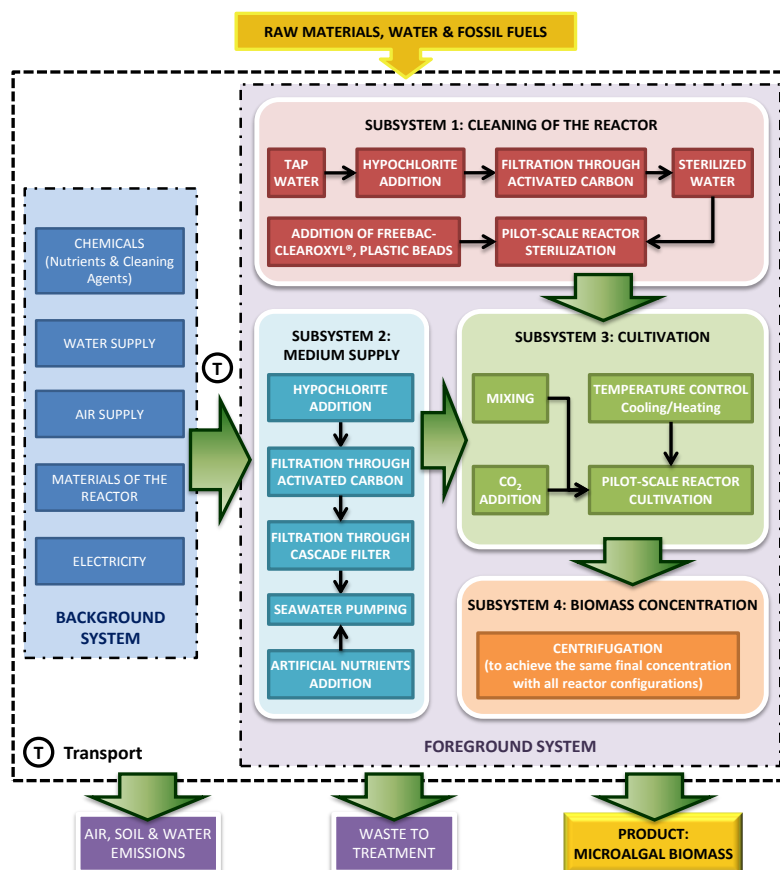
Highlights of the past year

Analysis of the drying behavior of starch rich yam which is a major element in African and South-American diets.

Halving the energy consumption in tubular algae cultivation systems by introducing smooth turbulence promoters (Algal Research 12 (2015) 1–9)

LCA for algae cultivation based on real time monitored data from AlgaePARC

Growth of duckweed in the ECOFERM circular farm. Winner of the Shell bachelor price 2015.



Overview of system aspects considered in the LCA for AlgaePARC (Applied Energy 154 (2015) 1122–1127)

Systems Theory

Name: Karel J Keesman

Involved PhD students: Nurul Khairudin, Rungnapha Khiewwijit, Elvira Bozileva, Jan Klok, Nik Grubben, Daniel Reyes Lastiri, Yu Jiang



Background and goal of project

In the past decade, there have been strong developments in communication (internet, e-mail, smart phones, wireless), computation (Moore's exponential law - processors, memory, storage capacity), sensor networks (data warehouses) and cyber science (integration of knowledge). These developments allow the implementation of smart, high-tech, cost-effective solutions to water/energy/material related problems in a bio-based/circular economy.

The objective of the project is to support new and innovative technological solutions to complex, dynamic, and possibly constrained, systems in a bio-based/circular economy, such as water-energy-material cycles in urban systems, S/N/P cycles in natural and industrial environments, storage and aquaponic systems, through **network modelling** and **data-model integration** techniques.

Highlight of the past year

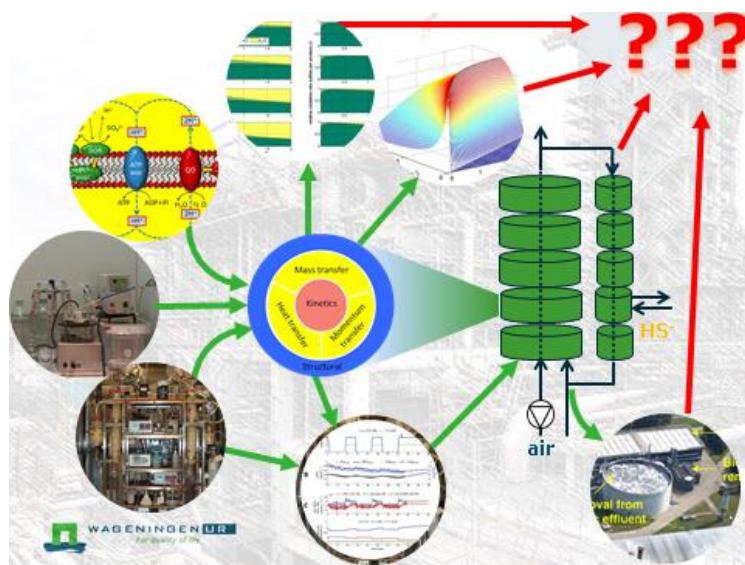


Figure 1. Progress in biological desulfurisation (Klok, 2015, PhD thesis)

In the past year, we made good progress on identifying biological reaction kinetics and pathways, reactor and full-scale modelling and on monitoring and control of the **biodesulfurization** process at haloalkaline conditions (Figure 1).

In addition, a review on mathematical models, monitoring and bioprocess control of automated biological **sulphate reduction** by Cassidy et al. was published in FEMS Microbiol Rev (2015) 39 (6).

Type of student projects envisioned

We can offer student projects on Big Data processing in drinking water industries and in fisheries, and on modelling and simulation in an urban and food production environment.

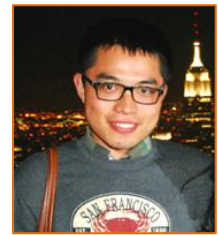
Bioenergy policies for achieving liveable and sustainable cities of the future: An integrated game-model-data approach (E-game)

Name PhD: Yu Jiang

Involved staff members: Dr. Karel Keesman

Project sponsor: Climate-KIC (EU)

Start/(expected) end date of project: 01-09-2014/01-09-2018



Background and goal of project

Three of the challenges we are facing are: first, climate change as a consequence of intensive use of fossil fuels; second, urgent need for energy independence and security due to international relation crisis; third, waste management challenge in urban areas because of rapid urbanization.

