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Chemical Engineering, As I like it

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Chemical Engineering has changed a lot in the fifty years spanning the time I entered it to now, when I am near my exit. I am sure it is a dynamic profession, and will change even more. In this article, I will focus on what changes I would like to see, and speculate a little on what role ChEs can play in India.

When I started as a student ChemEngg was quantitative, but largely empirical. Design, and scale-up were challenges. Focus was largely on heavy chemicals. One talked about $3H_2 + N_2 \rightleftharpoons 2NH_3$. A decade later, it transformed itself into an engineering science under the influence of transport phenomena, chemical reaction engineering, and tools of systems engineering. Chemical reactions were written as $aA + bB \ldots \rightleftharpoons \ldots yY + zZ$. This powerful transformation however seems to have run its course. On top of it, Biology has caught on the imagination of one and all, and ChemEngg has also come under its spell. Products seem to take over the center stage. However, history does not repeat itself. Now products are not just chemicals, but include biologicals, and devices. They are structured, and aim at meeting a perceived need. Scaling down is now equally important. How should a ChE train himself?

I would like that we view ourselves as problem solvers. Needs arise out of problems, and are fulfilled by products. Products are made through processes. ChemEngg through its umbilical linkage to chemistry, and through it to biology, has the intrinsic prerequisites to train its practitioners to imagine products needed, design them, and engineer processes to make them. We have to see ourselves as engineering physical and chemical changes using principles of chemistry, physics, and biology through our understanding of ceilings placed by ideas of reversibility, and restrictions placed by rates of irreversible processes.

Having said that, I would like to make a few comments about problems ChEs trained in *India* can and should solve. This aspect is becoming more and more central as governments expect engineering graduates to play an important role in the economic development of India. These problems can be classified broadly into two categories. First are those relating to problems arising in rural India. The other are those pertaining to the Indian chemical industry, security of the country, energy, environment *etc*. The former are peculiar to India and, solutions to them are most probably available, so to speak, but are expensive.[1] The latter are related closely to what ChEs do all over the world.[2]

Let us look at the first category of problems, and this was the focus of the Reflux 2017. Lack of economic growth is main problem in rural areas. Apart from that, there are problems in providing energy, drinking water, basic sanitation, and transport at affordable costs. The main approach will have to be about providing decentralized services, and development of value adding products from agricultural/dairy products. Gasification of agricultural residues, small photovoltaic or dye sensitized solar devices for lighting, pumping, and potable water generation, adsorption based devices for purification of drinking water, food preservation and packaging are areas where chemical engineers can contribute. In all these problems, the main hurdle will be reduction in costs, and that is where innovation is needed.[3]

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[1] Thus, one can always use RO membranes to produce potable drinking water, but would be very expensive for many in India.

[2] Thus, problems involved in developing batteries for cars or energy storage or solar panels for harvesting solar energy, or sequestering CO2 are the same everywhere in the world.

[3] I would like to add here latest news about prevention of stubble burning in Punjab, Haryana, and UP. It is being proposed that the stubble be collected and transported so that NTPC can use. Is there an opportunity to offset transport costs by decentralized energy generation by gasification?

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Let us now turn our attention to the second category of problems. The problems once again relate to energy, environment and health care. Here, however, advanced science and technology are available and restrictions posed by costs are less severe. Further, all disciplines focus on the same issues. Hence, the approaches needed are holistic and interdisciplinary in nature. Chemical engineers have to firmly place one of their feet on at least one basic science: physics, chemistry or biology. It is this that is enabling. Their focus has also to change from simple chemicals or mixtures to products with structure, complexity and need based. I give examples of chemical engineers, some of them trained in India, who could successfully use such an approach. These were development of asymmetric membranes for RO applications (Profs Sourirajan and Loeb), solid polymer lithium batteries to make them safer (Prof Nitash Balsara), development of cancer drugs based on reduction of tortuosity in blood vessels (Prof Rakesh Jain), controlled drug delivery and organ development (Prof Langer), structuring carbon nanotubes into nematic liquid phase for easy processing into devices (Prof Pasquali), and rechargeable structure for MnO2 for use in throw away alkaline cells (Prof Sanjoy Banaerjee).

This is an extended summary of the talk I gave in Reflux 2017 held by the Chemical engineering department of IIT Guwahati.

Coalbed methane (CBM) and Underground coal gasification (UCG) potential of India

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Coal plays a vital role in power sectors for the generation of electricity. India is the second largest coal producer in the world. Indian coal contains high ash content (~45%) and thus, its calorific value is low. The use of high ash coal in power plant industries reduces the net thermal efficiency and further, the handling of ash slag from boilers is a major problem. Also, 37% of Indian coal resources are found at a depth greater than 300m. Exploitation of these resources through conventional mining method is uneconomical. In order to fulfil our energy requirement, it is essential to focus the utilization of these unmineable coal reserves using unconventional technologies such as underground coal gasification (UCG) and coalbed methane (CBM). Implementation of these technologies could ensure the sustained production of high calorific value gases.

1. Coalbed methane (CBM):

CBM process involves capturing of methane gas from a coal seam. Methane gas formed during the coalification process get entrapped into the porous matrix of coal seams. And, these gases would release into the atmosphere during coal mining process. As a consequence, fire hazard and global warming would arise as major issues of CBM process. Alternatively, the capture of methane gas from coal beds would provide an energy source for the production of electricity. It may be a clean source of energy as it contains low sulphur content. Methane gas capacity of Indian coal seams is calculated based on the inherent properties of coal using Kim's correlation [1]. Further, CO2 sequestration capacity of a coal seam is calculated based on the volume of methane gas entrapment in coal beds.

Table 1a: CBM and CO_2 sequestration potential of Indian bituminous and sub-bituminous coal

S. No.	State	Total resource, million tonnes	Total CBM gas, billion m^3	CO_2 sequestration potential, million tonnes
1	West Bengal	27394	201	742
2	Jharkhand	71864	526	1938
3	Bihar	160	0.54	2
4	Madhya Pradesh	18660	59	217
5	Chhattisgarh	39545	111	407.5
6	Uttar Pradesh	1062	2.0	7.5
7	Maharashtra	8414	21	76
8	Orissa	60987	131	482
9	Andhra Pradesh	16697	61	224
10	Assam	340	2.4	9
11	Arunachal Pradesh	90	0.5	2
12	Meghalaya	459	1.7	6.5
13	Nagaland	20	0.06	0.23

Table 1a and 1b show the CBM gas and CO2 sequestration potential of Indian coal seams for bituminous and lignite coals, respectively. The state Jharkhand has huge coal reserves and accordingly, it has shown a high CBM capacity. In terms of lignite coal, Tamil Nadu possesses major coal resources with CBM capacity. It is estimated that 57% of total CBM gas of bituminous and sub-bituminous coal is found in deep coal seams at a depth higher than 300 m. In addition, 38.9% of total CBM gas of lignite coal is estimated that are found in between 300-600 m of depth.

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Table 1b: CBM and CO_2 sequestration potential of Indian bituminous and sub-bituminous coal seam[1]

S. No.	State	Total resource, million tonnes	Total CBM gas, billion m^3	CO_2 sequestration potential, million tonnes
1	Pondicherry	416.61	0.205	0.753
2	Tamil Nadu	32892.92	54.735	201.65
3	Rajasthan	4835.29	4.843	17.842
4	Gujarat	2722.05	2.769	10.194
5	Jammu & Kashmir	27.55	0.012	0.044
6	Kerala	9.65	0.004	0.015
7	West Bengal	1.79	0.0013	0.0048

2. Underground coal gasification (UCG):

UCG technology can be implemented in deep coal mines after the extraction of methane gas through CBM technology. After the recovery of the primary methane gas, the residual methane of the seam can be extracted using enhanced coalbed methane (ECBM) technology. The injection of CO_2 gas into the coal seam desorbs the residual methane with the adsorption of CO_2 gas. The adsorbed CO_2 gas in deep coal seams can be act as a gasifying medium during a UCG process. However, pure O_2 gas is required to supply as an oxidizing medium to neutralize the effect of CO_2 for sustaining the combustion front in a UCG seam. Laboratory scale borehole combustion experiments were carried out using CO_2, O_2 and air as the feed gas for high and low ash Indian coals and, the product gas composition and its calorific value are estimated[2].

Table 2: Laboratory scale based UCG product gas composition using CO_2 feed gas[2]

Coal used*	Feed flow rate (lpm)			Feed molar ratio (CO_2/oxidant)	Product gas composition (vol. %)						Average calorific value of product gas (kJ/mol)
	O_2	CO_2	Air		H_2	CO	CH_4	CO_2	C_2H_4	C_2H_6	
LAC	1	0.2	-	0.2	16.5	7.5	21.7	41.0	-	2.2	267.5
LAC	0.1	0.2	0.9	0.2	18.4	9.2	19.5	45.8	-	2.3	260.9
HAC	1.0	0.2	-	0.2	25.7	10.3	12.8	49.8	-	0.1	195.9
HAC	0.5	0.2	0.5	0.2	24.9	9.2	15.5	42.9	-	0.3	214.0

*LAC: low ash Assam coal, HAC: high ash Jharia coal

Table 2 shows the laboratory scale experiments based product gas composition using high and low ash Indian coals. Indian coal having 40% of ash content (HAC) has shown the production of syngas with 200 kJ/mol calorific value using CO2 with O2/air as the feed gas. A low ash Assam coal (~5% ash) generates a product gas with the calorific value as high as 265 kJ/mol. Hence, real UCG runs are needed to conduct in high ash Indian coal seams for examining the feasibility of the technology.

