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Professor Dr Jiří Jaromír Klemeš: Celebration of the Jubilee in Science and Engineering

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Following the spontaneous decision of the friends within the Process Integration community, the current Jubilee Part of the Chemical Engineering Transactions (CET) Vol. 45 has been created, to celebrate the scientific achievements and the personality of Professor Dr Jiří Jaromír Klemeš. Some of the authors have chosen to prepare scientific tributes and others have contributed personal congratulatory articles. As a result the current Jubilee Part is a multi-faceted presentation of all friends' perspectives.

This Editorial article introduces the celebration contributions. They are organised in scientific and personal parts, where the scientific part has a number of topical sections related to process design, optimisation and sustainability.

It is shown in the overview that the collaboration of the community established with the help of the PRES series of conferences founded by Professor Dr Jiří Jaromír Klemeš has been very useful and is very much needed in the future.

1. Scientific contributions

The scientific contributions cover a range of topics relevant to research and development in Process Integration, Process Optimisation and Sustainable Development. The topical groups are Heat Transfer and Heat Exchange, Process Integration, Sustainability contribution and use of renewables, Batch Process Optimisation, Conceptual Analyses.

1.1 Heat Transfer and Heat Exchange

This section comprises of several papers on Heat Exchanger Network Retrofit, application of heat transfer enhancement and intensification techniques, control and controllability of industrial processes with recycles. They have been authored by distinguished members of the PRES family from Slovenia, USA, Ukraine, and Slovak Republic.

Čuček and Kravanja (2015), from the University of Maribor have presented a study on Heat Exchanger Network Retrofit, based on a real case. Beside those works recently published as Nemet et al. (2015) and Liew et al. (2014) they have developed another procedure for retrofitting of large-scale heat exchanger networks within industrial plants and Total Sites by considering trade-offs between investment and operating cost. A transhipment-based framework TransGen for the energy targeting and retrofitting industrial plants and TSs has been developed for this purpose. Retrofitting of heat exchanger networks could be performed for problems of any size - from few heat exchange units up to hundreds of them. This procedure could be applied for both nominal designs under fixed conditions and under uncertain conditions for flexible designs by considering several scenarios. TransGen is illustrated on a simplified demonstration case study of two plants in order to clearly represent the features of the developed procedure. From the results from improved version of TransGen it was shown that significant energy and economic savings could be obtained, at modest payback times of maximum 15 months.

Kapustenko et al. (2015) present a survey of the recent advances in heat transfer intensification and enhancement techniques. The authors suggest that the selection of a particular method for heat transfer intensification depends on the process conditions where the heat transfer equipment is used. When

1718

retrofitting existing shell and tube heat exchangers, enhancing tube inserts can be employed or changing the tubes for enhanced tubes. Economic considerations of a new enhanced shell and tube heat exchanger; tube replacement with enhanced tubes; or the use of PHEs should also be considered in the evaluation of a heat exchanger. The authors also contributed to a book presenting comprehensive coverage has been just published by Klemeš et al. (2015).

Mészáros et al. (2015) have investigated the dynamic behaviour of industrial processes involving recycles from the perspective of stability and controllability. Investigation of influence of process recycle loop parameters have been carried out, applying simulation experiments on linear transfer function models. Stability and controllability considerations are provided in both, open and closed loop mode.

1.2 Process Integration

Process Integration has been an area of particularly intensive research by the Process Engineering community – covered by recent Handbook of Process Integration (Klemeš, 2013) and Process Integration and Intensification: Saving Energy, Water and Resources textbook (Klemeš, 2014). In the recent years it has received very considerable attention from researchers coming from South-East Asia – see e.g. Chew et al. (2015) and Mohammad Rozali et al. (2015). This trend has been reflected also in the current Jubilee part. This section presents several contributions from Malaysia, India, and China. Two of them are dedicated to strategic issues of Process Integration and another represents an attempt to combine Process Integration thinking and Mathematical Programming for solving Total Site Integration problems overviewed also by Klemeš and Kravanja (2013).

In a strategic research effort, Tan et al. (2015), have discussed the potential research areas that can benefit from further spread of the Pinch Analysis idea. Pinch Analysis was originally developed as a thermodynamically-based methodology for targeting and design of industrial heat recovery systems. The authors first analysed the already available Pinch Analysis extensions – most notable are those related to mass exchange. They have further identified as promising directions for future work methodological extensions, such as multiple-objective and multiple-quality index Pinch Analysis, as well as hybridization of Pinch Analysis with allied optimisation techniques, energy planning, production planning under uncertainty, and risk and safety management – for a wider overview see (Klemeš et al., 2013).

