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Bridging the Gap: Computer-Aided Engineering for Energy Security and Environmental Protection

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Abstract

Engineers use computational tools to address a variety of practical problems. Often, the role of computer aided engineering is to capture the opportunities for wealth creation, as well as societal and environmental impacts through integrating, otherwise disconnected, piece of knowledge and closing the gap between theoretical developments and corresponding applications. The present article reports some aspects of our research activities at Centre for Process Systems Engineering (CPSE), where Computer Aided Chemical Engineering is applied to address important problems, with energy and environmental implications. The discussed examples include (1) integrated design and control of industrial processes (2) biofuel production, (3) carbon capture from industrial processes. While the explored applications are by no mean exhaustive, they are illustrative examples of recent advancements in the field.

Introduction

The engineers' endeavours for delivering economic values as well as protecting environment and enhancing the quality of life require bridging over a variety of gaps. Examples include the gap between "theory" and "application", between "academy" and "industry", or between "economy" and "environment".

Figure 1. The role of Computer-Aided Chemical Engineering is to bridge over various gaps

Filling such gaps require a variety of skillsets including modelling, pilot plant trials, scale-up and optimization, which can be computationally demanding. Computer aided engineering (CAE) is an integrating branch of engineering, where the experimental knowledge developed in the engineering labs and workshops, as well as theoretical developments, are embedded into enabling software tools which enhance the computational capabilities of end-user engineers. CAE offers several advantages. Firstly, it makes large amount of information accessible, often in the form of data banks of materials and physical properties, as well as modelling libraries. Secondly, it enables knowledge scalability by providing links between the fundamental understandings of physical and chemical phenomena at different spatial and temporal scales. Thirdly, it provides the opportunity for knowledge integration in order to construct the whole-system scenario, required for uncovering true economic and environmental impacts. Most of all, computer aided engineering minimizes the required skill-set for the end users, and enable a larger group of engineers to solve practical problems to a high degree of accuracy.

The aim of the present publication is to illustrate the importance of Computer Aided Engineering by exploring a few challenging applications in Process Systems Engineering. The rest of this paper is organized as follows. The first example is concerned with the design and control of industrial processes. The fact that design engineers are often chemical or mechanical engineers and control engineers are often electrical and instrumentation engineers with different mind-sets, poses a cross-disciplinary gap. Here optimization programming offers the opportunity for systematic decision-making and considering the objectives and constraints of various engineering disciplines at the same level. Then, the discussions continue with the second example concerning biofuel production. Here, the design challenge is due to the fact that the focus of experimental data is rather limited to only key aspects (e.g., reactors) of biofuel production. Simulation software tools enable constructing whole-system analyses at the plant-wide level and supply chain level. The last presented example is concerned with commercialization of novel solvents for separation of CO_2 from power generation flue gas. The key observation is that the energetic requirement for CO_2 capture at the industrial scale depends on the intermolecular interactions between CO_2 and solvent. Such multi-scale analysis is not feasible without using powerful modelling and optimization programs. The final section of this paper provides an overview of various computational tools commonly used by Process Systems Engineers.

Integrated process design and control: bridging a cross-disciplinary gap

The traditional practice is that process design is conducted first and only after the details of process configuration and equipment specifications are decided, the corresponding control system is designed. However, such a sequential approach is unfortunate because design and control of industrial processes share important decisions. If the process specifications are fixed, there is little room left for control engineers to improve the control performance. Therefore, many commentators recommend that design and control of industrial processes should be conducted together [1]. The methodology in which design of process and its control system is conducted simultaneously is called integrated process design and control (IPDC). Here, the research gap is to some extent multidisciplinary (Figure 1), as the process designers are often chemical and mechanical engineers and control designers are instrumentation and electrical engineers. While the focus of the first group of designers is on the economic and environmental expectations, the second group have concerns regarding uncertainties, practicalities of the process operation. Page Buckley was among the pioneering industrial engineers who recognized the importance of integrated design and control. He achieved this integration by transferring to Design Division of DuPont's Engineering Department and coordinating the efforts of process and instrumentation engineers [2].