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Economics driven controlled variables selection – Self optimizing control in plantwide control

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Efficient process operation improves the operating margins, to be more competitive, and therefore profitability. The automation system designers assume that process outputs (controlled variables) are known during automation or controller design. But the control engineering practitioners face control structure design issue .The control structure design deals with the selection of controlled variables (CV/outputs) and manipulated variables (MV/inputs), and the pairings or interconnections between these variables. The number of alternative control structures are combinatorial in nature and there are combinations, where represent number of measurements and manipulated variables respectively. The control structure selection is a strategic decision, which gives the controlled variables for the plant.

The business objectives can be energy efficiency, environmental impact or sustainability of process plant. Let us denote the cost function representing the plant business objectives by J. Then for a range of disturbances $d_1, d_2, \cdots d_p$ the optimal cost with a chosen control structure are denoted by $J_{opt}(c^k, d_1), J_{opt}(c^k, d_1), \cdots, J_{opt}(c^k, d_p)$..Upon plotting the cost with disturbances for each control structure, the best control structure will be the flattest of all alternatives. Using this best control structure and keeping those control variables at constant set points guarantees operation to stay close to optimal operation. This best control structure is termed as self-optimizing control. To facilitate evaluation of alternative sets for CV_1, the controlled variables are linked to process measurements as $CV_1 = c = Hy$. Here H is selection matrix. Each control structure maps to a specific matrix. In addition to accounting for all ${n_y}C_{n_u}$ control structures, this representation can also be used to find controlled variables as combination of measurements subsets.

The controlled variables selection problem described above fits in the supervisory control layer of plantwide control system for a plant as shown in Figure 1a. The plant optimal operation can be viewed to constitute the control layer (supervisory layer plus regulatory layer) and optimization layer in the hierarchical decomposition of plantwide control. The task of control layer is to keep controlled variables at given set points and the task of optimization layer is to provide optimal set points. For simple implementation, we want to update the set points less frequently while obtaining an acceptable loss in the presence of disturbances. This approach is termed as “self-optimizing control” and this will automatically lead the operation close to optimal operation. To implement “self-optimizing control” policy the two major constituents are (1) appropriate controlled variables selection and (2) keeping them at constant set points. Physically, in self-optimizing control, the selected controlled variables will have optimal values are insensitive to disturbances and controlling these (at constant set point) would need fewer set point updates. The controlled variables in “self-optimizing control” link the optimization layer and the control layer. The interaction of controlled variables selection and the local optimization layer is depicted in Figure 1b. When a disturbance (d) affects the process, the controller K tries to keep the controlled variables c at their set points c^s using local feedback loop and above layer changes optimal set points c^s for the control layer.

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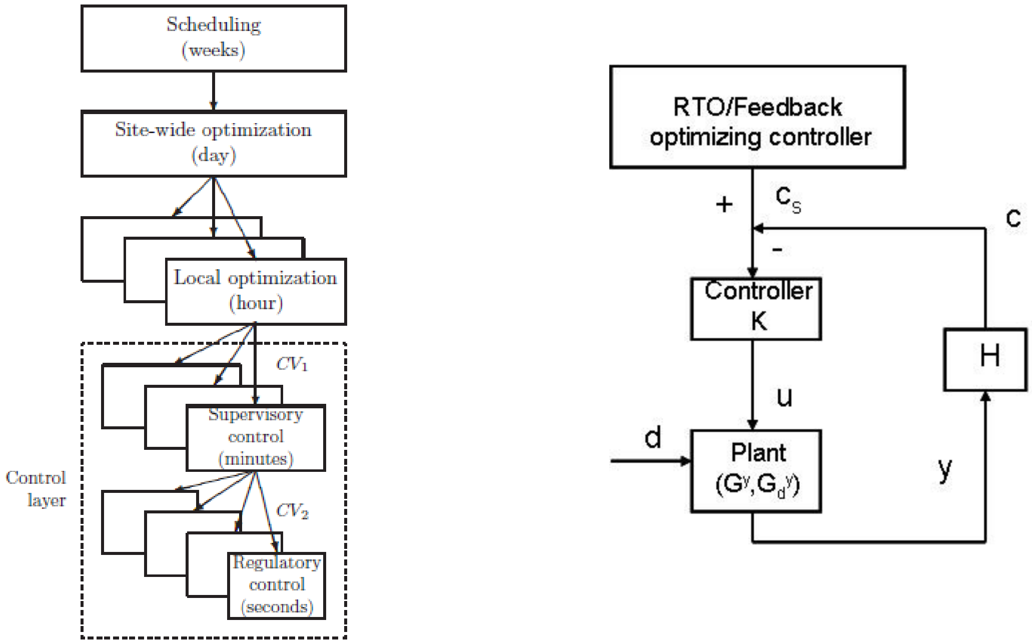

Figure 1. (a) Control system hierarchy for plantwide control in chemical plants (Findeisen et al., 1980, Skogestad and Postlewaite, 1996), (b) Feedback implementation of optimal operation with separate layers for optimization and control (Kassidas et al., 2000). K could be any controller including MPC. Self-optimizing control addresses selection of the controlled variables $c = Hy$

Every plant can be categorized as either constrained systems or unconstrained systems. Self-optimizing control is for unconstrained systems. For these systems, there is no systematic framework on how to utilize these unconstrained degrees of freedom (DOF) to meet the economic objectives. Self-optimizing control provides framework to find CV_1 that minimize the steady state loss in the economic objectives for these unconstrained DOF. For the fully or partially unconstrained systems the optimization problem in reduced space is

$$\min_u J(u, d) \tag{1}$$

where u is the unconstrained DOF. To keep the operation at optimum, the optimization problem (1) is solved for $u = u_{opt}(d)$ for any disturbance d and the resulting optimal cost is $J_{opt}\big(u_{opt}(d), d\big)$. The cost function J as a function of input u and disturbance d is shown in Figure 2. The optimal inputs for disturbances d^*(solid), and d (dotted) are $u_{opt}(d^*)$ and $u_{opt}(d)$ respectively, i.e optimal u varies for each disturbance. The loss by keeping the input u constant at $u = u_{opt}(d^*)$ when there is a disturbance d is also illustrated in Figure 3. Hence, for any disturbance d, u then we will incur loss from optimal operation as shown in Figure 2. The associated loss can be quantified as (Skogestad and Postlethwaite, 1996).

$$L = J(u, d) - J_{opt}(u_{opt}(d), d) \tag{2}$$

In self-optimizing control framework, input u is manipulated to keep Hy_m at constant set point c_s using a feedback diagram as in Figure 3 and the associated loss is defined as

$$L_c = J\left(\underbrace{u}_{to\ keep\ Hy_m at\ c_s}, d\right) - J_{opt}\big(u_{opt}(d), d\big) \tag{3}$$

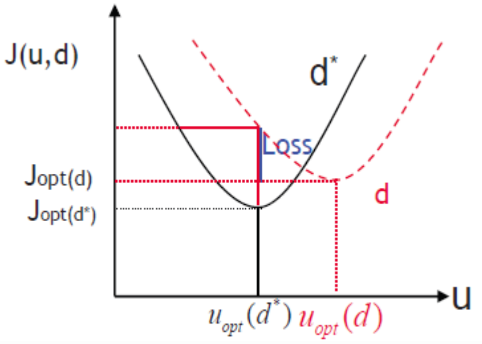

Figure 2. Cost function as a function of disturbances d^* and d and inputs u; Illustration of loss by keeping input u constant at $u = u_{opt}(d^*)$ when there is a disturbance d.

Mathematically, the optimal H that minimizes the average steady state loss from optimum may be obtained using minimum loss method by solving the following steady-state optimization problem (Halvorsen et al., 2003 Yelchuru., 2012).

$$\min_{H} \left\| J_{uu}^{1/2}(HG^{y})^{-1}HY \right\|$$

where $Y = [FW_d \; W_{n^y}], F = \frac{dy_{opt}}{dd}$ is the optimal sensitivity matrix with respect to disturbances, W_d and W_{n^y} are diagonal matrices with elements equal to the expected magnitude of disturbances and measurement noises(errors), G^y, G_d^y is the measurement gain matrices with respect to u , d and J_{uu} is the Hessian of the cost function J with respect to the unconstrained DOF u and $\|M\|_F = \sqrt{\sum_{i,j} M_{ij}^2}$ denotes Frobenius norm of matrix M. This framework allows formulation of four interesting problems in an increasing order of self-optimizing properties. They are (i) find CV_1 as individual measurements, (ii) find CV_1 as combinations of measurements subset of y, (iii) find CV_1 as combinations of all measurements, (iv) find CV_1 as combinations of measurements subset of y with a user specified structure in H. The specified structure in H is to avoid delays and for dynamic reasons between the CV_1 and u when combining measurements from different sections of the process plant.

