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IPESE
Industrial Process and Energy Systems Engineering

Development of Biorefineries and Energy Systems:

Energy Integration
Life Cycle Analysis
Thermodynamics in Biorefineries
Biochemical Routes for Biorefineries
Thermochemical Routes for Biorefineries

30th, 31st March and 1st April, 2016
EPFL, Sion
Switzerland

Prof. Francois Marechal (Chair)
Dr. Shivom Sharma

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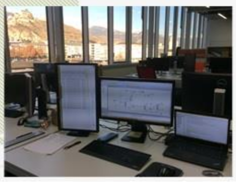
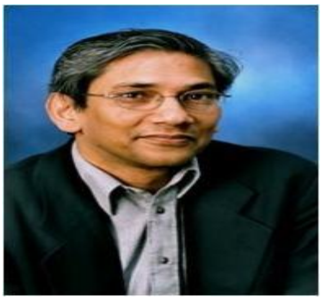


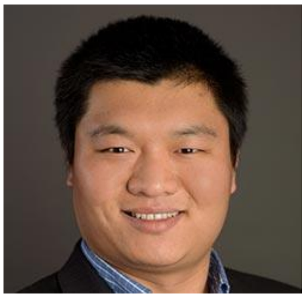
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Keynote Speakers

Prof. Antonios Kokossis



Prof. Rafiqul Gani



Prof. Fengqi You

Prof. Rakesh Agrawal

Prof. Mario R. Eden

Prof. A. V. Ensinas

	Registration	**13:15**
	Welcome (François Maréchal, IPESE-EPFL)	**13 :45**
30 March, 2016	**Keynote 1:** Design of Integrated Biorefineries Prof. Antonios Kokossis (NTUA, Greece)	14:00-14:40 (30 + 10 min)
	• Model-based optimization of microalgal biorefineries by dynamic flux balance analysis (DFBA) Melanie Fachet (Max-Planck-Institute for Dynamics of Complex Technical Systems, Germany) • Selection of optimally integrated biorefinery processes by early-stage design decision making approach Ayse Dilan Celebi (EPFL, Switzerland)	14:40-15:20 (15 + 5 min)
	Tea/Coffee break (15:20-15:40)	
	• Systematic process development of integrated first and second generation biorefineries Aikaterini Mountraki (National Technical University of Athens, Greece) • Production of sugar platforms from lignocellulosic biomass – energy analysis and techno-economic comparison Juan David Villegas (University of Geneva, Switzerland) • Integrated biomethanol production Andre F. Amaral (Politecnico di Milano, Italy) • Optimizing biomass-based energy supply chains for sustainable mobility Federico d'Amore (University of Padova, Italy)	15:40-17:00 (15 + 5 min)
31 March, 2016	**Keynote 2:** New Vistas in Chemical Product and Process Design Prof. Rafiqul Gani (Technical University of Denmark)	10:00-10:40 (30 + 10 min)
	• Rigorous optimization-based design of energetically intensified distillation processes for the separation of non-ideal mixtures Thomas Waltermann (TU Dortmund, Germany) • Shortcut-based evaluation of energetically intensified distillation processes under uncertainty Mirko Skiborowski (TU Dortmund, Germany)	10:40-11:20 (15 + 5 min)
	Tea/Coffee break (11:20-11:40)	
	• Process network flux analysis for an early design stage evaluation of biorefinery processing pathways Kirsten Ulonska (RWTH Aachen, Germany) • Computer-aided molecular design using process shortcut models and COSMO-RS Jan Scheffczyk (RWTH Aachen, Germany) • Synthesis and optimization of processing paths for specialty chemicals in microalgae biorefineries Melina Psycha (National Technical University of Athens, Greece) • Process design of 5-hydroxymethlfurfural (5-HMF) Process and integration in bio-refineries Masoud Talebi Amiri (EPFL, Switzerland)	11:40-13:00 (15 + 5 min)
	Lunch break (13:00-14:00)	
	Keynote 3: Life Cycle Analysis and Optimization for Sustainable Synthesis of Biofuels and Bioproducts Pathways Prof. Fengqi You (Northwestern University, USA)	14:00-14:40 (30 + 10 min)