The field of integrated process design and control is highly diverse, and the developed methodologies could have very different perspectives and engage with a variety of problems and sub-problems at different levels. Examples of the decisions involved in design of industrial processes include process configuration (e.g., reaction and separation networks), detailed design of process equipment, operational procedures and scheduling, supply chain optimization, and so on. Examples of decisions involved in the design of control systems, include selection of the control structure, i.e., manipulated variables (MV) and controlled variables (CV), setpoint policy (e.g., real-time optimization, self-optimizing control), controller degree of centralization, controller parameterization, and so on. Clearly there are many alternative solutions for both process and its control systems. It is said that the problem suffers from the so called “Curse of Dimensionality”, i.e., due to combinatorial characteristics, the number of alternative solutions grows sharply with the problem size and soon it becomes intractable. Therefore, complexity reduction is the leading frontier in this research area.

The early attempts for reducing the problem complexity was to deploy the insights and heuristics, developed over decades of engineering practice in order to enable conceptual as well as temporal and spatial decomposition of the problem. Examples include decomposition of the problem based on the production rate and inventory control, energy management, the causal relationship between control variables and so on. Further research was focused on the feasibility of controllability, which resulted in a variety of measures for controllability, operability, resiliency and switchability. For example, the characteristics

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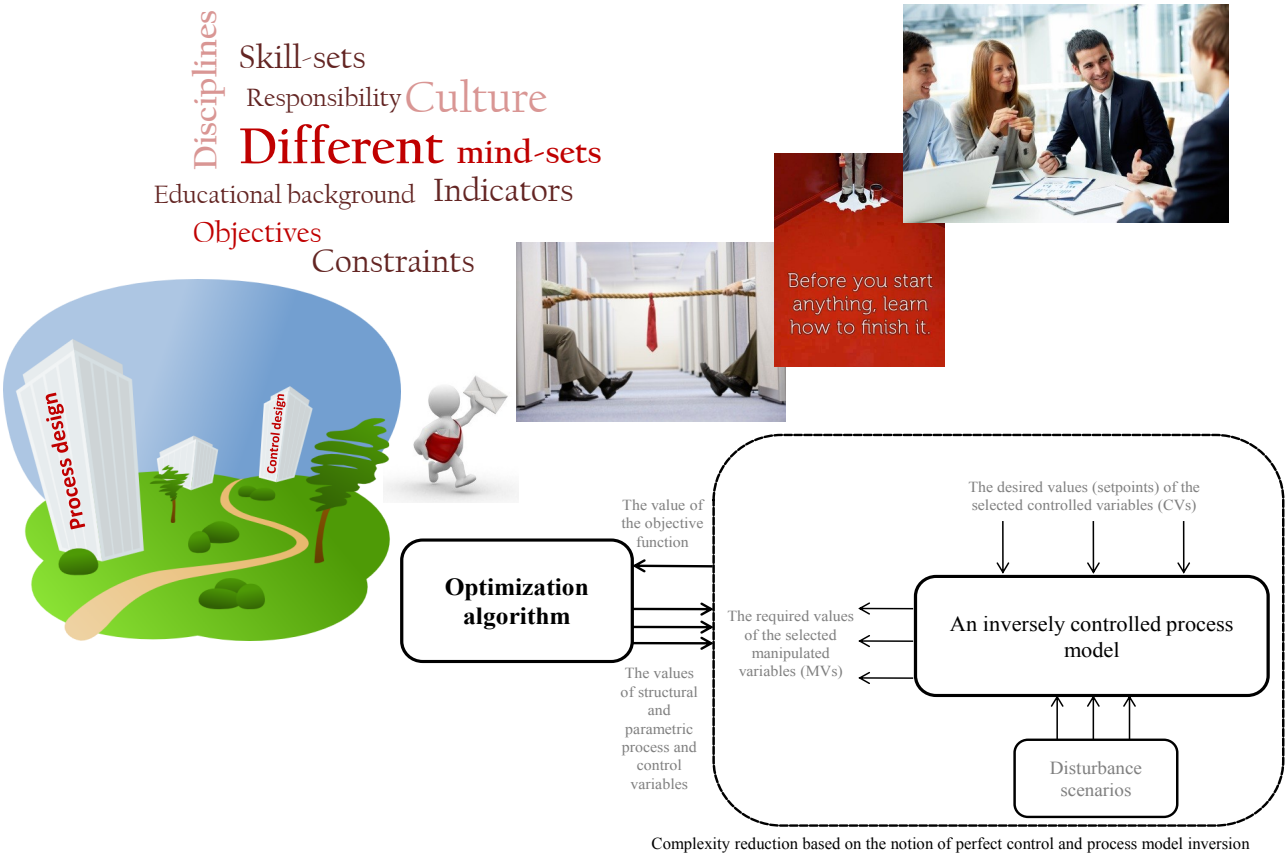