Promoting a transition to biobased urban energy system can allow us to “kill” three birds with one stone and help to achieve a circular economy.

This project aims at using various approaches including energy system modelling, agent based simulation and life cycle assessment in order to provide scientific insights into the contribution of waste biomass to urban energy system; sustainability performance of urban bioenergy supply chain; and bioenergy’s role in balancing the grid, thus supporting related policy-making process.

Highlight of the past year

We built a biobased urban energy system planning model to analyze the contribution of waste biomass in future urban energy supply with a case study in Amsterdam.

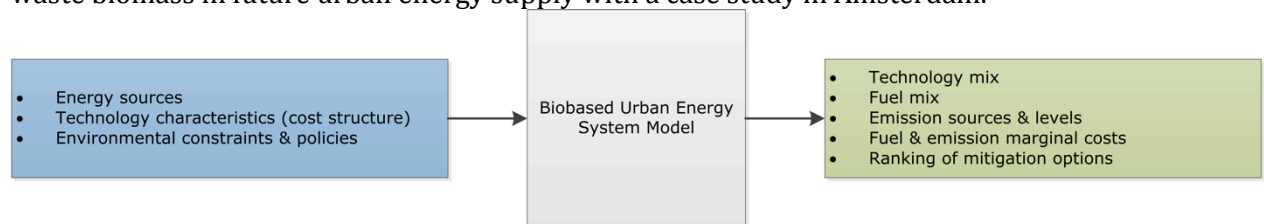


Figure 4 Input and output of biobased urban energy system model

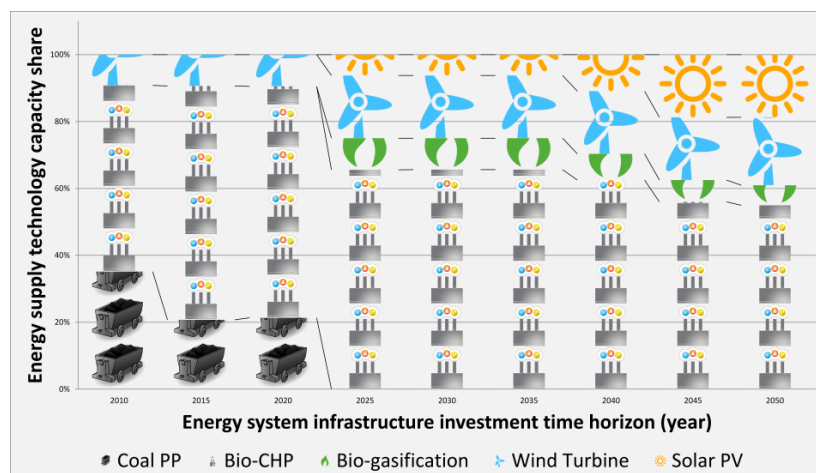


Figure 5 Technology mix under the policy scenario of 80% emission reduction (Our GAMS model calculation)

Type of student projects envisioned

Possible topics for students’ thesis: (1) Application of Energy Returned on Energy Invested indicator on urban energy system evaluation; (2) Sustainability analysis of urban bioenergy supply chain; (3) Multi-criteria analysis of bioenergy technology selection for urban energy system.

Modelling aquaculture-hydroponic systems

Name PhD/Postdoc: Daniel Reyes Lastiri (PhD),
Hans Cappon (part-time Postdoc)

Involved staff members: Karel J. Keesman

Project sponsor: INAPRO
(EU 7th Framework Programme for Research)

Start/(expected) end date of project:

Daniel - 15 June 2014/15 June 2018

Hans - 1 April 2014 - 1 April 2018



Background and goal of project

Current food production systems are unsustainable. About 70% of the fresh water used worldwide is destined to agriculture, largely for animal feed, and almost three quarters of the global fish stocks are overfished.

Aquaponics is a technique that can help decreasing the ecological impact of food production by combining aquaculture (farming of aquatic organisms) with hydroponics (farming of plants without soil) in a single water cycle. Today, aquaponics is mainly used in small scale, remote systems.

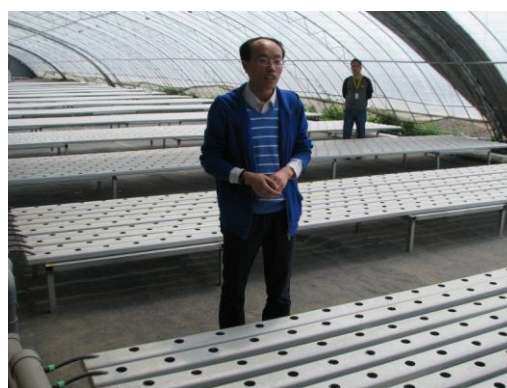
Our research is part of the EU project INAPRO, which aims at developing aquaponics towards a commercial state based on simultaneous modelling and demonstration approaches. Our group works in modelling and simulation of water, nutrient and energy flows in aquaponic systems. In parallel, our project partners build and operate pilot systems.

The main target of the model is to minimize water, nutrient and energy consumption in the aquaponic cycle.

Highlight of the past year

The general code for the full model has been completed in Python, an open source programming language. The model has a modularity approach, i.e. every component of the system is programmed as a single, interchangeable unit, which will allow us to simulate different equipment, scenarios, species to grow and locations in the world.

Daniel has worked in the overall Python structure while Hans has simulated separate modules.



Daniel and Karel had the pleasure to visit the completed construction of an INAPRO demonstration system in Beijing, as part of the collaboration between theoretical and practical approaches.

Type of student projects envisioned

Our student projects are focused on modelling. We also have collaboration with research institutes in Europe and China involved in INAPRO, which could provide experimental data to validate models.

Real-time accounting and simulation of dynamic energy-water-material balances for achieving liveable and sustainable cities of the future

Name PhD/Postdoc: Elvira Bozileva
Involved staff members: Karel J. Keesman
Project sponsor: Climate KIC
Start/(expected) end date of project: 09-2013/09-2017



Background and goal of project

Many of us envision living in a future where covering our needs for energy, water and food does not result in deteriorating environmental systems. Transition towards such future would undoubtedly require updating current technological infrastructure and implementing technological solutions that make use of renewable sources of energy, water and nutrients. Many such solutions are already available (solar energy harvesting through photovoltaics or solar collectors, reusing greywater, nutrient recovery from waste). These technologies, however, are not sustainable *per se*. Nevertheless they can be sustainably implemented in a specific context depending on a local climate and availability of other technologies. For example, even in the areas with abundant insolation, having photovoltaic modules does not ensure self-sufficiency of the urban system, as long as harvested solar energy storage is not addressed.