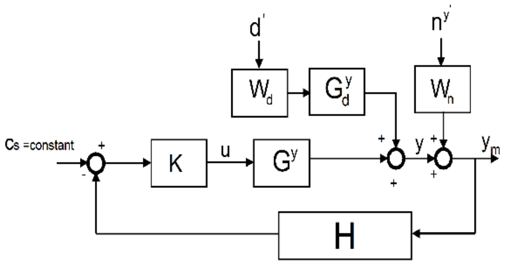

Figure 3: Feedback diagram

Conclusion

The control practitioners' challenges in deciding the controlled variables are highlighted. A mathematical framework to evaluate control structure alternatives is discussed. The interesting problems in self-optimizing control framework in plantwide control are listed.

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Integration of Planning, Scheduling &Control: Answering the 5 'W'

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Why it is needed?

Chemical supply chains are complex interconnected systems and a systematic review of the operational procedure offers significant opportunities to reduce costs. According to, Shobrys & White (2000), any sustainable manufacturing supply chain depends on the way the production management system counters the following questions: 1) what are the raw materials? 2) When to buy it? 3) How much time needed to make the product? 4) What equipment to run? 5) What are the products? 6) How to ensure the quality of the products? An informed and optimized answer to these questions, even for a medium scale chemical process, can increase profit as much as 10$ per ton of the products, if not more[2]. Before getting into more details, let us look into the different sections of production management system, which depicted in Figure 1.

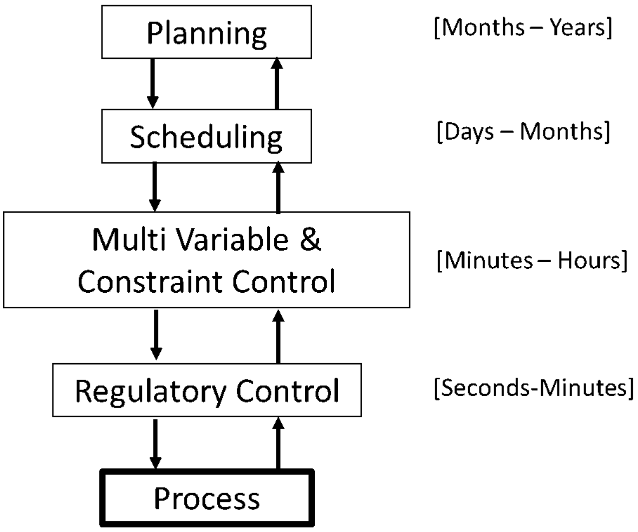

Figure 1: The automation hierarchy, adapted from Seborg et al. (2010)[3].

The top layer of the production management system deals with the strategic & tactical planning of the whole process and maintains coordination amongst the entire supply chain over a long horizon of time, ranging from months to years. The subsequent scheduling layer assignees specific activities to each resources over a time scale of days to weeks. The lower layers or the control layers help the process to achieve the targets set by the upper layers, and the decision making time in these layers ranges from seconds to minutes.

Traditionally decision support tools for these tasks have been operated separately using local optimization models and the need for sharing information between these layers has been so far ignored[2]. However, to exercise the automation in its entirety, information exchange between this layers are crucial and integrating these layers will help to facilitate transparent information exchange, which eventually helps in reaching overall goal.

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The need for information sharing between these layers can be understood by evaluating the following scenario. The solution of scheduling problem consists of optimal production time, sequence, allocation of resources, however, they do not provide any idea about the dynamic behaviour of the plant. Whereas, strict control policies to meet required product specifications may disrupt the whole schedule. So, it is evident that to execute automation in its entirety the integration between these layers are very important.

According to Shobrys & White (2000), *"Companies aggressively pursuing integration report substantial financial incentives for better integration. Exxon Chemicals estimated that a major integration initiative reduced annual operating costs by 2%, and operating inventory by 20%. Du Pont aggressively pursues the improvement and integration of these functions. An indication of the resulting financial impact is that a single polymers business reduced working capital tied up in inventory from $160 million to $95 million."*

Scheduling and plant wide control both seek to achieve the optimal operating conditions and it is reasonable to expect that an integration or merger of them will help in achieving more economically viable process. With integrated modelling, information can be exchanged between these layers without delay, ensuring more economical operation[4]. There are several variables which actually connect control and scheduling layer, such as, the state variables at the start and end of the transient periods, duration of the periods, and amount of material processed in units etc. The integration of scheduling and control results in better modelling since, transitions are accounted for, which are not incorporated in traditional approaches.

When the idea came?

Though the first mention of integration of scheduling and control dates back to 1970-1980s, [5,6] however, the following technical issues have hindered the advancement in this process,

- The necessary analytical abilities were weak and underdeveloped.
- Computer hardware was of limited capacity and expensive.
- Data storing and management capabilities were inadequate.
- Connectivity between applications were hard to achieve and user interface was also poor.

However, the wave of new innovations in information technology sector in recent years has really helped in overcoming these barriers, so the prospects of integration is now becoming more and more realizable and lucrative to researchers of academic as well as industrial communities. The first proper documentation citing the prospect as well as the key issues with integration can be found in Shobrys & White (2000)[2]. After 2000, there are several attempts that have been reported in literature, on implementation of integration between planning, scheduling & control layer for both continuous processes[4,7-10] as well as batch processes[11,12]. In 2009, Harjunkoski et al. wrote a seminal review paper enlisting all the important achievements in this area till then[1]. Baldea and Harjunkoski (2014) also present a review paper on integration of scheduling and control giving more preference to the integration approaches used in continuous processes over the years[13]. These review papers enlist all significant contributions in this fields and identify the most favourable solution approaches.

Where to improve?

The major complexities that arise when formulating an integrated problem is the difference between the time scales amongst the layers. While the control layer operates in the range of seconds to minutes, the horizon in the scheduling layer can extend up to months. Another major setback comes from the solution perspective. The planning or scheduling aspects of a process are largely formulated as mixed integer linear programming problem, whereas, the process dynamics that needs to be captured to design and evaluate the controller performances lead to dynamic optimization problems. Approaches that combine the planning or scheduling aspects with control layers essentially formulate a mixed integer dynamic optimization (MIDO) problems, which are very difficult to solve. The major solution approaches that have been reported over the years are of three types: 1) Converting MIDO to large MINLP problems[7, 8, 12], 2) decomposition into scheduling & control subproblems[14], 3) Heuristics, such as, agent based or logic based methods[9,15]. However, more efficient formulation & solution approaches are needed to properly apply integration in real-life complex processes.

Who holds the key?

Traditionally, the control problems are investigated by the researchers of chemical engineering (process system engineering) community, while planning/scheduling comes under the operation research domain. People from completely different domain have sought to optimize each of these problems locally, which upon implementation may lead to suboptimal results. However, integration amongst these layers demands collaboration between these two separate research tracks that have not been well – or hardly at all – coordinated but might offer a good potential. Grossmann (2005) introduces the concept of enterprise wide optimization from a process system engineering point of view which essentially hails the idea of integration between the layers of automation hierarchy[16]. According to Grossmann (2005*): "…in enterprise wide optimization, the emphasis is on the manufacturing facilities with a major focus being their planning, scheduling and control which often requires the use of nonlinear process models, and, hence, knowledge of chemical engineering."*

What is the future?

According to Harjunkoski et al. (2009)[1] *"The field of integrating scheduling and control is a very challenging research area, as it needs to combine several problem aspects, dimensions and research disciplines. Thus, an active research collaboration between industry and academia also plays a key role for the success of this topic".*

Though there are several research works that are going on simultaneously all over the world, there are still lots of opportunities that are unexplored. Harjunkoski et al. (2009)[1] concluded their seminal review paper as: *"Even though some formal steps have successfully been taken and a number of methods already exist, there are many theoretical questions as well as practical issues to be solved for the future. This research is still at its early phase".*

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Journey from Chemical and Materials Engineering to Nanotechnology: Motivation and Experience

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Have you ever thought why taste of cooked food depends on its ingredients, why nail polish doesn't dissolve in water, and the cause behind the first rain drop after a harsh summer? If you have, pursuing a research in Chemical Engineering and Materials Science can be good for you as it has been awesome for me. I have always been passionate in doing things which I like, be it dancing or be it analysing interesting things. It is this passion to know the unknown, the creative personality within and the strong liking for teaching, which drove me towards pursuing research.

My M. Tech. research work under Professor G. Pugazhenthi involved utilizing carbon and layered double hydroxide nanoparticles as fillers to reinforce pliable polymers like polystyrene by preparation of a composite using solvent blending method. Nanoparticles are good as a filler essentially due to their greater surface area and higher degree of reinforcement at low quantities. In Situ Polymerization, Anionic polymerization and ATRP (Atom transfer radical polymerization) requires high temperature, initiator, and terminator whereas melt mixing gives good yield, but difficult to overcome viscous forces and process parameters make it complex. As opposed to the latter methods, solvent blending is a simpler, easy to control process which when assisted by ultrasonication gives a stable nanotube dispersion. cMWCNT(Carboxylic acid functionalized multiwalled carbon nanotubes) was used as a nanofiller due to their high tensile strength, temperature tolerance and electrical conductivity.

The first challenge faced was prevention of nanofiller agglomeration by overcoming strong electrostatic and interlayer van der Waals forces followed by selection of a proper dispersant to stabilize the dispersed particles. Proper dispersion was ensured by magnetic stirring and sonication followed by characterization of its morphology by Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy and X-Ray diffraction (XRD).