Figure 2. Different mind-sets (objectives and concerns) between design and operational engineers can cause inconsistencies in design and controls of industrial processes. Optimization programming provides a systematic approach for considering the design and control of industrial processes simultaneously.

which limit process controllability can be screened and rejected from the candidate solutions. They include interactions between control loops, disturbances, the constraints on the manipulated variables, delays and unstable zero dynamics, which can be quantified using a variety of measures and indicators such as various types of relative gain arrays (RGAs), minimum and maximum singular values, Niederlinski index, right-half plane zeros, and so on.

All the aforementioned methods have qualitative or yes/no attitudes. Each measures only concerns a certain limiting factor of controllability. Most of all, despite nonlinear behaviour of industrial processes, they are based on linear control theory. This is unfortunate because the results of linear control analyses are valid only locally and therefore, are incapable of capturing the interactions between design and control of industrial processes. Acknowledging these limitations, recent research activities have focused on application of Computer-Aided Engineering for developing algorithms which can establish a trade-off between (1) process objectives in terms of profitability and environmental foot-print, and (2) control objectives in terms of dynamic performance, resiliency and controllability. Examples of these efforts include multi-objective optimization[3] (including controllability indices), developing methods for inferring undesirable nonlinear behaviour from steady-state analysis[4], applying process model for geometric analysis of operability[5], parameterization of controller and simultaneous optimization with process design decisions[6], flexibility optimization[7,8] and optimization based on inverse process modeling[9-11]. Nevertheless, the important characteristics of all these new methods is application of nonlinear (mixed-integer) optimization programming for systematic generation of alternative solutions and screening them based on performance analysis of nonlinear models[1].

It is expected that the notion of integrated design and control of industrial processes will be even more important in the near future. This is due to the fact that as industrial processes become more energy efficient, their control also becomes more challenging. Modern processes are multipurpose and multiproduct. Furthermore, the existence of several energy and material pathways due to the application of heat integration and material recycling result in propagation of disturbances in multiple pathways. In addition, in order to enhance safety measures and save energy, often less material inventories are held. However, small liquid and gas

holdups are less tolerant of disturbances. Another emerging technology is process intensification. For example conducting various phenomena in the same unit operation (e.g., reaction and separation in a reactive distillation column) may save energy. However, intensified processes have significantly narrower operating window compared to the equivalent multi-unit processes. The key observation is that as the efficiency and profitability of industrial processes is increased, their control becomes more challenging and it is essential to consider the design of their control systems at the same level of process design in order to ensure the operability and profitability under uncertain conditions. While, Computer-Aided Engineering has been crucial for the advances in this field, it is anticipated that future developments, particularly in the area of dynamic optimization and off-the-shelf libraries for control analysis will facilitate industrial integrated process design and control.

Biofuel production: bridging a system integration gap

The production of liquid fuels from biomass has the potential to diversify energy resources and mitigate the environmental impacts associated with consumption of fossil-based energy resources. Amongst various biomass conversion pathways, pyrolysis offers the cheapest route to renewable liquid fuels. Despite such economic incentives, commercialization of biomass pyrolysis poses significant challenges. In the following, several instances of such challenges are outlined and then it is explained how Computer Aided Engineering (CAE) enables addressing them.