The goal of this project is, therefore, to develop a model-based framework that would allow to systematically identify the most suitable combinations of technologies for a specific urban system (e.g., building or district), taking into account intermittency of renewable sources of energy, water and nutrients, as well interconnected nature of urban energy, water and nutrient cycles.

Highlight of the past year

The model, implemented in Matlab, to simulate water and energy flows within residential buildings was used to study the relationship between technological factors (PV efficiency, water and electrical energy storage capacity, etc) and the extent to which external water and energy demand can be reduced within the building. This relationship was studied via Response Surface Methodology using full factorial design.



Type of student projects envisioned

Student projects will involve modelling of water, energy and nutrient cycles in an urban environment using Matlab software. High proficiency in Matlab is not required, however, previous experience is welcomed.

Smart ventilation for safe and sustainable food storage

Name PhD: N.L.M. Grubben

Involved staff members: Karel Keesman

Project sponsor: Omnivent techniek b.v.

Start/(expected) end date of project: 01/04/2014-01/04/2018



Background and goal of project

Most agricultural products are season-dependent. To overcome seasonality of the harvested products and to guarantee a continuous flow of food products to the consumers and of biomass, in general, to bio-based industries, storage of primary food products and biomass is crucial.

This study focuses on the understanding and design of optimal ventilation strategies for safe and sustainable storage of primary food products. Computational fluid dynamics (CFD) simulation is used to provide physical insight between the product quality and the climate numerically and via visualisation. The CFD model, including product quality processes, is spatially distributed and suitable for model-based quality control.

Highlight of the past year

A review article about modelling ventilated bulk storage of agro-materials has been published (Grubben & Keesman, 2015). This includes a broad investigation on CFD simulations, used in food storage applications.

A complete 3-D CFD simulation model has been developed, including ventilators and moving hatches.

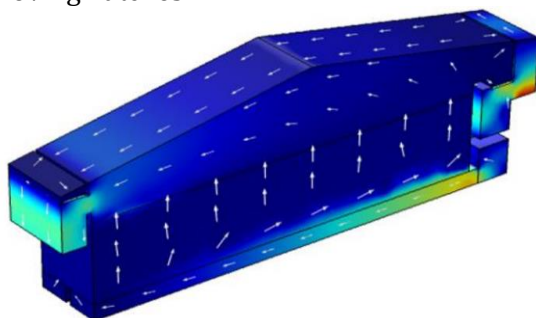


Figure 1. Air velocity profile in a food storage facility obtained by CFD simulation.

To calibrate and validate the spatially-distributed model of potatoes, data of a full scale test-storage facility is processed. One of the quality aspects of potatoes is the sugar content. For the validation of the sugar content in potatoes the sugar content is frequently measured with HPLC analyser.

Type of student projects envisioned

Related to the topic this project, several MSc projects can be defined. Detailed models of product specific processes are often absent, but needed for quality control. Modelling these processes can be conducted and implemented in CFD simulations.

Grubben, N. L. M., & Keesman, K. J. (2015). Modelling ventilated bulk storage of agromaterial: A review. *Computers and Electronics in agriculture*, 114.

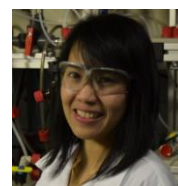
Computer - aided design and monitoring of WWTPs towards energy and nutrient recovery

Name PhD: Rungnapha Khiewwijit

Involved staff members: Huub Rijnaarts, Hardy Temmink, Karel Keesman

Project sponsor: IMD B.V.

Start/end date of project: September 2011 - August 2015



Background and goal of project

Although conventional activated sludge (CAS) systems are widely applied to treat municipal wastewater, CAS systems cannot be considered sustainable because they consume large amounts of energy (mainly for aeration and sludge treatment), have a high CO₂ emission and do not recover a potential resource of water, energy and nutrients, such as nitrogen (N) and phosphorus (P). Therefore, the main goal of this project was to (re)design new municipal wastewater treatment concepts that combine treatment with recovery of valuable resources and can save considerable amounts of energy, by modelling and experiments.

Highlight of the past year

Quantitative numerical results showed that the feasibility of two novel wastewater treatment configurations, including combined bioflocculation and anaerobic digestion but with different nutrient removal technologies, i.e. partial nitrification/ Anammox or microalgae treatment, is strongly dependent on the locations and wastewater composition. For example, the configuration with microalgae treatment is only applicable in tropical regions that are close to the equator line. The experimental results showed that a combined process with bioflocculation, using a high-loaded membrane bioreactor (HL-MBR) to concentrate sewage organic matter, and anaerobic fermentation, using a sequencing batch reactor to produce volatile fatty acids (VFA), is technologically feasible (Figure 1).

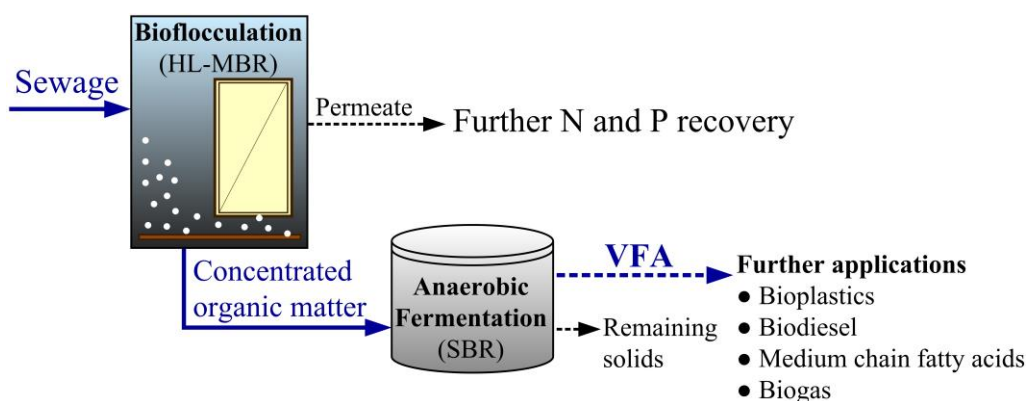


Figure 1: Combined bioflocculation using a high-loaded MBR (HL-MBR) to concentrate sewage organic matter and sequencing batch reactor VFA production reactor (SBR).