To improve the interfacial interaction between nanofiller and polymer, functionalized fillers were employed which also preserves their intrinsically high tensile strength, elasticity, thermal and electrical conductivity. The improvement in thermal stability based on the weight percentage of nanofiller incorporated was investigated by Thermogravimetric analysis assisted by Coats Redfern and Criado method to witness the thermal degradation kinetics and mechanism for inferring about the range of temperature tolerance and reason of reinforcement.

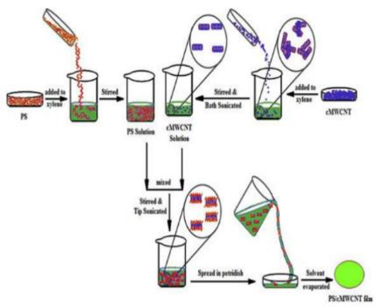

Figure. 1. Schematic of solvent blending method for nanocomposite preparation (Journal of Science: Advanced Materials and Devices, 2016: 1(3), 311-323)

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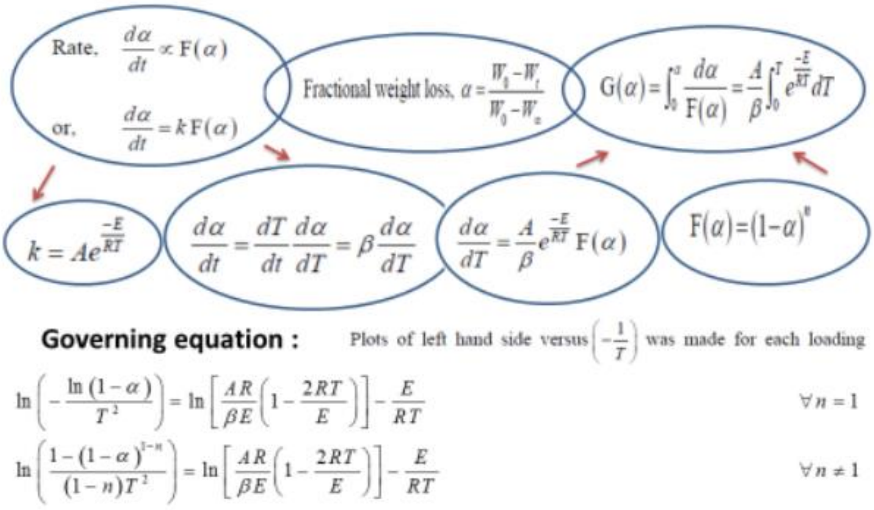

Figure 2: Schematic of Coats Redfern method for thermal degradation kinetic

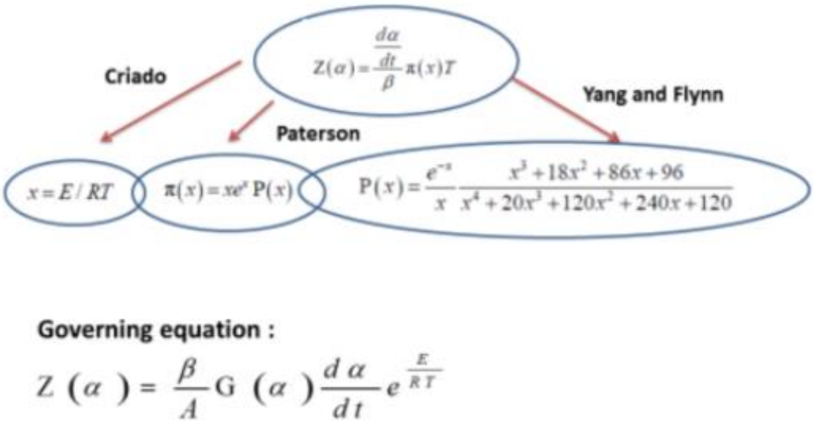

Figure 3: Schematic of Criado method for thermal degradation mechanism

Melt rheological investigation was also conducted to witness the microstructural reinforcement proportional to filler concentration.

The aim was to achieve significant property improvement by maximizing dispersion and incorporation at low filler content to control the cost of production too. The precision and challenge was mainly centred on optimization and maintenance of reproducibility of the fabrication parameters, processing times and characterization techniques. The focus of this work was synthesis of a nanocomposite with a thermo-mechanical strength and application scope which cannot be achieved by the polymer matrix acting alone

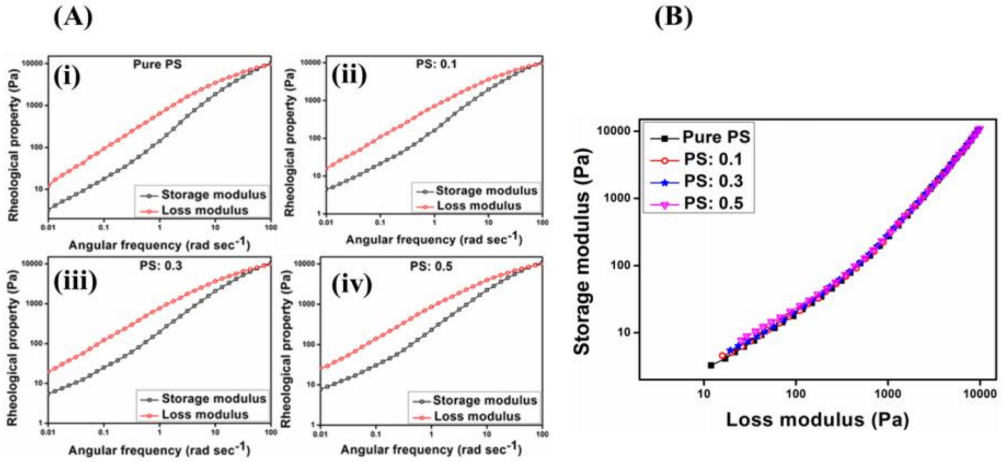

Figure. 4: (A) Shift in crossover of Storage and loss moduli curves to lower frequency with greater filler loading indicates greater rheological reinforcement, (B) Cole-Cole plot signifying microstructural homogeneity before and after filler addition [,Pure PS: Pristine polystyrene, PS: 0.1 – Polystyrene with 0.1 wt. % COOH-MWCNT, PS: 0.3 – Polystyrene with 0.3 wt. % COOH-MWCNT, PS: 0.5 – Polystyrene with 0.5 wt. % COOH-MWCNT]

The most critical part was testing electrical conductivity of the nanocomposites. Making the nanotubes perfectly dispersed and connected to give a good conductivity at small nanotube content was vital. I immensely thank my guide for believing in me, providing valuable suggestions at each step of the research and helping me throughout the course.

The search and re-search for solutions to achieve desired Fabrication and Characterization results inspired me to extend my current interest to Nanopore sequencing in University of Alberta, Canada. Fabrications and measurement at nanoscale, implementing all microscopic, lithographic, etching and thermo-mechanical and morphological characterization techniques for best results has been the prime focus of my PhD research, which improved my knowledge on Nanotechnology, Polymer Science and Bio-nanotechnology, the foundation of which was laid at IIT G during my M. Tech. tenure.

Non-Dimensional Numbers in Fluid Mechanics

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Dimensionless numbers often compare different scales in a problem and give important information about the dominant forces or physical effects for a particular system. An important application of non-dimensional numbers is in similitude, a concept often used in the scaling up of the prototype to the real model. The dynamic similarity requires the ratio of all the forces acting on the prototype and the real model to be same. The ratio of the different forces are given in terms of different dimensionless number. Dimensionless numbers relevant for a particular problem can be identified using Buckingham Pi theorem or by non-dimensionalisation of the equations governing the phenomena.

In this article, the non-dimensional numbers frequently used in different fields of fluid mechanics have been discussed.

1. **Knudsen number (*Kn*):** Knudsen number is the ratio of two length scales: mean free path (λ) of molecules in a fluid to the length scale of the problem (L). A Knudsen number sufficiently smaller than one suggests that the mean free path of molecules is very small when compared with the system dimension and the system under consideration can be described using continuum assumption. Continuum assumption suggests that there are sufficiently large number of molecules present in the system to consider the material properties, velocities and stresses as smoothly varying functions of position.

2. Reynolds Number (*Re*): Reynolds number is the ratio of inertial and viscous stresses. Inertial stress is the force per unit area required to bring a change in the momentum of a fluid. For a fluid element having characteristic length L, velocity U and density ρ, the force required to bring the fluid element to a stationary state (or for that matter to double the velocity to $2U$) is equal to the rate of change of momentum i.e. $[\rho UL^3/(L/U)]$. The inertial stress therefore is ρU^2. From Newton's law of viscosity, the viscous stress can be written as $\mu(U/L)$ for a Newtonian fluid. The ratio of the inertial stress to viscous stress is therefore $\frac{\rho UL}{\mu}$. Reynolds number can also be represented as the ratio of the viscous $(L^2/(\mu/\rho))$ and convective (L/U) time scales.

3. Drag Coefficient (C_D): The non-dimensional drag force on an object or particle is often given as drag coefficient. It is defined as the ratio of drag force per unit projected area of the particle to the dynamic pressure ($\rho U^2/2$). Note that the drag coefficient includes both forms of drag: skin friction caused by viscous forces and form or pressure drag.