First of all, the products of pyrolysis reactions, called pyrolysis oil (PO), features undesirable properties such as chemical instability, high acidity, low heating value and immiscibility with petroleum-derived fuels. The technologies for the removal of oxygen and other heteroatoms from pyrolysis oil are referred to as “upgrading”. Hydrodeoxygenation is the most common upgrading technology and was originally inspired by hydrodesulfurization (HDS) and hydrodenitrogenation (HDN) from the petroleum refining industry. However, the amount of heteroatoms (i.e., oxygen) is an order of magnitude larger in the case of PO. The high oxygen content can lead to excess coke formation. As a resolution multistage hydrodeoxygenation is recommended in which first the PO is stabilized in a low temperature reactor and then a deeper hydrodeoxygenation (HDO) is accomplished in the second-stage reactor at a higher temperature[12]. An alternative upgrading technology is hydrothermal upgrading, in which hot compressed water (HCW) is used as a reaction medium. This technology dates back to pioneering research into coal liquefaction during the 1970s to 1990s by Shell[13]. Changes in the physical and chemical properties of HCW become very apparent at around 300^{o}C and it is widely observed that at these conditions water features enhanced and tunable properties (e.g. solubility, solvent polarity, transport properties), and ease of solvent removal. Other advantages of this technology include avoiding phase change and parasitic energy losses due to high-pressure processing, versatile chemistry to existing chemical and fuel infrastructure, enhanced reaction rates, and minimal hydrogen consumption[14].

Hydrodeoxygenation (HYD) of pyrolysis oil has a high biomass to fuel yield. However, it requires large amounts of hydrogen and its economic viability is highly sensitive to the hydrogen price. By comparison, hydrothermal upgrading (HTU) requires little or no hydrogen. However, its fuel yield is relatively lower. Recently, we conducted a comprehensive set of experimental and modelling analyses on both upgrading technologies [15]. The observation was that in both scenarios, the product of short-residence time upgrading separates to aqueous and organic phases. However, the separated phases have different potentials for biofuel and hydrogen production. Based on a series of preliminary studies and key process indicators, an integrated scheme which exploits the synergies between HTU and HYD technologies was developed. Detailed process modelling and techno-economic analysis showed that biofuel can be produced at competitive prices while the overall process is self-sustained with respect to the required hydrogen.

Nevertheless, the chemistry of biomass poses an additional fundamental challenge; the ratio of hydrogen atoms available for combustion to carbon atoms, (H-2×O)/C, of biomass is significantly smaller than fossil fuels. For example, the effective hydrogen to carbon ratio for hybrid poplar ($C_{4.1916}H_{6.0322}O_{2.5828}$) is as low as 0.207. By comparison the same value for Octane (a representative component of Gasoline) is 2.25. As a result, in order to convert biomass to liquid fuels, compatible with current energy infrastructure, all the oxygen atoms and a large portion of carbon atoms should be removed as carbon dioxide which deteriorates economic competitiveness of the biomass conversion processes. For example for the case of hybrid polar pyrolysis 45% of initial carbon atoms in the biomass end up in the greenhouse gas emissions. Therefore, CO_2 utilization is crucial for profitability of future biorefineries. In a recent study [16], we investigated the carbon footprint of biofuel production through biomass pyrolysis. The research importance is due to the fact that various types of biomass contain large quantities of oxygenates. As a result, application of biomass for producing biofuel can result in large CO_2 emissions. For example, in the pyrolysis pathway from each two carbon atoms in the biomass almost one of them ends up in the atmosphere as CO_2 [17]. Therefore, CO_2 capture and utilization will be an indispensable element of future biorefineries. In this study, an integrated scheme was developed in which the CO_2 produced during biomass pyrolysis and upgrading was captured and utilized for microalgae cultivation via photosynthesis process. Then, the cultivated microalgae biomass is used for additional fuel production. It was shown that in the new

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refinery, the CO_2 emissions is reduced from 45% to only 6%. Furthermore, under certain economic assumptions, the extra produced fuel compensates the costs of CO_2 capture and utilization. Nevertheless, pyrolysis oil is a rich source of hydrocarbons and can be used for producing olefins and aromatics. Sharifzadeh et al.,[18] showed that it is possible to retrofit an existing olefin process using multi-stage catalytic upgrading of biomass pyrolysis oil. Detailed technoeconomic analysis as well as environmental assessment suggested that the greenhouse gas emissions are up to 44% less than conventional olefin processes, and the produced biochemical are economically competitive. The research significance is due to the fact that the olefin process is highly energy-intensive and its products are essential for polymer production.