An HL-MBR operated at a hydraulic retention time (HRT) of 1 hour and a sludge retention time (SRT) of 1 day resulted in very good performance, because as high as 75.5% of the sewage COD (chemical oxygen demand) was diverted to the concentrate and only 7.5% was mineralized into CO₂. Moreover, it was found that application of a pH shock of 9 in the first 3.5 hours of a sequencing batch cycle followed by a pH uncontrolled phase for 7 days gave the highest VFA yield of 440 mg VFA-COD/g VSS and this was equivalent to 52% of the biodegradable sewage COD.

Modelling of ammonia volatilisation in fertilised and flooded rice systems

Name PhD: Nurulhuda Khairudin

Involved staff members: Karel J. Keesman

Project sponsor: Ministry of Higher Education Malaysia

Start/(expected) end date of project: January 2011 – September 2016



Background and goal of project

Estimates of ammonia (NH_3) volatilisation in fertilised and flooded rice systems range from 2 % to 60 % of total N applied. A reasonable estimation of NH_3 volatilisation is important in order to quantify the N loss to the environment and to pre-determine how much N is available for uptake by rice crop. Hence, one of our objectives is to determine an appropriate model structure for estimating NH_3 volatilisation in fertilised and flooded rice systems, given limited availability of observational data sets. Previously, a process-based model for estimating NH_3 volatilisation in fertilised and flooded rice systems and is of complexity appropriate for small data sets was developed. The model was calibrated with data sets from the Philippines.

Highlight of the past year

The proposed model was co-validated with modelling concepts developed by Chowdary et al. (2004) with respect to their common outputs: concentrations of urea-N in the floodwater, concentrations of total ammoniacal-N in the floodwater, and cumulative NH_3 volatilisation. The key question then is: Can the proposed model produce comparable or better estimations than Chowdary's model?

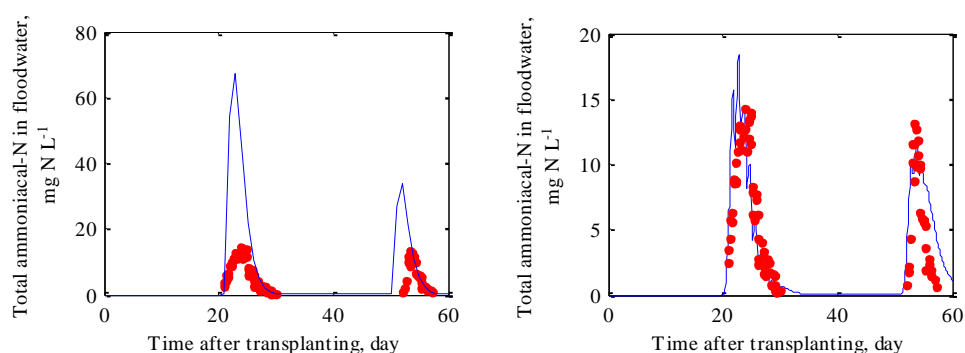


Fig. 1 Concentrations of total ammoniacal-N in floodwater: a) Simulated using Chowdary et al. (2004) and b) simulated using the proposed model, against observations reported by Fillery et al. (1984).

Unlike the proposed model, the model of Chowdary et al. (2004) could not properly predict the trend of total ammoniacal-N in floodwater observed (Fig. 1). The result supports the concept of two-step urea hydrolysis for rice systems with low urease activity. Nevertheless, the cumulative NH_3 volatilisations estimated by both models are comparable. The calibrated value of constant rate coefficient of NH_3 volatilisation of each model differed due to the underlying concepts.

References

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Education

Bachelor and Master courses BCT and contribution to other courses

Code	Course title
BCT-20306	Modelling Dynamic Systems
BCT-21306	Control Engineering
BCT-22306	Sensor Technology
BCT-22803	Physical Transport Phenomena
BCT-23306	Biorefinery
BCT-30806	Physical Modelling
BCT-31306	Systems and Control Theory
BCT-31806	Parameter Estimation and Model Structure Identification
BCT-32306	Advanced Biorefinery
BCT-50306	Renewable Resources and the (Bio)Chemical Production of Industrial Chemicals
BCT-50806	Sustainability Analysis
BCT-51306	Biobased Economy

Code	Course title
BPE-10305	Process Engineering Basics
BPE-12806	Bioprocess Engineering Basics BT
BPE-60312	Bioprocess Design
FTE-12803	Introduction Biosystems Engineering part 2
FTE-13807	Engineering 2 (Electronics)
FTE-32806	Automation for Bioproduction
FTE-34806	Modelling of Biobased Production Systems
MAT-24803	Mathematics for Time-dependent Systems
ORC-13803	Bio-organic Chemistry for Life Sciences
XWT-21305	Process Dynamics (Wetsus)

BCT: Biobased Chemistry and Technology

FTE: Farm Technology

BPE: Bioprocess Engineering

MAT: Mathematics

ORC: Organic Chemistry

XWT: Wetsus Academy

PhD courses

Uncertainty analysis of dynamic models

Dynamic modelling plays a crucial role in life science research, for example for predicting or hypothesis testing. A key feature of biosystems is parameter uncertainty, arising from biological variation, or a lack of knowledge. It is generally hard to foresee how parameter uncertainty propagates into model predictions, especially when a model contains a lot of complex interactions. Some predictions may be sharp, others highly uncertain. Some parameter uncertainties make all predictions uncertain, whereas others may have no influence at all.

The purpose of this course is to make the participants familiar with general statistical concepts describing uncertainty, and methods to compute prediction uncertainty coming from uncertain parameter values. We introduce dynamic input-state-output systems and methods to write your model in this format. Also methods are presented to obtain parameter uncertainty from input-output data in case some system states are not measurable, and in case of noise in the data. The methodology is illustrated with realistic examples.

This course was in renewed form given in 2015 with Biometris as course coordinator.