4. Friction Factor (*f*): Friction factor is the ratio of local shear stress (τ) and local kinetic energy per unit volume of the fluid flowing in a channel. There are two different friction factor definitions commonly used in fluid mechanics: Darcy friction factor and Fanning friction factor. Fanning friction factor is defined as $\tau/\frac{1}{2}\rho U^2$ whereas Darcy friction factor is four times the Fanning friction factor. For laminar flow in a channel of circular cross section, the Fanning friction factor is $16/Re$.

5. Stokes Number (*St*): Stokes number characterises the behaviour of a particle suspended in the flow. It is the ratio of the relaxation time of the particle (t_{relax}) to the characteristic time of the flow (L/U). The relaxation time of a particle is the time constant in the exponential decay of the particle velocity due to drag. If the Stokes number for a particle is low, the particle follows the fluid streamline.

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6. Strouhal Number (*Sr*): The Strouhal number is defined to characterise the oscillatory unsteady flow. In terms of time scales, it is the ratio of the flow time scale to the oscillation time scale i.e. $(L/U)/(1/f)$, where f is the frequency of the oscillatory phenomena.

7. Womersley Number (α^2): Womersley number is often used in cardiovascular fluid mechanics to compare the pulsatile flow time scale (or frequency) with the viscous time scale. It is defined as $\alpha^2 = \frac{\rho(\omega L)L}{\mu}$. It can also be thought of as an oscillatory Reynolds number and is the ratio of transient or oscillatory inertial stress to viscous stress. It can be rearranged as the ratio of channel radius to the oscillatory boundary layer thickness.

8. Froude Number (*Fr*): Froude number is the ratio of inertial stress to that generated due to an external field. In many circumstances, the external field is gravity and therefore a common definition of Froude number is $(\rho U^2/\rho g L)$. Sometimes, it is also defined as $Fr = U/\sqrt{gL}$ i.e. the ratio of the flow velocity to that induced by the gravitational field. In flows involving free surface, a surface subjected to zero shear stress, the flow becomes unstable above $Fr > 1$.

9. Bond Number (*Bo*): Bond number is the ratio of the stresses caused by the buoyancy and surface tension $Bo = \Delta\rho g L/\left(\frac{\sigma}{L}\right)$. It is also known as Eötvös number. It determines the relative importance of surface tension and gravity in two-phase flow. As the Bond number is proportional to square of length scale, gravity is dominated by surface tension in small size channels.

10. Capillary Number (*Ca*): Capillary number is the ratio of viscous stress to the stress caused by surface (or interfacial) tension between a gas and a liquid (or two immiscible liquids) i.e. $Ca = \frac{\mu\frac{U}{L}}{\frac{\sigma}{L}}$.

11. Weber Number (*We*): Weber number is the ratio of inertial stress to that caused by surface tension and is given by $We = \frac{\rho U^2}{\sigma/L}$. It can also be rearranged as the product of Capillary and Reynolds numbers.

12. Morton Number (*Mo*): Unlike many other non-dimensional numbers described above, Morton number is not the ratio of any two physical effects but is a combination of fluid properties and gravity. It is defined as $Mo = \frac{g\mu^4\Delta\rho}{\rho_c^2\sigma^3}$. It is used to describe the bubbles and drops rising or freely falling in an infinite fluid.

13. Deborah Number (*De*): Deborah number characterises the fluid-like behaviour of a material. It is the ratio of the relaxation time to the characteristic time of the process under consideration. At lower Deborah number, the material behaves more like a fluid whereas higher Deborah number indicates that the material behaviour is more solid like and is dominated by elasticity. It can be thought of as a non-dimensional measure of the rate of change of flow conditions. The name 'Deborah' is inspired by a verse in the Bible, stating "The Mountains flowed before the Lord" in a song by the prophet Deborah.

14. Weissenberg number (*Wi*): It is the ratio of a characteristic relaxation time of fluid to a characteristic time measure of shear rate (*L*/*U*). It compares viscous and elastic stresses and indicates the degree of anisotropy or orientation generated by the deformation.

On the optimization of integrated biorefineries

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The uncertainty in availability of fossil fuels as well as an increasing awareness of their adverse effects on the environment has led to a steady increase in the interest shown towards the production of fuel and utilities through renewable sources. One such abundantly available renewable resource is biomass, which is organic waste generated from human or natural processes. Biomass can be processed to produce a large variety of useful products, including fuel.

A processing plant which converts biomass into valuable products is termed as a biorefinery, and a biorefinery which combines several conversion technologies in order to process a variety of biomass feedstocks is termed as an integrated biorefinery. Apart from the direct combustion of biomass in order to produce heat and electricity, it may be processed to produce fuel such as syngas (mixture of hydrogen, carbon monoxide and carbon dioxide), ethanol and biodiesel (mixture of mono-alkyl esters of long-chain fatty acids). In addition, biomass may be processed to produce value added chemicals such as furfural and levulinic acid which are important raw materials for various chemical industries. The general schematic of a biorefinery is shown in Figure 1[1].

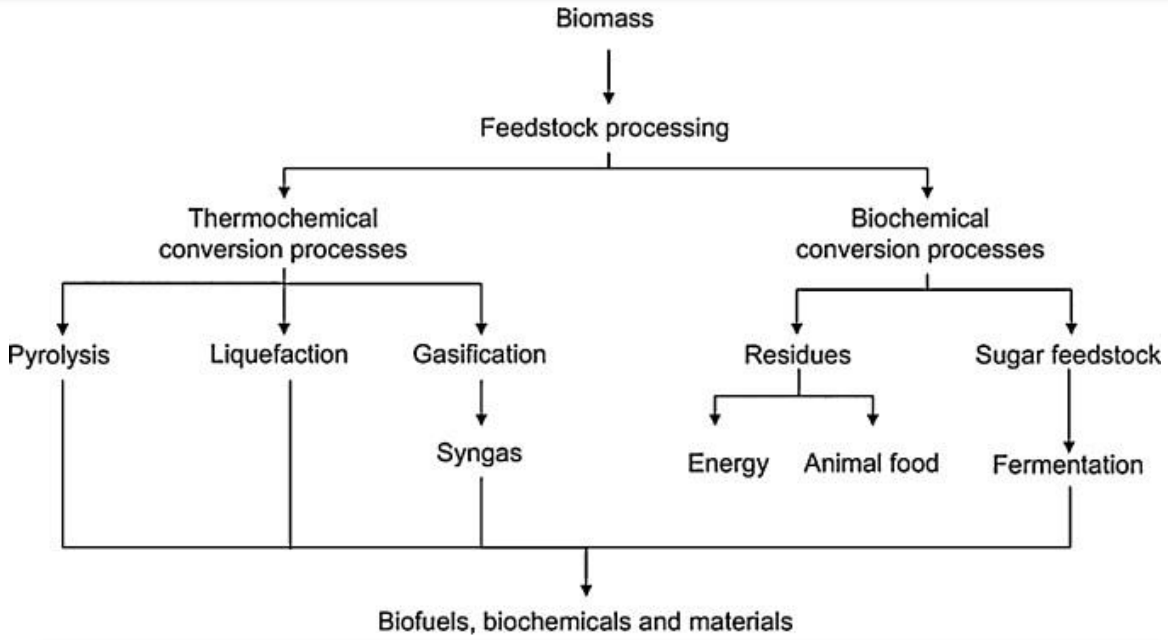

Figure. 1. Schematic of a biorefinery

There are numerous factors, which need to be taken into consideration while designing a biorefinery system. The transportation of biomass over vary large distances is not viable in most cases; hence it is generally preferable to locally source the biomass. For instance, in the Indian context, the biomass is generally some form of agricultural residue. To meet the product demands, it may be required to procure the biomass from various farms, thus leading to a highly distributed logistical network. In such cases, it may be profitable to have several regional biomass pre-processing depots (RBPD) at various locations. Additionally, agricultural residues are subject to seasonal variation and prone to disruptions due to external factors.

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The conversion technologies utilized by the biorefinery should be selected to account for such fluctuations in the composition and availability of biomass. The product demand may be met by designing a single large capacity biorefinery, or a network of distributed biorefineries of smaller scale based on the economics of the problem. Lastly, designers may consider multiple objectives at the optimization stage to account for the economic, environmental and social impacts of such an undertaking. The general schematic of the supply chain for a biorefinery system is shown in Figure 2 [2], where the location of the collection facilities or RBPDs and biorefineries are to be selected by the designer.uncertainty in availability of fossil fuels as well as an increasing awareness of their adverse effects on the environment has lead to a steady increase in the interest shown towards the production of fuel and utilities through renewable sources. One such abundantly available renewable resource is biomass, which is organic waste generated from human or natural processes. Biomass can be processed to produce a large variety of useful products, including fuel.