In addition, biomass resources are dispersed and subject to seasonal and geographical uncertainties. Therefore, supply chain network design and management can significantly influence the economic viability of a biofuel technology. Fast pyrolysis offers several advantages for biofuel production. It is a relatively cheap process and can be conducted using centralized, decentralized, or remote production strategies. Centralized production strategy refers to the scenario where biomass pyrolysis and upgrading are conducted at the same location. Decentralized production strategy is when biomass pyrolysis is conducted at a separate pyrolysis plant and the pyrolysis oil is transferred to the upgrading centres. Finally, remote production strategy refers to the scenario when pyrolysis oil produced by the mobile pyrolyzers is sent to upgrading centres for biofuel production. The trade-off between these strategies lies in the different transportation and production cost of the materials and economies of scale. Recently, we investigated the economic performance of pyrolysis supply chain network[19]. Various options including centralised, decentralised and mobile production strategies were considered. The formulated program was applied to the case of 290,000 m^3 biofuel per annum in the United Kingdom. It was observed that there is an important trade-off between the costs of biomass transportation and economies of scale. In addition, it was shown that in the presence of uncertainty, flexible operation of the supply chain has economic significance.

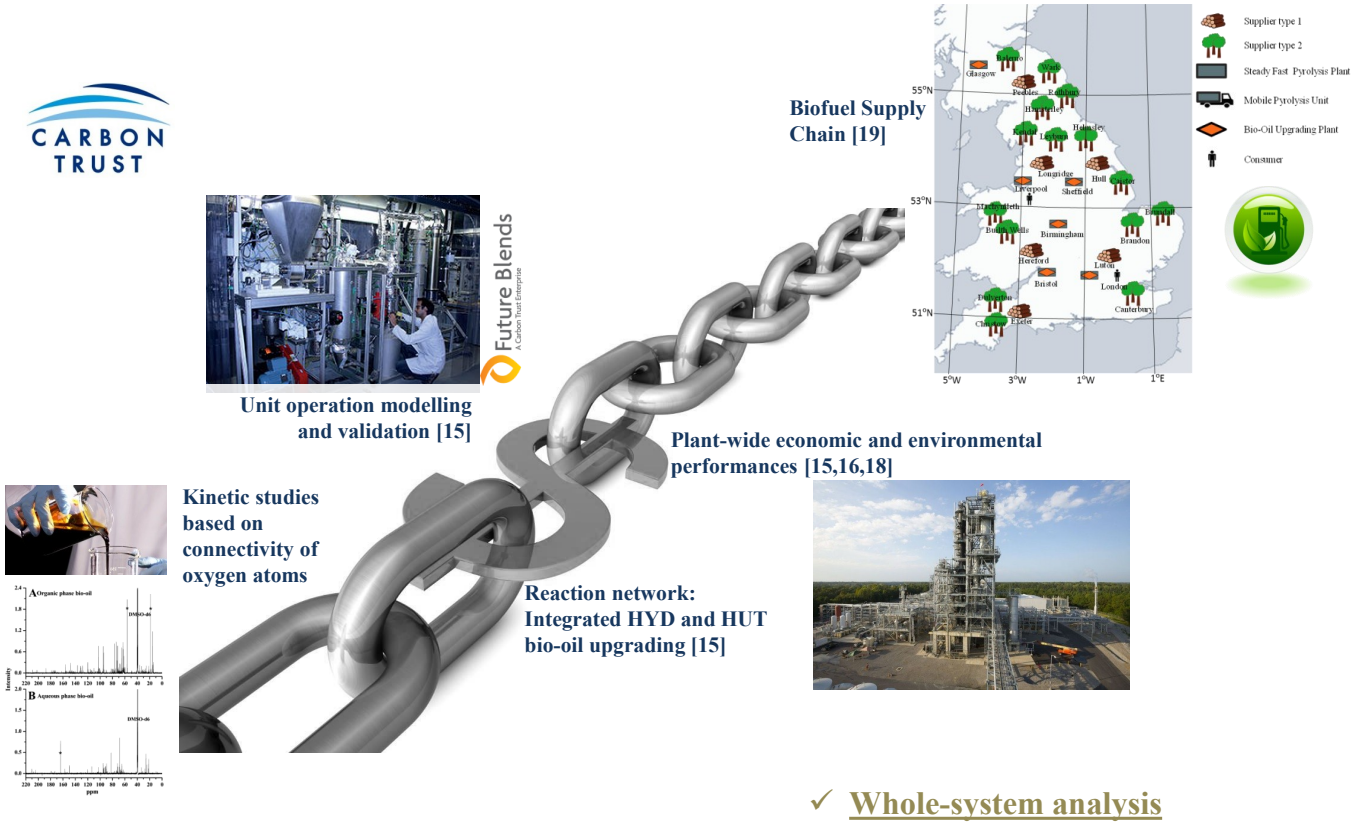

Figure 2. Uncovering the economic and environmental impacts of biofuel production requires reconciliation of experimental data, model development and validation and whole-system analysis.

The common observation is that biofuel pyrolysis is a multifaceted technology. Here the role of Computer Aided Engineering is to integrate the otherwise scattered, pieces of knowledge and enable systematic whole-systems analysis. Otherwise, isolated, mono-dimensional studies could result in unrealistic and uninformed decisions. The idea is shown in Figure 2. The first step is to study the key performance indicators of through experimental programs, which is often focused on key conversion reactions. The results will illustrate the yield of the products and the feed (i.e., hydrogen) requirements, or the kinetics of reactions.