VLAG Advanced Chemistry Course

The Wageningen Graduate school VLAG organizes several courses for PhD students within the fields of VLAG (Food sciences, Nutrition, Agro-biotechnology and Health sciences). One of the new courses in 2015 was the Advanced chemistry course. Every year this course will focus on a relevant topic for chemists and the topic in 2015 was 'characterization of nanomaterials'. The BCT group participated in this course with a lecture and case studies on texture and structure analysis by physisorption and electron microscopy.

The course was closed with a lecture by Prof. Petra de Jongh from the Utrecht University, a renowned speaker from the nanomaterials field.

BSc Theses

- Adamson, Lara; The influence of storage on algae biomass composition
- Goedhart, Joost; Analysing the robustness and flexibility of lipid biorefineries using response surface methodology
- Ruigrok, Thijs; Temperature response of duckweed growth at the Ecoferm greenhouse
- Slinkert, Thomas; Modelling of an integrated plant-fish system
- Stockmann, Jeroen; Possibilities of using pulsed electric field in leaf biorefinery

MSc Theses

- Beus, Niels de; Modelling of a Dutch agricultural region containing grass and maize biorefineries
- Gerritsen, Casper; Design of an in vivo controller
- Guzman, Maria; Membrane Distillation in Milk Powder Production
- Haanstra, Lennaert; Storage of arable products; optimal climate control with focus on renewable energy
- Holgueras Ortega, Juan; Conversion of PHB in cells into methyl crotonate as first step to obtain biobased acrylates and propylene

Process design of lignocellulosic biomass fractionation into cellulose, hemicellulose and lignin by prehydrolysis and organosolv process

- Hoogstad, Tim; A framework for formulating and optimising a superstructure
- Houthoff, Iris; Development of a sustainable biorefinery process from microalgae
- Karrenbelt, Michiel; Optimal input design for discrimination of feed-forward loops in genetic transcription networks
- Martinez, Iris; Modelling for assessing and reducing energy requirements in four standard PBR designs
- Mol, Jordi; Dynamic simulation and control of potato bulk storage
- Peterhans, Thomas; Aquaponic nutrient model
- Poletto, Francesca; Sustainable co-production of H₂O₂ and chemicals by oxidases
- Rijn, Rick van; Optimization of the extraction procedure of lignin from different agroindustrial residues
- Saglibene, Marco; Modelling a type 1 diabetes mellitus patient based on physiological knowledge
- Stolp, Femke; Modelling and improving the nutritional content of yam during drying
- Trebuch, Lukas; Validation of Algae Productivity Models for Outdoor Conditions
- Visser, Quirien; Energy efficient drying process for milk powder
- Wieneke, Kira; Productivity of microalgal biomass constituents in simulated simulated day night cycles
- Wijst, Evie van der; Biobased nitrile production from amino acids: influence of side-chain and halide on reactivity
- Yao, Xinyi; Uncertainty analysis for biorefineries

PhD Theses

- Klok, Jan; Modeling studies of biological gas desulfurization under haloalkaline conditions
- Marasabessy, Ahmad; Valorization of Jatropha fruit biomass for energy applications
- Sari, Yessie; Biomass and its potential for protein and amino acids: valorizing agricultural by-products

Scientific Publications 2015

Refereed article in a journal

- [Optimal control of greenhouse climate using minimal energy and grower defined bounds](#)
Beveren, P.J.M. van; Bontsema, J. ; Straten, G. van; Henten, E.J. van (2015)
Applied energy 159 . - p. 509 - 519.
- [Minimal heating and cooling in a modern rose greenhouse](#)
Beveren, P.J.M. van; Bontsema, J. ; Straten, G. van; Henten, E. van (2015)
Applied energy 137 . - p. 97 - 109.
- [The potential of optimized process design to advance LCA performance of algae production systems](#)
Boxtel, A.J.B. van; Perez-Lopez, P. ; Breitmayer, E. ; Slegers, P.M. (2015)
Applied energy 154 . - p. 1122 - 1127.
- [Automated biological sulphate reduction: a review on mathematical models, monitoring and bioprocess control](#)
Cassidy, J. ; Lubberding, H.J. ; Esposito, G. ; Keesman, K.J. ; Lens, P.N.L. (2015)
FEMS Microbiology Reviews 39 (6). - p. 823 - 853.
- [Hybrid Constraints of Pure and Mixed Pixels for Soft-Then-Hard Super-Resolution Mapping with Multiple Shifted Images](#)
Chen, Yuehong ; Ge, Yong ; Heuvelink, G.B.M. ; Hu, Jianlong ; Jiang, Yu (2015)
IEEE Journal of Selected Topics in Applied Earth Observation and Remote Sensing 8 (5). - p. 2040 - 2052.
- [Deoxygenation of biobased molecules by decarboxylation and decarbonylation – a review on the role of heterogeneous, homogeneous and bio-catalysis](#)
Dawes, G.J.S. ; Scott, E.L. ; Notre, J.E.L. Le; Sanders, J.P.M. ; Bitter, J.H. (2015)
Green Chemistry 17 . - p. 3231 - 3250.
- [Spatial boundary of urban ‘acid islands’ in China](#)
Du, E. ; Vries, W. de; Liu, X. ; Fang, J. ; Galloway, J.N. ; Jiang, Y. (2015)
Scientific Reports 5, 12625, doi:1038/srep12625
- [CFD simulation for reduced energy costs in tubular photobioreactors using wall turbulence promoters](#)
Gomez Perez, Cesar ; Espinosa, J. ; Montenegro Ruiz, L.C. ; Boxtel, A.J.B. van (2015)
Algal Research 12 . - p. 1 - 9.
- [Modelling ventilated bulk storage of agromaterials](#)
Grubben, N.L.M. ; Keesman, K.J. (2015)
Computers and Electronics in Agriculture 114 . - p. 285 - 295.
- [Supporting data of spatiotemporal proliferation of human stromal cells adjusts to nutrient availability and leads to stanniocalcin-1 expression in vitro and in vivo](#)
Higuera, Gustavo A. ; Fernandes, Hugo ; Spitters, Tim W.G.M. ; Peppel, Jeroen van de; Aufferman, Nils ; Truckenmueller, Roman ; Escalante, Maryana ; Stoop, Reinout ; Leeuwen, Johannes P. van; Boer, Jan de; Subramaniam, Vinod ; Karperien, Marcel ; Blitterswijk, Clemens van; Boxtel, Ton van; Moroni, Lorenzo (2015)
Data in Brief 5 . - p. 84 - 94.
- [Spatiotemporal proliferation of human stromal cells adjusts to nutrient availability and leads to stanniocalcin-1 expression in vitro and in vivo](#)
Higuera, G.A. ; Fernandes, H. ; Spitters, T.W.G.M. ; Boxtel, A.J.B. van (2015)
Biomaterials 61 . - p. 190 - 202.
- [Production of volatile fatty acids from sewage organic matter by combined bioflocculation and alkaline fermentation](#)
Khiewwijit, R. ; Temmink, H. ; Labanda, A. ; Rijnaarts, H. ; Keesman, K.J. (2015)
Bioresource Technology 197 . - p. 295 - 301.