1 April, 2016

• A supply chain optimization approach to the design of lignocellulose-based products Anna Panteli (Imperial College London, UK) • Development of semantically-enabled community hubs in biorefineries and biorewables Eirini Siougkrou (National Technical University of Athens, Greece)	14:40-15:20 (15 + 5 min)
Tea/Coffee break (15:20-15:40)	
• Rapid capital and operating cost estimation for biorefinery processes under development Mirela Tsagkari (CRRA- Arkema, France)	15:40-16:00 (15 + 5 min)
Keynote 4 & Seminar Series ChE 602: Solar Energy to Fuels, Chemicals and Electricity Prof. Rakesh Agrawal (Purdue University, USA)	16:00-17:00 (60 min)
Panel Discussion with Keynote Speakers: Process Systems Engineering in Energy Systems	17:00-18:00 (60 min)
DINNER (Start at 18:30)	
Keynote 5: Gas-To-Liquids (GTL) Technologies for Production of Fuels and Chemicals from Lignocellulosic Biomass Prof. Mario Richard Eden (Auburn University, USA)	10:00-10:40 (30 + 10 min)
• Discovering valorization paths in waste biorefineries using an ontology engineering approach Foteini Barla (National Technical University of Athens, Greece) • An ontology supported model discovery and data integration Linsey Koo (University of Surrey, UK)	10:40-11:20 (15 + 5 min)
Tea/Coffee break (11:20-11:40)	
• Techno-economic evaluation of consolidated bioprocessing of lignocellulosic biomass: Katelyn McClung (EPFL, Switzerland) • Novelty in reactor design and optimization for biotechnology applications using a systems approach Georgios Panayiotou (NTUA, Greece) • Holistic syntheses of more sustainable renewable-based supply networks Žan Zore (University of Maribor, Slovenia) • Optimal management of raceways using meteorological forecasts Riccardo De Luca (University of Padova, Italy)	11:40-13:00 (15 + 5 min)
Lunch break (13:00-14:00)	
Keynote 6: Integral valorization of biomass as the key for sustainable biorefineries Prof. Adriano Viana Ensinas (UFABC, Brazil)	14:00-14:40 (30 + 10 min)
• General superstructure synthesis for combined mass and energy integration in industrial processes Maziar Kermani (EPFL, Switzerland) • Retrofitting of large-scale total site heat exchanger networks for fixed and flexible designs Lidija Cucek (University of Maribor, Slovenia) • Climate, Energy, and Food Security from the Sea Prof. Deborah Sills (Visiting Prof. at IPESE-EPFL, Switzerland)	14:40-15:40 (15 + 5 min)
Closing Words (François Maréchal, IPESE-EPFL)	**15 :40**
APERITIF (15:45-16:30)	

Keynote 1: Design of Integrated Biorefineries

Prof. Antonios Kokossis
School of Chemical Engineering, National Technical University of Athens, Greece

The design of biorefineries from pilots and installed facilities bears tremendous social and economic benefits. By 2020, Bloomberg predicts that, only in Europe, there would be around 1,000 of such new units bringing €32.3 trillion revenues and 1 million new jobs. Process systems engineering has a pivotal and critical role in the development of biorefineries. The general view is increasingly supported by results and analysis that prove the significance of systems engineering in future developments. The design and synthesis of biorefineries constitutes a complex problem challenged to cope with the large and unknown product portfolios as they arise from different chemical itineraries and processing paths (value chain analysis) as well as process engineering options to select units and integrate them into a plant (process synthesis, process integration). In all cases, the designs are required to match maximum efficiencies in the use of materials/energy and to assess uncertainties in processing and economic parameters that may affect the selected designs and the level of integration. The presentation explains a systems framework tested on real-life applications. The work combines methods in process synthesis and integration, optimization and process modelling. At a conceptual level, process synthesis determines process and products to use, enabling a systematic screening with a simultaneous approach and the systematic use of optimization. Process integration, integrates for maximum efficiency in raw materials and energy, as well as for the maximum performance against environmental targets. Process flowsheeting validates with process simulation and enables improvements with parametric optimization. The coordinated use of the systems methods constitutes a significant advancement in the state of the art, currently relying on case-by-case analysis (flowsheeting) or the experimentation with commercial simulators.

The systematic methodology is already applied to several real-life biorefineries that include lignocellulosic and oleochemical biorefineries, halophytic algo-biorefineries and, more recently, waste biroefineries. The lignocellulosic applications involve chemistry paths with 70-odd chemicals that include basic intermediates (sugars, lignin, ethylene, oils), bulk chemicals (ethanol, butanol, propanol, isopropanol), bio-based polymers (PVC, resins, polyamides, PEIF, polyacrylates, PUs), and a wide range of chemicals (xylitol, xylonic acid, itaconic acid, sorbitol, isosorbide, hydrogel etc). Preliminary results are often impressive. Other than systematically screening and scoping integrated paths for the plant, the analysis reduces energy by 70% and the water use by 50-60%. Research is strongly coordinated with LCA. Results demonstrate that, unless fully integrated, biorefineries remain unsustainable. Instead, fully integrated biorefineries stand as viable and operational options, offering a strong promise to the development of sustainable industries in the future.