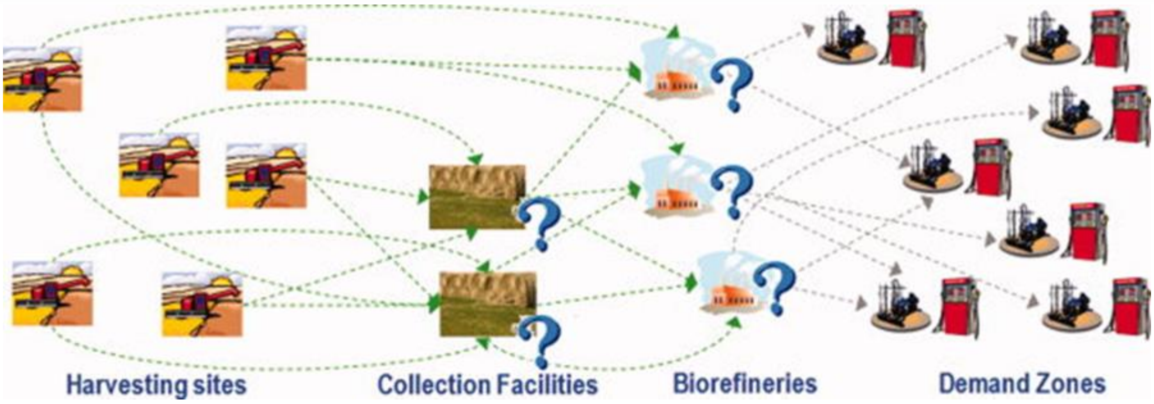

Figure. 2. Schematic of the supply chain system^2

There are a large variety of processing steps described in literature for the conversion of biomass to useful products. Triglyceride based feedstock (such as oil seeds) can undergo processes such as transesterification, hydrolysis, pyrolysis/cracking or steam/dry reforming to produce biodiesel, glycerol, syngas and a variety of fatty acids which may be utilized to produce value added products. The oil cake from the extraction stage is rich in lignin and may be processed for the production of fertilizers, hydrogen and methane. Lignin based biomass (such as the oil cake and agricultural wastes) generally undergoes pretreatment and hydrolysis to obtain lignin and pentose and hexose sugars. They can subsequently be converted a variety of products such as ethanol, hydrogen, furfural and levulinic acid to name a few. Lignin based biomass can be processed via an alternate thermochemical route as well, which can result in the production of hydrogen, various alcohols or FT-oil. Sugar and starch based feedstock (such as potato or sugarcane) generally undergo hydrolysis to produce hexose sugars, which can then be utilized to produce products such as ethanol, butanol, acetone and a variety of other organic acids such as lactic, succinic and levulinic acid. Thus, we see that an optimal configuration for a biorefinery is significantly dependant on the type of biomass which is available for processing and the set of chemicals which the biorefinery is to produce. The complete biorefinery design problem can be broadly divided into two parts: the supply chain and process synthesis problems. The supply chain problem deals with the logistics involved in procurement, transportation and storage of raw materials as well as intermediates. In addition, it considers the distribution of the products to their respective markets. The process synthesis problem involves the selection of the optimal technological pathway within the biorefinery to produce the desired products and the flow of material between various equipments.

Ideally, these two sub-problems should be solved in an integrated manner in order to obtain a comprehensive and accurate model of the overall system. The drawback of such an approach is that the problem size (in terms of number of constraints and variables) can scale up very fast. The inherent integrality of certain decision variables (such as the selection of biomass, selection of products, selection of RBPD locations, etc.) results in the problem being formulated as an MILP/MINLP problem, which falls in the NP-hard class in terms of complexity. This implies that the computational time required to solve such problems can increase exponentially with increase in problem size.

Many works in literature consider specific cases and simplifications of the complete biorefinery problem in order to have a manageably sized model. Another approach is to solve the supply chain and process synthesis problems separately. This approach accommodates detailed problem models, but the resultant solution may be sub-optimal for the complete problem as the interactions between the two sub-problems can be lost. Thus, the optimization of integrated biorefineries is an active field of research, with attempts being made to develop simpler and accurate problem models while improving the problem solution methodology.

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Safe handling of Volatile Liquid Petroleum Products

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There is a trend these days to minimize the quantity of sulfur in the distilled petroleum products such as petrol, kerosene and diesel in order to mitigate the environmental problem associated with the oxides of sulfur. However, with the decrease in the sulfur content, the electrical conductivity of the liquid hydrocarbon decreases and could accentuate the problems of accidental fire and explosions during the handling. The causes of such accidental ignition during the handling of the volatile distilled liquid petroleum products and remedial methods to be adopted to prevent such fires and explosions are dealt with in this article.

Electrical charges can accumulate in insulating media irrespective of whether they are in liquid, solid or gaseous phase. Under normal circumstances, the insulating medium is always neutral – neither positively nor negatively charged with the relatively heavier protons in it getting balanced by the lighter electrons. But any act of rubbing with some other medium, be it a conductor or an insulator, leads to a migration of the electrons across the interface. This could readily take place during flow of the volatile liquid petroleum in pipelines or through filters or injectors and flow control devices. When the insulating substance loses some electrons, which are very mobile, from the rubbing at its surface, it becomes positively charged while if it acquires the mobile electrons it gets negatively charged.

Charge can also be acquired or lost inductively when the medium is in an electric field. The field attracts the protons in the direction of the field making the distribution of the electrons and protons in the medium to be non-uniform. If in the presence of the electric field, the medium breaks up into smaller volumes either through crushing, flow diversion or otherwise, the portion having excess protons becomes positively charged while those having more electrons are negatively charged.

The charged medium on coming into contact with ungrounded conductors or insulators transfers the charge to them and accumulation of charge takes place. When the charge density exceeds a critical threshold, electrical discharge takes place from the ungrounded conductors or insulators to grounded objects or otherwise in its vicinity. The discharge could be in the form of a spark discharge as between two metallic objects, a distributed brush discharge between a grounded conductor and a charged insulator, a lightning-like discharge or a corona discharge due to ionization of air surrounding an electrically charged conductor. The energy release from the discharge could ignite the flammable vapor–air mixture, formed from the mixing of the vapor of the volatile petroleum fuel with air. The ignition could lead to a fire or an explosion. The lower flammability limit of most of the hydrocarbon vapors with air is very low of the order of about 2% by volume of the vapor. It is therefore essential to ensure that accumulation of electrical charges do not occur during the handling of the low volatile petroleum products.

The ability of a medium to hold electrical charge is called electrical permittivity. It is defined by the constant ‘ε’ in the Coulombs law which states that the force ‘F’ in Newton between two charges of ‘q_1’ and ‘q_2’ Coulombs separated by a distance ‘*r*’ meters is given by $\frac{1}{4\barwedge\varepsilon}\frac{q_1 q_2}{r^2}$. The permittivity of free space denoted by ‘ε_0’ is 8.852×10^{-12} Farads/m. For media other than free space, the permittivity $\varepsilon = \varepsilon_r \times \varepsilon_0$,

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where ε_r is the relative permittivity or dielectric constant for the given medium. It does not vary significantly and is 189 for the paraffinic hexane, 2.3 and 2.38 for the aromatic benzene and toluene, is about 3 for rubber and 80 for water.

The drift velocity of a charge ‘v’ in a medium is proportional to the electric field ‘E’ to which it is subjected and is given by $v = \mu E$, where the parameter ‘μ’ is known as mobility. It varies with temperature, pressure and nature of the medium. The drift velocity ‘v’ is related to the current density ‘j’ and charge density ‘ρ’ by $j = \rho v$. Substituting the value of drift velocity ‘v’ gives $j = \rho\mu E$ and the product ρμ is denoted by ‘σ’, which has units of $\frac{1}{ohm-m}$ and is the specific electrical conductivity. The value for water is 5.5×10^{-4} while for hexane and toluene the values are about 10^{-16} and 10^{-12} $\frac{1}{ohm-m}$ respectively. The higher value of water explains why the charges generated in water get dispersed away.

The ability of a medium to hold the charge is given by the permittivity ‘ε’ while the ability to diffuse the charge away is given by it specific electrical conductivity ‘σ’. The rate of generation of the charge must not exceed the rate of dissipation to prevent accumulation of the charge. If the permittivity of the medium is significantly larger compared to the specific electrical conductivity, it can hold on to the charge. A typical time constant ‘τ’ for the charge to get dissipated away in a medium is the relaxation time and is the ratio of the permittivity to the specific electric conductivity$(\tau = \frac{\varepsilon}{\sigma})$. The values of relaxation times for hexane and toluene are very large about $1.67\times10^{+5}$ and 21.07 seconds respectively, while for water it is small at 12.9×10^{-7} seconds.

Substances having long relaxation times can retain charges for long and have adequate time to transfer them to neighbouring ungrounded surfaces with which they come in contact. The residence time of the flow, if greater than the relaxation time will not allow the carry over of the charge and eliminates charge build up in the ungrounded elements. A slower volume flow rate of transfer of the petroleum products is therefore necessary and the American Petroleum Institute recommends the rate of filling for road tankers and rail cars to be below a threshold value. Similarly there must be an upper limit for the filling rate of aviation kerosene in airplanes and rocket grade kerosene in rockets. The problem will become more crucial as the specific electrical conductivity of the volatile petroleum products used in different propulsion systems employing volatile petroleum products decrease due to further removal of sulfur.