- [Volatile fatty acids production from sewage organic matter by combined bioflocculation and anaerobic fermentation](#)
Khiewwijit, R. ; Keesman, K.J. ; Rijnaarts, H.H.M. ; Temmink, B.G. (2015)
Bioresource Technology 193 . - p. 150 - 155.
- [Energy and nutrient recovery for municipal wastewater treatment: How to design a feasible plant layout?](#)
Khiewwijit, R. ; Temmink, B.G. ; Rijnaarts, H.H.M. ; Keesman, K.J. (2015)
Environmental Modelling & Software 68 . - p. 156 - 165.
- [Selective terminal C-C scission of C5-carbohydrates](#)
Klis, F. van der; Gootjes, L. ; Haveren, J. van; Es, D.S. van; Bitter, J.H. (2015)
Green Chemistry 17 . - p. 3900 - 3909.
- [Connecting and unmasking relativity and quantum theory](#)
Koning, W.L. de; Willigenburg, L.G. van (2015)
Physics Essays 28 (3). - p. 392 - 398.
- [Economic valuation of potential products from Jatropha seed in five selected countries: Zimbabwe, Tanzania, Mali, Indonesia, and The Netherlands](#)
Lestari, D. ; Zvinavashe, E. ; Sanders, J.P.M. (2015)
Biomass and Bioenergy 74 . - p. 84 - 91.
- [The urban harvest approach as framework and planning tool for improved water and resource cycles](#)
Leusbrock, I. ; Nanninga, T.A. ; Lieberg, K. ; Agudelo, C. ; Keesman, K.J. ; Zeeman, G. ; Rijnaarts, H. (2015)
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- [Particle suspension concentration with sparse obstacle arrays in a flow channel](#)
Lubbersen, Y.S. ; Fasaei, F. ; Kroon, P.J. ; Boom, R.M. ; Schutyser, M.A.I. (2015)
Chemical Engineering and Processing 95 . - p. 90 - 97.
- [Analysis of sustainability metrics and application to the catalytic production of higher alcohols from ethanol](#)
Patel, A.D. ; Telalovic, S. ; Bitter, J.H. ; Worrell, E. ; Patel, M.K. (2015)
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- [Effect of Methanethiol Concentration on Sulfur Production in Biological Desulfurization Systems under Haloalkaline Conditions](#)
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Environmental Science and Technology 49 (15). - p. 9212 - 9221.
- [Towards plant protein refinery: Review on protein extraction using alkalo and potential enzymatic assistance](#)
Sari, Y.W. ; Mulder, W.J. ; Sanders, J.P.M. ; Bruins, M.E. (2015)
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- [Toward concise metrics for the production of chemicals from renewable biomass](#)
Sheldon, R.A. ; Sanders, J.P.M. (2015)
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- [Comparison of first principles model of beer microfiltration to experiments via systematic parameter identification](#)
Sman, R.G.M. van der; Willigenburg, G. van; Vollebregt, H.M. ; Eisner, V. ; Mepschen, A. (2015)
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- [Stability of Transition-metal Carbides in Liquid Phase Reactions Relevant for Biomass-Based Conversion](#)
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ChemCatChem 7 (18). - p. 2816 - 2823.
- [Conversion of polyhydroxybutyrate \(PHB\) to methyl crotonate for the production of biobased monomers](#)
Spekreijse, J. ; Notre, J.E.L. Le; Sanders, J.P.M. ; Scott, E.L. (2015)

- Journal of Applied Polymer Science* 132 (35). - 8 p.
- [Structure-performance relations of molybdenum- and tungsten carbide catalysts for deoxygenation](#)
Stellwagen, D.R. ; Bitter, J.H. (2015)
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 - [Simultaneous and selective decarboxylation of l-serine and deamination of l-phenylalanine in an amino acid mixture—a means of separating amino acids for synthesizing biobased chemicals](#)
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New Biotechnology 33 (1). - p. 171 - 178.
 - [Metabolic engineering of the mixed-acid fermentation pathway of *Escherichia coli* for anaerobic production of glutamate and itaconate](#)
Vuoristo, Kiira S. ; Mars, Astrid E. ; Sangra, Jose Vidal ; Springer, Jan ; Eggink, Gerrit ; Sanders, Johan P.M. ; Weusthuis, Ruud A. (2015)
AMB Express 5 (1). - 11 p.
 - [Heterologous expression of *Mus musculus* immunoresponsive gene 1 \(irg1\) in *Escherichia coli* results in itaconate production](#)
Vuoristo, K.S. ; Mars, A.E. ; Loon, S. ; Orsi, E. ; Eggink, G. ; Sanders, J.P.M. ; Weusthuis, R.A. (2015)
Frontiers in Microbiology 6:849
 - [Metabolic engineering of itaconate production in *Escherichia coli*](#)
Vuoristo, K.S. ; Mars, A.E. ; Vidal Sangra, J. ; Springer, J. ; Eggink, G. ; Sanders, J.P.M. ; Weusthuis, R.A. (2015)
Applied Microbiology and Biotechnology 99 (1). - p. 221 - 228.
 - [Temporal stabilizability and compensatability of time-varying linear discrete-time systems with white stochastic parameters](#)
Willigenburg, L.G. van; Koning, W.L. De (2015)
European Journal of Control 23 . - p. 36 - 47.
 - [U-D factorisation of the strengthened discrete-time optimal projection equations](#)
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International Journal of Systems Science 47 (5) p. 1032 – 1041.
 - [Optimal adaptive scheduling and control of beer membrane filtration](#)
Willigenburg, L.G. van; Vollebregt, H.M. ; Sman, R.G.M. van der (2015)
Control Engineering Practice 34 . - p. 77 - 87.
 - [How Does Alkali Aid Protein Extraction in Green Tea Leaf Residue: A Basis for Integrated Biorefinery of Leaves](#)
Zhang, C. ; Sanders, J.P.M. ; Xiao, T.T. ; Bruins, M.E. (2015)
PLoS One 10 (7).
 - [Effects of Granule Size of Cross-Linked and Hydroxypropylated Sweet Potato Starches on Their Physicochemical Properties](#)
Zhao, J. ; Chen Zenghong, ; Jing, Z. ; Buwalda, Piet ; Gruppen, H. ; Schols, H.A. (2015)
Journal of Agricultural and Food Chemistry 63 (18). - p. 4646 - 4654.
 - [Level and position of substituents in cross-linked and hydroxypropylated sweet potato starches using nuclear magnetic resonance spectroscopy](#)
Zhao, J. ; Chen, Z. ; Jin, Z. ; Waard, P. de; Buwalda, Piet ; Gruppen, H. ; Schols, H.A. (2015)
Carbohydrate Polymers 131 . - p. 424 - 431.
 - [Exergetic comparison of food waste valorization in industrial bread production](#)
Zisopoulos, F.K. ; Moejes, S.N. ; Rossier Miranda, F.J. ; Goot, A.J. van der; Boom, R.M. (2015)
Energy 82 . - p. 640 - 649.