A study on "Reconfiguration of Cooling Water Networks in Retrofit Scenarios" has been contributed by Kim (2015). This field had been previously overviewed by Klemeš (2012). This study investigates impacts resulted from the reconfiguration of cooling water network when cooling water reuse is introduced for debottlenecking of existing cooling water systems. Conceptual design guidelines are provided to regain driving force of heat transfer for coolers by increasing cooling water flowrate for the cooler. A case study has been presented to explain how reduced temperature difference in coolers can be compensated by increasing cooling water flowrate, and to demonstrate the applicability of the proposed design method in practice.

Bandyopadhyay (2015) has presented a study titled "Mathematical Foundation of Pinch Analysis", in which the mathematical derivation of Pinch Analysis tools for Resource Allocation Networks. In this paper, a mathematical basis for three different graphical methods of Pinch Analysis and their interrelations are established. The proposed mathematical foundation can be used to extend the applicability of Pinch Analysis to complex problems such as conservation of multiple resources.

Chang at al. (2015) have performed a study on the use of a Heat Recovery Loop on Total Sites. This has been a topic previously tackled by Varbanov and Klemeš (2000). As this work concentrates on heat recovery in low temperature range, hot water is selected as the heat transfer medium. The solved results can give the mass flow rate of intermediate-fluids, diameter of pipeline, temperatures of the heat transfer medium and the configuration of heat exchanger networks (HENs). An industry case study with three plants is used to demonstrate the model.

1.3 Sustainability contribution and use of renewables

The industry contribution to sustainability including the use of renewables has become a traditional part of the PRES conference (PRES, 2015). This section presents papers on biorefinery concept development, improved gasification processes, Organic Rankine Cycles using solar energy, carbon capture. The contributions have come from University of Pannonia in Veszprém – Hungary, Politecnico di Milano – Italy, CERTH – Thessaloniki, Greece, University of Paderborn – Germany.

In this topical section first is the paper by Nagy and Hegedüs (2015), who have studied biorefinery concepts with a focus on Central Europe. The paper provides a brief survey on the possible future processes, which are recommended to be developed in the future for this region in order to make the utilization of lignocellulosic biomass profitable, which should use several types of membranes in competition or in synergy with distillation.

Pierucci et al. (2015) have directed their attention toward tools for simulating gasification processes for materials such as biomass, coal and waste. The waste to energy problem had been overview previously by Fodor and Klemeš (2012). Pierucci et al. (2015) have extended the scope and formulated a multiscale mathematical model for the simulation of solid fuels thermochemical conversion processes. The novelty of this approach relies on a kinetic modelling approach, which can characterize, with a reasonable detail, also the devolatilisation and pyrolysis steps, as well as the secondary gas phase reactions. The model has been applied to the gasification of biomass and coal in an updraft fixed-bed reactor. Comparisons with experimental data show the viability of the approach although some further comparisons should be done in order to improve the reliability of the model.

Flexible Solar Rankine Cycles have been studied by Mavrou et al. (2015). They have proposed a systematic method for the selection of working fluid mixtures in a solar Organic Rankine Cycle (ORC) under operating variability. The method is based on a sensitivity analysis procedure where several operating and design parameters that affect the cycle performance are assessed and investigated through an appropriate sensitivity index, which quantifies their impact on several important system performance indices. The proposed method has been applied to 11 mixtures, which were previously identified to present increased energy and exergy performance in solar ORC systems. Among those the mixture containing 70 % 1,1,1-trifluoro-propane and 30 % 1-Fluoromethoxy-propane was found to combine good performance at steady state conditions with reduced sensitivity to variability.

Hüser and Kenig (2015) have performed "A Comparative Study of Carbon Capture for Different Power Plants". This is a study within the framework of the EU-funded project CAPSOL and well compels with the other works developed in this project. Capture units for three different power plants were designed. The solvents used were aqueous amine solutions; feed compositions and main process conditions were first determined using equilibrium-based simulations. As the main evaluation criterion, reaching a CO_2 absorption level of 90 % with minimum energy requirements was selected. It is shown in the paper that an absorption level of 90 % is not always feasible and even not always required. It was shown, that in case of coal-fired power plants, an absorption level of 90 % could be reached with industrially feasible column heights. On the other hand, for the gas-fired power plant, such a level could only be achieved with an unrealistically high column. However, for a reduced absorption degree of 86 %, a fully feasible column height has been obtained, with a low CO_2 concentration of only 600 ppm in the outlet gas stream. These results demonstrate how important the determination of the column height for the feasible industrial design of capture plants is. Furthermore, it is illustrated that an extremely high absorption degree is not always meaningful.