Reduction of the relaxation times is achieved in practice by enhancing the specific electrical conductivity by adding additives such as ionizing liquids or electrical conducting materials. In the case of aircrafts, static dissipaters such as STADIS are added to decrease the relaxation times. The kerosene fuel used is termed as jet-mixed products and several nomenclatures of the kerosene fuel such as Jet A, Jet A1, JP etc., are used. In the case of rockets, rocket grade kerosene is referred to a rocket propellant (RP).

Bonding and grounding reduce the voltage and help to alleviate the electrostatic discharge problem. In the bonding process, two or more conductive objects are connected together with conductors so that they are at the same potential, though not at the same potential as Earth. However, it is essential to have a safer technology of handling with reduced flow rates of the volatile petroleum products especially in the high-energy propulsion systems in aerospace and rockets employing hydrocarbon fuels by an increase of the residence time of the flow. A review of the flow processes and the additives in the volatile fuels would be in order.

TRANSFORM

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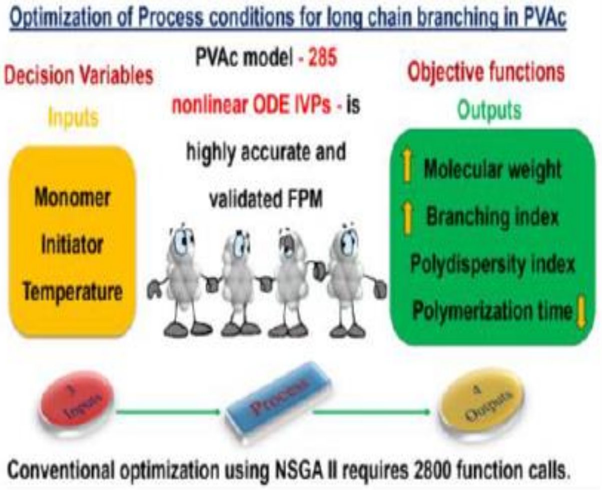
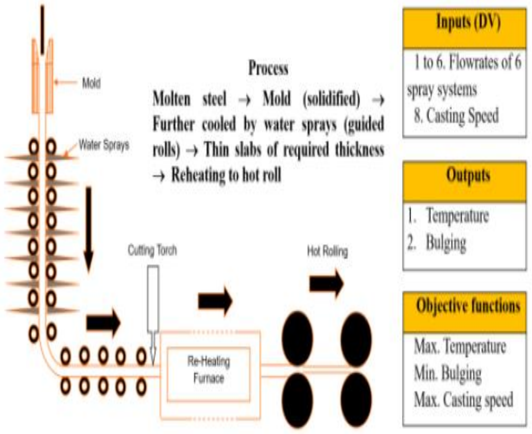
With the onset of high performance computing machines, research in engineering and science is witnessing a rapid growth in applicability of computationally expensive first principle models (FPMs). However, the optimization, control and parametric sensitivity analysis with these time intensive models still remains to be an arduous task due to the iterative nature of these algorithms which demands repeated high fidelity function evaluations. For instance, a multi-objective optimization exercise for determining the operating conditions to induce long chain branching in Polyvinyl Acetate (PVAc) polymer required approximately 2500 function evaluations when solved using Non-dominated sorting Genetic Algorithm (NSGA–II), an efficient population based evolutionary optimizer (see Fig. 1). The first principles based PVAc model which was used to generate the high fidelity solutions consisted of 285 highly nonlinear, coupled, stiff ordinary differential equations which consumed 10 minutes on an average to cater one function call. Thus the optimization exercise ran for approximately 15 days on an Intel(R) Xeon(R) CPU E5-26900 @ 2.90GHz (2 processors) 128 GB RAM machine[1].

There is no dearth of FPMs in literature which are computationally intensive to this and probably several orders higher in magnitude. Scenarios such as that in PVAc optimization, are neither limited to the Chemical engineering domain nor they appear as a direct result of using evolutionary optimization solvers. This issue is truly interdisciplinary in nature. For example, consider the Continuous Casting model (Fig. 2) from steel industry hosting a system of Partial Differential Equations[2]. This model simulated using the Finite Element Method (FEM) was considered for solving the industrial optimization problem of minimizing energy loss and maximizing productivity. When solved using the ε-constrained method and fmincon optimization solver with Sequential Quadratic Programming algorithm, the FPM was called nearly 3600 times. This number is slightly less than what was reported by the NSGA-II solver.



Conventional optimization using NSGA II requires 2800 function calls.

Figure 1. First principle model for PVAc polymerization. The optimization problem maximizes the molecular weight, branching index and minimizes the reaction time with a constraint on polydispersity index[1].



Process
Molten steel → Mold (solidified) → Further cooled by water sprays (guided rolls) → Thin slabs of required thickness → Reheating to hot roll

Figure 2. First principle model for Continuous casting process from Steel making industry[2].

Without going into further details on comparative studies across several engineering domains and optimization algorithms, the message in gist is, the process optimization of computationally intensive FPMs is confined to theoretical studies and there is a strong need for addressing this issue in order to implement them in practise in real time.

A practical solution to such problems is Surrogate assisted optimization. Surrogate models are data based mathematical functions which learn to emulate the FPMs with high accuracies. They are tremendously fast and once trained efficiently, they can replace the FPMs in iterative procedures such as optimization, thus earning the name “surrogate” models.

One classic example of surrogate models wherein one can find a blend of principles from machine learning and artificial intelligence is the Artificial Neural Networks (ANN). They are well known for their credible ability to capture the nonlinear behaviour of complicated models. However, neural networks suffer with major disadvantages such as those listed in Fig. 3 below, which not only degrade the performance of ANNs but also prevent them from qualifying as potential surrogates for optimization.

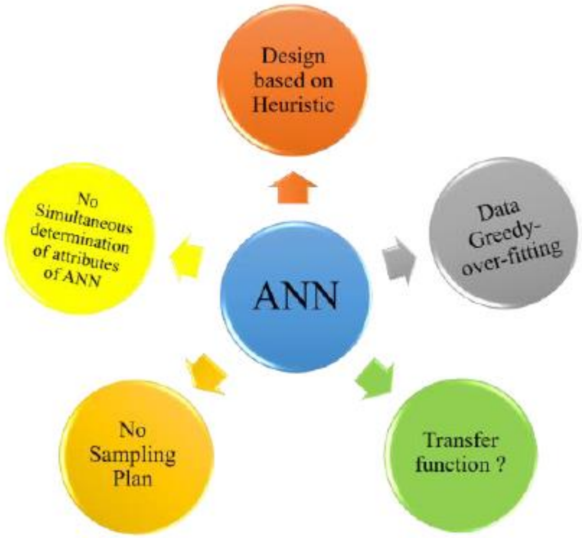


Figure. 3. Challenges associated with ANN

We present TRANSFORM (TRade-off between Accuracy, Nodes and Sample size FOR Meta-modelling), a novel ANN building framework which estimates the best configuration along with optimal training size and transfer function, simultaneously. While doing this, TRANSFORM ensures a balance between the aspects of over-fitting and prediction accuracy. It implements a novel sample size determination (SSD) techniques based on Sobol sampling plan and designed using the potential concepts of hypercube (HC) sampling and space filling. The modular nature of TRANSFORM does not put a hard constraint on usage of HC based SSD, thereby allowing the training with any available experimental data.

The decision boundary formed by an ANN classifier represents an n-dimensional hyperplane which can only segregate the linearly separable data. Since the nature of data to be modelled cannot be known apriori, it becomes imperative to design an automatic and intelligent technology which determines the optimal number of hidden layers and number of neurons in each hidden layer. Furthermore although the predictability can be improved by providing large number of training data points or by ensuring enough handles in the model to capture the dynamic trend, it is important to realize that increase in sample size and/or the number of parameters in the model tend to overfit the model.

Thus the technology need is to design such a parsimonious ANN model that is capable of maximum predictability. The trade-off between accuracy of validating a held out set, total nodes and training sample size is what propels the TRANSFORM algorithm[2].

	TRANSFORM – ANN			
	Architecture	N	r^2	Size
t_{poly}	3-5-1-1	6	0.9993	70
M_w	3-3-3-8-1	14	0.9979	50
B_n	3-2-1	2	0.9981	60
PDI	3-2-1	2	0.9979	80
Total function calls = 80 (Sobol-training) + 200 (validation) = 280				

Table 1. Architectures obtained from TRANSFORM for each of the outputs in PVAc FPM.

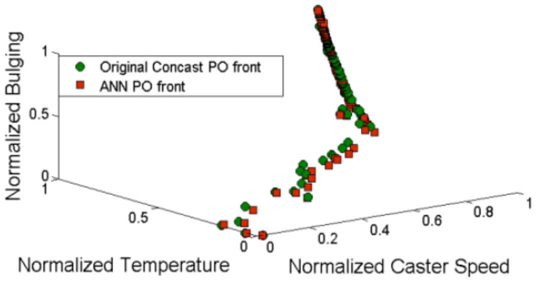


Figure 4. Results of ANN surrogate assisted optimization of casting model and comparison with conventional Pareto front.

TRANSFORM results in a 3 Dimensional Pareto front in which each solution corresponds to an optimal ANN architecture along with optimal transfer function and training sample size. One ANN architecture selected based on some appropriate higher order information will serve as Surrogate model. The models obtained in case of PVAc test case are presented in Table 1. Such a model is used as surrogate and the optimization results in case of continuous casting are presented in Fig. 4.