Non-refereed article in a journal

- [Set-membership identification of an agro-ecosystem from a small data set: The case of ammonia volatilisation in a flooded rice field](#)
Khairudin, N.B. ; Struik, P.C. ; Keesman, K.J. (2015)
IFAC Papers Online : Agricontrol 48 (1). - p. 580 - 585.
- [Sustainability metrics of chemicals from renewable biomass \(editorial\)](#)
Sheldon, R.A. ; Sanders, J.P.M. ; Marinas, A. (2015)
Catalysis today 239. - p. 1 - 2.

PhD Theses internally prepared

- Modeling studies of biological gas desulfurization under haloalkaline conditions
Klok, J.B.M. (2015)
Wageningen University. Promotor(en): Albert Janssen, co-promotor(en): Karel Keesman. - Wageningen : Wageningen University, - 158 p.
- [Valorization of jatropha fruit biomass for energy applications](#)
Marasabessy, A. (2015)
Wageningen University. Promotor(en): Johan Sanders, co-promotor(en): Ruud Weusthuis; M. Moeis. - Wageningen : Wageningen University, - 147 p.
- [Biomass and its potential for protein and amino acids : valorizing agricultural by-products](#)
Sari, Y.W. (2015)
Wageningen University. Promotor(en): Johan Sanders, co-promotor(en): Marieke Bruins. - Wageningen : Wageningen University, - 146 p.

Refereed conference paper

- On-line parameter and state estimation in membrane bioreactor systems
Keesman, K.J. ; Brink, Paula van den (2015)
17th IFAC Symposium on System Identification, Beijing International Convention Center October 19-21, 2015. Beijing, China
- Optimal input design for parameter estimation in nonlinear state-space models using Pontryagin's minimum principle
Keesman, K.J. (2015)
17th IFAC Symposium on System Identification, Beijing International Convention Center October 19-21, 2015. Beijing, China
- From bounded-noise data to robust PI-controller design
Steinbuch, Luc ; Keesman, K.J. (2015)
In: European Control Conference, ECC 1999 - Conference Proceedings. - - p. 1988 - 1993.
- Optimal parametric sensitivity control for a FED batch reactor
Stigter, J.D. ; Keesman, K.J. (2015)
In: 2001 European Control Conference, ECC 2001. - - p. 2841 - 2844.
- A Kalman decomposition to detect temporal linear system structure
Willigenburg, L.G. Van; Koning, W.L. De (2015)
In: 2007 European Control Conference, ECC 2007. - - p. 1721 - 1726.

Non-refereed conference paper

- [Membrane distillation for milk concentration](#)
Moejes, S.N. ; Romero Guzman, Maria ; Hanemaaijer, J.H. ; Barrera, K.H. ; Feenstra, L. ; Boxtel, A.J.B. van (2015)
29th EFFoST International Conference Proceedings 10-12 November 2015, Athens, Greece

Professional publications 2015

Article in journal

- Optimale besturing kasklimaat met minimale energie
Beveren, P.J.M. van; Bontsema, J. ; Straten, G. van; Henten, E.J. van (2015)
Kas techniek 2015 (12). - p. 28 - 30.
- ['We weten precies hoe we het productieproces kunnen sturen'](#)
Bitter, J.H. (2015)
Kennis & Innovatie (2). - p. 6 - 7.
- Concurrenieren met olieprijs? Hoe biobased concurrentie uit de weg kan gaan (interview met Harry Bitter)
Didde, R. ; Bitter, J.H. (2015)
MilieuMagazine: vakblad voor milieumanagement 2015 (4). - p. 24 - 25.
- Op het grensvlak van chemie en biotechnologie (interview met Harry Bitter)
Gool, J. van; Bitter, J.H. (2015)
Petrochem 2015 (6). - p. 8 - 9.
- [How biomass composition determines protein extractability](#)
Sari, Y.W. ; Syafitri, U. ; Sanders, J.P.M. ; Bruins, M.E. (2015)
Industrial Crops and Products 70. - p. 125 - 133.
- Bioplastic niet altijd groen (interview met Harry Bitter)
Versluis, K. ; Bitter, J.H. (2015)
Bionieuws 25 (23 mei 2015). - p. 11 - 11.
- Pernis voeden met suikerbieten (interview met Harry Bitter)
Versluis, K. ; Bitter, J.H. (2015)
Bionieuws 25 (23 mei 2015). - p. 10 - 10.

Book chapters

- [Towards bioeconomy development in Latin America and the Caribbean](#)
Trigo, E.J. ; Henry, G. ; Sanders, J.P.M. ; Schurr, U. ; Ingelbrecht, I. ; Revell, C. ; Santana, C. ; Rocha, P. (2015)
In: Towards a Latin America and Caribbean knowledge based bio-economy in partnership with Europe / Hodson de Jaramillo, E., Bogota Colombia : Pontificia Universidad Javeriana, - p. 15 - 41.