1.4 Batch Process Optimisation

Batch processes are also important for the chemical and process industries. This section presents two contributions dealing with patch process optimisation more generally and batch reactive distillation. They have been contributed by researchers from Universitat Politècnica de Catalunya – Spain as well as from National Oil Corporation, and Libyan Petroleum Institute, Tripoli, Libya, in a team with the University of Bradford – United Kingdom.

Moreno-Benito et al. (2015) have contributed an article on integrated process and plant design optimisation for batch processes. The work explores stochastic and hybrid solution approaches for dealing with integrated batch processes development and plant design. The simultaneous optimisation of the synthesis of batch processes, combined with task allocation and plant design has been formulated in the literature as a mixed-logic dynamic optimisation (MLDO) problem, including dynamic control profiles, continuous variables, integers and Booleans as degrees of freedom. In industrial scale situations, this formulation leads to numerically intractable problems when mathematical programming solution strategies are used. So, this contribution has formulated a two-step approach that combines a differential genetic algorithm (DGA) with a deterministic direct-simultaneous solution that transforms the problem into a non-linear programming (NLP) problem. A comparative study of the stochastic and hybrid strategies with the purely deterministic solution is made for the specific case of primary copolymerization for acrylic fibre production. The results show that local optimal solutions of the deterministic method can be beaten by the proposed optimisation strategy, becoming a suitable option for solving cases of industrial size.

The stochastic and hybrid approaches presented in this paper (Moreno-Benito et al., 2015) have been characterised by the authors as providing a powerful option for solving complex integrated problems as these of batch process development and plant design, where the mathematical complexity may require problem decomposition or recipe approximations. Both proposed strategies, based on DGA with random initial populations, have been reported as providing promising results, with improvements in the objective function of more than 40 % compared solutions from deterministic solvers. This indicates that the new algorithm is capable of overcoming certain local optima. The authors attribute this achievement to the

1720

applied hybrid strategy. Several directions have been suggested for further research – for instance the use of adaptive penalty factors or other strategies to balance the order of magnitude of the objective function and the penalties in the fitness function.

Edreder et al. (2015) have considered the use of several indicators and criteria for evaluating the performance of reactive batch distillation processes. The combination of distillation and reaction reduces the capital and operating cost considerably. Among many different types of batch reactive distillation column configurations, conventional and middle vessel batch reactive distillation columns are considered in this contribution for hydrolysis of methyl lactate and only conventional is considered for an esterification of acetic acid and ethanol. Several criteria such as maximum profit under fixed demand, maximum productivity and minimum batch time are used to evaluate the performance of different column configurations. Optimal design and or operation policies are obtained by applying these criteria and are compared. A detailed rigorous dynamic model, consisting of mass, energy balances, chemical reactions and thermodynamic properties, is used for evaluating the column performance. It was observed by the authors that multi-reflux ratio operation always led to better performance in terms of productivity or batch time for all reaction schemes compared to that obtained using single reflux operation. Feed dilution (in the case of ethanol esterification) led to more profit even though productivity was found to be lower. This was explained as due to reduction in feed price because of feed dilution. Optimisation of design and operation (for ethanol esterification) clearly showed that a single column will not lead to profitable operation for all possible product demand profile.

1.5 Conceptual Analyses

Two conceptual analysis papers have also been written. They are both focusing on the definition and analysis of indicators of economic and environmental performance. The articles come from Austria and Slovenia.

Glavič (2015) has contributed a conceptual paper on the relation of chemical and process industry and conventional accepted economic indicators, mainly on the case of Gross Domestic Product. A lot of research has previously been carried out on eco-innovation, sustainable development and the associated indicators. However, it still needs more widely to be implemented into practice. Economic indicators such as Gross Domestic Product (GDP) were not fully designed to be comprehensive measures of prosperity and well-being. RIO+20 discussions have resulted in the call for development of a possible set of indicators to measure progress on Sustainable Development Goals. The EU Beyond GDP initiative is about developing indicators that are as clear and appealing as GDP, but more inclusive of environmental and social aspects of progress. Society needs adequate indicators to monitor the progress in addressing the global challenges of the 21st century such as climate change, poverty, resource depletion, health, and quality of life. A critical review of sustainability measurement using methods, tools and indicators for CPI is presented. Possible responses are investigated in this paper, ranging from short-term ones like resource efficiency and circular economy, via medium-term ones like renewable energy and material sources, to long-term ones such as adapting to changing consumption patterns by the products portfolio of these industries and their volume of production. The author provides an analysis, which leads to a number of conclusions for significant changes in the way of conducting the business as well as the life style of all society parts. This work can be considered as an interesting contribution to recently published book "Assessing and Measuring Environmental Impact and Sustainability" (Klemeš, 2015).