The development of the system framework relied on a new generation of methods that combine synthesis and process integration at different levels, further building high-throughput capacities using ontology engineering. Semantics and ontology engineering are intended to compound the screening of engineering options with a parallel screening for materials, strains, resources, and chemistries (biology, biochemistry node). They are also intended to capitalize and link the systems methodology with other systems methods around the world. Design work is being recently extended to address retrofit applications with a purpose to upgrade first generation plants into second (or higher generation) biorefineries. The methodology is also tested in the context of Industrial Symbiosis where the biorefineries are deployed to explore links (mass and energy exchanges) between industries and resources available at urban sites. Results and applications in that context will be presented from recent work to evaluate the bioenergy potential at four different EU ports. Other work in progress includes data modelling to develop Class 4 and Class 5 estimates for CAPEX and OPEX, data modeling to calculate LCA metrics at early stages, and the extension of FineChem to biorenewables.

Keynote 2: New Vistas in Chemical Product and Process Design

Prof. Rafiqul Gani
PSE for SPEED Project, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kgs. Lyngby Denmark.

Design of chemicals based products is broadly classified into those that are process centric and those that are product centric. In this presentation, the designs of both classes of products will be reviewed and a timeline in terms of key contributions in chemical product-process design will be presented. While significant advances have been made in the development of systematic model-based techniques for process design and also for optimization, operation and control, much work is needed to reach the same level for product design. In terms of current challenges and opportunities, issues related to integrated product-process design, the modelling challenges related to product properties and functions, and the motivation to find novel, innovative and sustainable solutions will be highlighted. The need for an integrated model-experiment based design approach will be presented together with benefits of employing a systematic computer-aided framework with built-in design templates. A chemical product design simulator will be presented.

Keynote 3: Life Cycle Analysis and Optimization for Sustainable Synthesis of Biofuels and Bioproducts Pathways

Prof. Fengqi You
Northwestern University, USA

Biomass-derived chemical products may offer reduced environmental impacts compared to their fossil-derived counterparts and could improve profit margins at biorefineries when coproduced with higher-volume, lower-profit margin biofuels. This presentation will begin with our recent life cycle analysis (LCA) study on assessing the life cycle energy and environmental impacts of 8 bioproducts selected on the basis of technology readiness and market potential. We developed high-fidelity process simulations to obtain energy and material flows in the production of each bioproduct and examined sensitivity of these flows to process design assumptions. Conversion process data were combined with upstream and downstream life cycle environmental impact parameters to determine the cradle-to-grave environmental impacts of each bioproduct. Data and results of this study have now been included in Argonne GREET model.

Building on the data and approach of the LCA study, we further develop a superstructure-based computational framework for sustainable design and synthesis of algal biorefineries that produce fuels and value-added chemicals. This framework simultaneous models detailed mass and energy flows within the biorefinery, and organically integrates with technoeconomic analysis and LCA. It systematically evaluates various technology alternatives and determines the optimal product portfolio for making different biofuels and bioproducts from a given algal feed.

At the end of the presentation, we will discuss a comprehensive biofuels and bioproducts conversion network, with 200 conversion technologies and 142 compounds (feedstocks, intermediates, and final products). This bioconversion network represents various pathways for making 4 types of biofuels and 9 bioproducts from 11 terrestrial and aquatic biomass feedstocks. We develop a network-based life cycle optimization framework to identify the most cost-effective and environmentally sustainable production pathways for a given feed or a specific demand. We will discuss general modeling frameworks, efficient solution algorithms, and case studies illustrate the applications of these frameworks.

Keynote 4 and Seminar Series ChE-602: Solar Energy to Fuels, Chemicals and Electricity

Prof. Rakesh Agrawal
School of Chemical Engineering
Purdue University, West Lafayette, IN 47907, USA

In the long run, it is likely that all the basic human needs will be met by renewable sources like solar energy. However, there are several challenges associated with harness, storage and use of solar energy to meet our daily needs for food, chemicals, heat, electricity and transportation. In a sustainable future, all these usage must coexist.

We will first present some results from our energy systems modeling highlighting the synergistic interactions that exist for transportation sector and production of chemicals. This will be followed by a discussion and analysis of candidate processes to produce hydrogen from solar energy, our modeling results for energy storage at giga Watt-hour levels and uninterrupted around the clock electricity production using new solar thermal power cycles with internal hydrogen circulation. Such cycles have a potential to not only supply solar thermal electricity at an unprecedented efficiency during the period while solar energy is available but have a potential to supply around the clock electricity with efficiencies similar to that from batteries storage, however, here energy is stored at a much higher density. We will then discuss our vision of how to use solar thermal processes to meet demand for water, chemicals and food.