Other output

Inaugural speech

- [Chemicals from biobased feedstocks : integration on multiple length scales](#)
Bitter, J.H. (2015)
Wageningen : Wageningen University, Wageningen UR, - 24 p.

Remaining Output/Presentations

- [Optimal control of greenhouse climate with grower defined bounds](#)
Beveren, P.J.M. van; Bontsema, J. ; Straten, G. van; Henten, E.J. van (2015)
- Exopolysaccharides from *Botryococcus braunii* and the production of bioplastics
Broek, L.A.M. van den; Klis, F. van der; Stoutjesdijk, J.H. ; Boeriu, C.G. ; Blaauw, R. (2015)
In: Exopolysaccharides from Botryococcus braunii and the production of bioplastics Warsaw, Poland, 19-22 October 2015 : 4th EPNOE International Polysaccharide Conference, 2015-10-19/ 2015-10-22
- [Economic viability of aquaponics](#)

- Stadler, M. ; Vermeulen, T. ; Keesman, K.J. ; Baganz, D. (2015)
 USA : ICES2015 Hydroponics and Aquaponics at the Gold Coast, 2015-07-05/ 2015-07-08
- Exergy analysis of industrial bread waste minimization technologies
 Zisopoulos, F.K. ; Moejes, S.N. ; Rossier Miranda, F.J. ; Goot, A.J. van der; Boom, R.M.
 (2015)
 Quebec city, Canada : 12th International Congress on Engineering and Food (ICEF 12),
 2015-06-14/ 2015-06-18
 - Towards non noble metal based catalysts for biobased conversions – role of TIPTOP chemistry, Harry Bitter, Ningbo Institute of Materials Technology, Ningbo, China, 2015-01-09
 - Towards non noble metal based catalysts for biobased conversions – role of TIPTOP chemistry, Harry Bitter, Shenyang National Laboratory for Materials Science, Shenyang, China, 2015-01-13
 - Towards non noble metal based catalysts for biobased conversions – role of TIPTOP chemistry, Harry Bitter, Tsinghua University, Beijing, China, 2015-01-16
 - Deoxygenation in biobased conversions, Harry Bitter, Biorenewables Business Platform, The Hague, The Netherlands, 2015-04-02
 - Biobased chemistry and technology – TIPTOP to food feed and chemicals
 Harry Bitter, WUR alumni meeting Den Bosch, The Netherlands, 2015-04-15
 - Hydrogen and oxygenates from polyols over Ni and Cu catalysts in aqueous alkaline media,
 T. van Haasterecht, C.C.I. Ludding, T. van Deelen, K.P. de Jong and J.H. Bitter,
 ISGC, La Rochelle, France, 2015-05-05
 - Selective terminal C-C scission of C5-carbohydrates
 Frits van der Klis, Linda Gootjes, Daan S. van Es, Jacco van Haveren, Johannes H. Bitter,
 ISGC, La Rochelle, France, 2015-05-07
 - Selective terminal C-C scission of C5-carbohydrates
 Frits van der Klis, Linda Gootjes, Daan S. van Es, Jacco van Haveren, Johannes H. Bitter,
 NAM (North American Meeting of the North American Catalysis Society), Pittsburgh,
 USA, 2015-06-17
 - Homogeneous, heterogeneous and bio catalytic deoxygenation of biobased feedstocks,
 E.L. Scott, R.W. Gosselink, S.A.W. Hollak, G. Dawes, J. Le Notre, D.S. van Es, J. van Haveren
 and J.H. Bitter
 International Symposium on relations between Homogeneous and Heterogeneous
 Catalysis (ISHHC-17), Utrecht, The Netherlands, 2015-07-14
 - Where can chemo and biocatalysis meet
 J.H. Bitter, Symposium on Integration and Synergy between Biocatalysis and Chemical
 Catalysis for Biorenewable Conversion, Utrecht, The Netherlands (invited talk), 2015-
 07-16
 - TIPTOP Chemistry: Towards non noble metal based catalysts for biobased conversions,
 J.H. Bitter, Instituto Nacional de Tecnologia (INT), Rio de Janeiro, Brazil (invited talk) ,
 2015-11-19
 - Texture , Piet Buwalda (invited talk) Haagse Hogeschool, Den Haag , The Netherlands,
 2015-09-28
 - Aqueous phase reforming/processing of bio-feedstocks, Neus Blanch Raga (Speaker)
 N. Blanch Raga, T. van Haasterecht, T.W van Deelen, C.C.I. Ludding, K.P. de Jong, J.H
 Bitter,
 CHAINS 2015 1/12/15 - 2/12/15
 - Biobased industrial nitriles from biomass by vanadium chloroperoxidase, Andrada But
 (speaker)
 But, A.; Wijst, E. van der; Notre, J.E.L. le; Scott, E.L.; Wever, R.; Sanders, J.P.M. (2015)
 Vienna, Austria: BIOTRANS, 26-30 July 2015
 - Biocatalytic formation of industrial nitriles from biomass, Andrada But (speaker)
 But, A.; Notre, J.E.L. le; Scott, E.L.; Wever, R.; Sanders, J.P.M. (2015)

- Noordwijkerhout : Netherlands Catalysis & Chemistry Conference XVI, 2-4 March 2015
 • Biobased nitrile production by enzymatic oxidative decarboxylation of amino acids: effect of side chain on the conversion and selectivity, Evie van der Wijst (Speaker)
 Wijst, E. van der; But, A.; Scott, E.L.; Bitter, J.H.; Sanders, J.P.M. (2015)
 Noordwijkerhout : Netherlands Catalysis & Chemistry Conference XVI, 2-4 March 2015
- Optimisation of water, energy and nutrient requirements in an aquaponic system with interacting production loops, Daniel Reyes Lastiri (speaker)
 Slinkert, T. ; Reyes Lastiri, D. ; Keesman, K.J. ; Cappon, H. (2015)
 2nd New Developments in IT & Water, IWC.

Press clippings

- Duurzaam verdwijnen in een kist van bioplastic, Harry Bitter, (Robin van Wechem)
 Trouw, 15 Jan 2016
- De afval race, Harry Bitter,(Enith Vlooswijk)
 KIJK magazine 1 (2016), 17 Dec 2015
 Muurverf op plantaardige basis is een stap vooruit, maar kan nog beter, Harry Bitter ,
 (Robin van Wechem)
 Trouw, 4 Dec 2015