Another work related to Assessing Sustainability is presented by Narodoslawsky and Shahzad (2015). They have taken a little different perspective on sustainability measurement and evaluation by analysing the essence of ecological indicators. Ecological evaluation has become a valuable tool for Process Engineering, as environmental concerns stimulate more and more the formulation of critical constraints for process design. Currently a wide variety of different indicators are available that may be used to support process engineers in making their design decisions. They offer, however, conflicting advice in many cases as presented by Čuček et al. (2012). The paper analyses the normative assumptions of single issue indicators (e.g. Carbon Footprint and Global Warming Potential), efficiency indicators (e.g. Material Input per Service Unit), thermodynamic ones (e.g. Emergy) and complex, highly aggregated indicators such as Ecological Footprint and the Sustainable Process Index. The paper attempts to provide guidelines for the choice of environmental indicators as well as for interpretation of the obtained results. The authors conclude that the normative basis of environmental indicators adds to the responsibility of those using these decision support instruments and that it requires from them awareness of the fact that they build their judgements and decisions on normative principles.

2. Personal

A number of contributions have followed the line of expressing their personal accounts and impressions from the work with Professor Dr Jiří Jaromír Klemeš. These contributions have been from

- Prof David Reay from Newcastle University, United Kingdom, founding Editor in Chief of Applied Thermal Engineering
- Prof Sharifah Rafidah Wan Alwi Director of PROSPECT and Prof Zainuddin Abdul Manan, Dean of Chemical Engineering Faculty from Universiti Teknologi Malaysia, Johor Bahru, Malyaisa
- Prof Petr Stehlík from Brno University of Technology, Czech Republic
- Prof Leonid Tovazhnyanskyy, Honorary Rector from National Tech University "Kharkiv Polytechnic Institute"
- Prof Petro Kapustenko CEO of AO Spivdruzhnist-T LLC, Kharkiv, Ukraine
- Prof Alájos Mészáros, Prof Monika Bakošová, Prof Miroslav Fikar from Slovak University of Technology, Bratislava, Slovak Republic
- Prof Vincenzo Dovì from Università di Genova, Italy
- The SDEWES Centre lead by Prof Neven Duić from the University of Zagreb, Croatia
- · AIDIC represented by Prof Sauro Pierucci and Dr Raffaella Damerio, Milan, Italy
- Prof Subhas Sikdar from the US Environmental Protection Agency, Cincinnati, USA
- Prof Eugeny Kenig, Chair Holder from the University of Paderborn, Germany
- Prof Otto Nowak, CEO of Nowak Waste Water Consult, Eisenstadt, Austria; previously TU Dresden, Germany
- Prof Qiuwang Wang, Dr Min Zeng, Dr Jin Yang, Dr Ting Ma from Xi'an Jiaotong University, P.R. China
- Prof Dominic Foo, University of Nottingham, Malaysia Campus
- Dr Petar Varbanov and DDr Andreja Nemet from University of Pannonia, Hungary
- DDr Hon Loong Lam from University of Nottingham, Malaysian Campus

3. Conclusions

The current Editorial Article has introduced the Special Jubilee part celebrating the 70-th anniversary of Professor Dr Jiří Jaromír Klemeš. He has been the driver of many scientific initiatives and as a result he has managed to form an active and vibrant Process Integration community around the PRES series of conferences (PRES, 2015). A number of researchers have united in contributing research and personal tributes to the current Jubilee part of the CET Vol.45 for the occasion.

The scientific part has presented a range of topics very much in line with the PRES conference and reflecting the current needs of the scientific and engineering communities. This includes fifteen articles from distinguished researchers and friends treating problems on heat transfer, Process Integration, sustainability, use of renewables and waste, batch, as well as strategic analyses.

The Guest Editors of this special part of CET Vol.45 Petar Sabev Varbanov, Hon Loong Lam and Andreja Nemet would like to express their sincere gratitude to all friends who have contributed to this celebration effort. It is their firm belief that the well-established collaboration has to be carried on further, uniting researchers and industry for even better serving the industry, society and our planet in the future. In completing this mission the collaboration under the guidance of Professor Dr Jiří Jaromír Klemeš has been and will be an invaluable vehicle for scientific and engineering success.

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1722

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