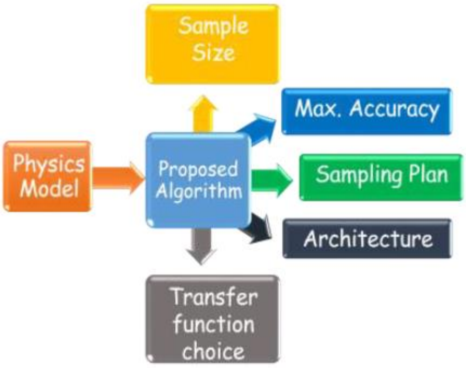


Figure. 5. Salient features of proposed algorithm - TRANSFORM

TRANSFORM is tested on 4 industrial models of varying difficulty levels and it could successfully build 25 optimal ANN surrogates so far with an average RMSE less than 3%. These ANN models are used in various applications mostly spawning from but not limited to process optimization, control and uncertainty analysis. All this was possible with TRANSFORM which is generic enough to be applied for any problem without a condition on input output dimensions (see Fig. 5).

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2. Miriyala SS, Subramanian V, Mitra K. TRANSFORM-ANN for online optimization of complex industrial processes: Casting process as case study. European Journal of Operational Research. 2018 Jan 1;264(1):294-309.

Guwahati Regional Centre Activities

Seminar Series

Science Friction: A Tale of Two Surfaces

Prof. Partho S G Pattader, Department of Chemical Engineering, IIT Guwahati delivered this talk on November 1, 2017.

Friction is a well-known (?!) phenomenon to the science and engineering community. Along with the known facts about friction, he talked about its appearance in our everyday life and its association with other closely related phenomena such as adhesion, locomotion, wear and tear etc. The conventional methods to characterize friction and a novel methodology to identify the salient features were also discussed. He also showed that noise can be used to mitigate the effect of friction and how one can exploit these findings to facilitate the transportation of macro scale objects for example particles, liquid droplets to the locomotion of micro/nano scale molecules.

Understanding Creative Design and Innovation as a trans-discipline

Prof. P. G. Yammiyavar, Department of Design, IIT Guwahati delivered this talk on November 3, 2017.

This presentation intended to give an insightful overview of what actually creative Design constitutes of - as a discipline. The wide range of niches in Technology that Design influences was illustrated with examples including one that proposes a possible role for an 'Interaction Designer' in a Chemical plant control room. That Design is a collaborative trans-discipline was explained through design case studies. Role of Innovation and creativity, which are the DNA of Design, were highlighted in the context of learning experiences from DoD IITG.

Language and mind: A handmaid's tale?

Prof. Bidisha Som, Department of Humanities & Social Sciences, IIT Guwahati delivered this talk on November 8, 2017.

Language, both verbal and non-verbal, is a communicative device. It 'says' what we think. However, the debate about the true nature of language has been fiercely debated, since the time of Plato. From being subservient to other higher mental functions, like 'thought', it has moved to a higher plane these days to a role of facilitator/ inhibitor in other cognitive functions. A sharp turn came around the time of advent of AI, when the debate centered on the underlying algorithm of language function. How is language intertwined with other mental functions? Does it merely give those processes a 'voice'? Or Does it play a role in facilitating/inhibiting those processes? Seems language never really wanted to be a sidekick! Language is a key player in our power to cognize. Category formation, attentional mechanism and executive function are some of the fundamental human cognitive abilities and findings point to a strong relationship between these and language. In this talk, she discussed some of these interesting relationships.

Growth of Indian Education System

Prof. Mihir Kumar Purkait, Department of Chemical Engineering, IIT Guwahati delivered this talk on November 10, 2017.

Polymeric Membranes for Water Purification

Prof. Suryasarathi Bose, Department of Materials, IISC Banglore delivered this talk on November 13, 2017.

This lecture comprehensively highlighted the various fundamental aspects of polymer blends from molecular level miscibility to the evolution of bi-phasic morphology, under different processing conditions, that are essential for exploring their potential in membrane applications. The key role of rheology on the evolution of morphology during processing and post-processing operations like compression molding, annealing etc. were discussed under the framework of different technique for the preparation of thin membranes. The different hierarchical porous structures (micro and nano), developed by selectively etching one of the components from binary blends, and their application in separation technology were discussed and the results were compared with the existing solutions. The unimpeded permeation of fluids was discussed with respect to the different morphology that is generated during their fabrication and the reasons for their clogging, fouling etc. were extensively discussed. In this context, various in situ and ex situ strategies to render the surface antibacterial were elaborated with respect to water purification applications using few model systems based on PVDF.

Controlled Movements in Interlocked Molecular Systems as Molecular Machines

Prof. Jubaraj Bikash Baruah, Department of Chemistry, IIT Guwahati delivered this talk on November 17, 2017.

Path, fuel and motion are three functional requirements of a molecular machine. The talk focussed on these three aspects taking examples from interlocked molecular systems. Preliminary aspects to define molecular machines and fundamental aspects to make improvised molecular machine were discussed. Specific examples on controlling catalytic activity, molecules walking along a path, protein synthesis, combination of rotational and translational motions were discussed.

Laboratory Safety

Prof. Sumana Dutta, Department of Chemistry, IIT Guwahati delivered this talk on November 22, 2017.

Upcoming Lectures

Quantification of Biological Systems: Systems Biology Approach

This talk will be delivered by **Prof. Kalyan Gayen**, Department of Chemical Engineering, NIT Agartala on December 8, 2017.

Engineering systems are getting quantified, optimized and optimally operated, where as biology is evolving to be a quantitative science. Engineering principles can be applied to the biological systems in analyzing the working principles of living systems. In other words, nature has created the biological systems and there are constant efforts to understand the working principles of biological systems, which are working efficiently in micro / nano scale with high degree of robustness. Systems biology approach is the application of engineering approachs to understand the biological systems. Challenges lie on the prediction of phenotypes incorporating genome, transcriptome, proteome and metabolome of one complex living system.

Lecture will broadly cover about the motivation of systems biology and the different mathematical approaches applied to understand the living systems. In this connection, one case study on the effect of endocrine disrupting elements on steroidogenesis using dynamic modeling will be presented.

In an another case study, quantification of bio butanol synthesis using steady state modeling namely elementary mode analysis will be presented. Further, highlights about the microalgae based bioproducts and conversion of lignocellulosic materials into value added chemicals will be delivered.

Introduction to structural biology

This talk will be delivered by **Prof. Akio Ebihara**, Faculty of Applied Biological Sciences, Gifu University, Japan on December 13, 2017. This Lecture mainly focusses on two topics relating to structural biology.

a) Deciphering a code of protein

Interestingly, in all genomes sequenced, a large portion of predicted proteins are functionally-unknown proteins, called as “hypothetical proteins”. X-ray crystallography, a powerful tool for structural biology, can determine the shape of protein at atomic level, which tells how the functional groups of a protein are well defined in 3-D space to exert its original function.

(b) Observing a protein complex

The most broadly used method to determine the atomic-resolution macromolecular structures is X-ray crystallography. However, this approach is limited by the bottleneck of protein crystallization. This constraint has imposed limitations in the application to large protein complexes and integral membrane proteins for which multiple conformational or compositional states coexist; these complexes are very difficult to crystallize. The recent advances in single-particle cryo-electron microscopy (cryo-EM) are solving this limitation. Cryo-EM now provides us a near-atomic resolution structure of protein complexes and membrane proteins.

Upcoming Events

CHEMCON – 2017

The Indian Chemical Engineering Congress, CHEMCON – 2017, along with the 70th Annual Session of the Indian Institute of Chemical Engineers will be organized by the Haldia Regional centre at Haldia, West Bengal during December 27-30, 2017.

The theme for CHEMCON-2017 is ‘*Versatility of Chemical Engineering to Meet Societal Challenges*’. Besides the regular events, such as Memorial Lectures, Chemcon Distinguished Speaker Lectures,Technical Sessions etc., there will be Indo –Canda Joint Symposium on ‘Chemical Engineering in Development of Energy and Environmental Technologies ‘.

Additional details can be obtained from www.chemcon2017.com

Advances in Sustainable Polymers

Fourth International Symposium on Advances in Sustainable Polymers will be jointly organized by Centre of Excellence for Sustainable Polymers, Department of Chemical Engineering, Indian Institute of Technology Guwahati and Polymer Processing Academy during January 8-11, 2018.

The symposium will include plenary talks on recent advances in several aspects of sustainable polymer-based technologies.

Additional details can be obtained from www.iitg.ernet.in/asp17

Indo-Japan Bilateral Symposium on Future Perspective of Bioresource Utilization

"Indo-Japan Bilateral Symposium on Future Perspective of Bioresource Utilization" with special reference to North Eastern Region will be jointly organized by Indian Institute of Technology Guwahati, India and GIFU University Japan during February 1-4, 2018.

The symposium includes the discussion on the lines: Frontier in bio-resource in NER, Harnessing of bio-resource in NER, bio-industries and bio-based economics for further agriculture in NER, bio-based processing and production, Functional food, Food development and Agrofood science. The symposium will be dedicated towards comprehensive elaboration on production and processing of bio-based resources and their utilization.

Additional details can be obtained from www.iitg.ernet.in/ijbs2017/

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