An exciting aspect of producing fuels and chemicals from biomass is learning to produce the array of molecules that we need with minimum process transformation steps and energy use while maximizing biomass carbon recovery. In this aspect, recent advancements at Purdue by a team of chemists, biologists and chemical engineers will be presented. We will show the new pathways along with the associated catalysts and reactors that have been developed for the production of fuel and chemicals from biomass. More importantly, we will showcase how modelling has been used to identify, design and guide the experiments.

Keynote 5: Gas-To-Liquids (GTL) Technologies for Production of Fuels and Chemicals from Lignocellulosic Biomass

Prof. Mario R. Eden
Department Chair, Joe T. & Billie Carole McMillan Professor
Director, NSF-IGERT on Integrated Biorefining, Department of Chemical Engineering, Auburn University, USA

The large amounts of underutilized woody biomass available (14.6 million tons annually in Alabama alone) can contribute significantly to societal goals for energy security and economic viability if technological advances are achieved in the thermochemical conversion platforms. In this work, we are developing viable hydrocarbon production strategies by integration of biomass fractionation technologies followed by technically well-informed application of thermochemical conversion approaches and associated catalyst structures.

Our multidisciplinary team has established significant synergies in our research efforts particularly in catalyst development and characterization, chemical/fuels production and process systems engineering. This work leverages ongoing research by taking advantage of a unique set of testbeds in the Auburn University Center for Bioenergy and Bioproducts consisting of biomass fractionation and several conversion technologies, most notably a pilot-scale gasification unit that will be used to produce the synthesis gas for supercritical phase Fischer-Tropsch synthesis and high value chemical co-production.

Biomass fractionation technology coupled with a pilot-scale gasification unit enables systematic analysis of the downstream conversion viability and potential for value addition for each feedstock constituent, i.e. cellulose, hemicelluloses and lignin. As a specific example, we have studied an innovative supercritical phase Fischer-Tropsch Synthesis (SCF-FTS) process developed at AU using biomass derived syngas with particular attention on the impact of novel nanoscale catalysts on reaction performance. This dense supercritical media enables significant enhancement of middle distillate products while drastically reducing undesired methane formation, thus improving the overall carbon utilization. Additionally, we have demonstrated that the use of properly selected Fe-based catalysts in supercritical fluid reaction media results in a product stream consisting of more than 30% aldehyde species plus significant concentrations of 1-olefins. This affords higher value than conventional FTS approaches. We have also studied Higher Alcohol Synthesis (HAS) under supercritical conditions and this process has been found to be particularly well suited for biomass derived syngas.

Synergistic collaboration between experts in chemical engineering and biosystems engineering allows for a systems level approach to the optimization of the biomass to hydrocarbon chemical/fuel lifecycle including design/characterization of the enabling catalysts. Our team employs a holistic methodology utilizing a systematic and flexible process integration/optimization based framework to identify product distributions and processing routes for integrated biorefineries.

This presentation will provide an overview of the biorefining activities at Auburn University with particular emphasis on the fundamentals of thermochemical conversion and gas-to-liquids technologies for the production of fuels and chemicals.

Keynote 6: Integral Valorization of Biomass as the Key for Sustainable Biorefineries

Prof. Adriano V. Ensinas
UFABC, Brazil

The green economy is growing as alternative to traditional fuels and chemicals markets based on fossil carbon conversion technologies. Its full implementation will allow producing organic products in large scale based on the principle of photosynthesis, like a huge recycling device able to recover carbon from the atmosphere and make it available for the society.The biorefinery concept allows multiple use of “green carbon” present in biomass, bringing flexibility to a system that is able to produce green energy and several biobased products. Local and global markets for biorefineries are being created worldwide but sustainable growth of this industry requires cost-effective products and energy-efficient plants that can reduce effective greenhouse gases emissions in a carbon neutral loop. The development of novel products from biorefineries usually focus the conversion of only some parts of the biomass composition and selection of pathways that can leads to the maximum reaction yield. This approach is useful for starting the learning process of new technologies but in further steps, an integral process design approach is needed, which can allow engineers to tackle the problem of industrial utilities integration, mass recovery and waste treatment. Throughout a biorefinery process, frequently, precious amount of valuable carbon fixed by photosynthetic process is lost when a waste stream is released from the biorefinery process. Furthermore, heat produced in exothermic reactions and heat transfer processes are big contributors for plant inefficiency. Hence, an integral use of biomass, with valorization of carbon and energy available in the conversion process, is crucial for the feasibility of a biorefinery.

In this presentation, the concept of integral valorization of biomass will be discussed with the help of some biorefinery case studies. Importance of integrated technologies for finding cost competitive and energy-efficient biorefinery plants will be shown using computer aided methods for modelling and process design optimization.

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