Furthermore, a major achievement of this step is characterization of the feedstock, intermediate products and fuel. Reconciliation of experimental data in the form of mixture properties such as elemental compositions, boiling point distributions, molecular weight distributions, or atomic connectivity (NMR) into a set of real species opens up routes to a wealth of thermodynamic property package and data banks. Then, the preliminary models are constructed and validated using bench-scale or pilot plant data. The validated model is later used for scale-up and constructing the plant-wide model which also include the feedstock pre-treatment as well as product purification up to the grade required by consumers. The outcome of plant-wide analysis is economic performance measures such as operational costs and required capital investment, in addition to environmental measures such as overall carbon balance. The knowledge associate with the design and operational of conversion processes will be later embedded in the supply chain network. The decisions involved in design and operation of supply chains include the selection among available biomass feedstock resources, mode of transportation, production strategy (centralized, decentralized, and mobile, as discussed earlier), the flowrates of feedstock, intermediate products, and fuel between resources, processing sites and consumers, production scheduling and potentials for feedstock and products storage. The outcome of these analyses is the overall picture of fuel economy in terms of the net present value (NPV) or internal rate of return (IRR) of the total supply chain network and environmental measures such as greenhouse gas emissions and carbon footprint.

Carbon Capture from power plants: bridging a multi-scale knowledge gap

Increasing energy demand and associated pollution have posed a paradoxical challenge toward the security of energy supply and environmental protection. This has translated into various national and global policies and regulations. The instances of these international regulations include the so-called Europe 2020 which targets 20% reductions in greenhouse gases, 20% energy supply from renewables, and 20% improvement in energy efficiency. In the UK, the Climate Change Act 2008 mandates an 80% overall cut in six greenhouse gases by 2050 compared to the 1990 baseline. While integration of renewable energy resources can moderate the problem to some extent, the Intentional Energy Agency (IAE) asserts that in a foreseeable future, fossil fuels remain the dominant source of energy supply, and application of carbon capture technologies will become increasingly urgent [20].

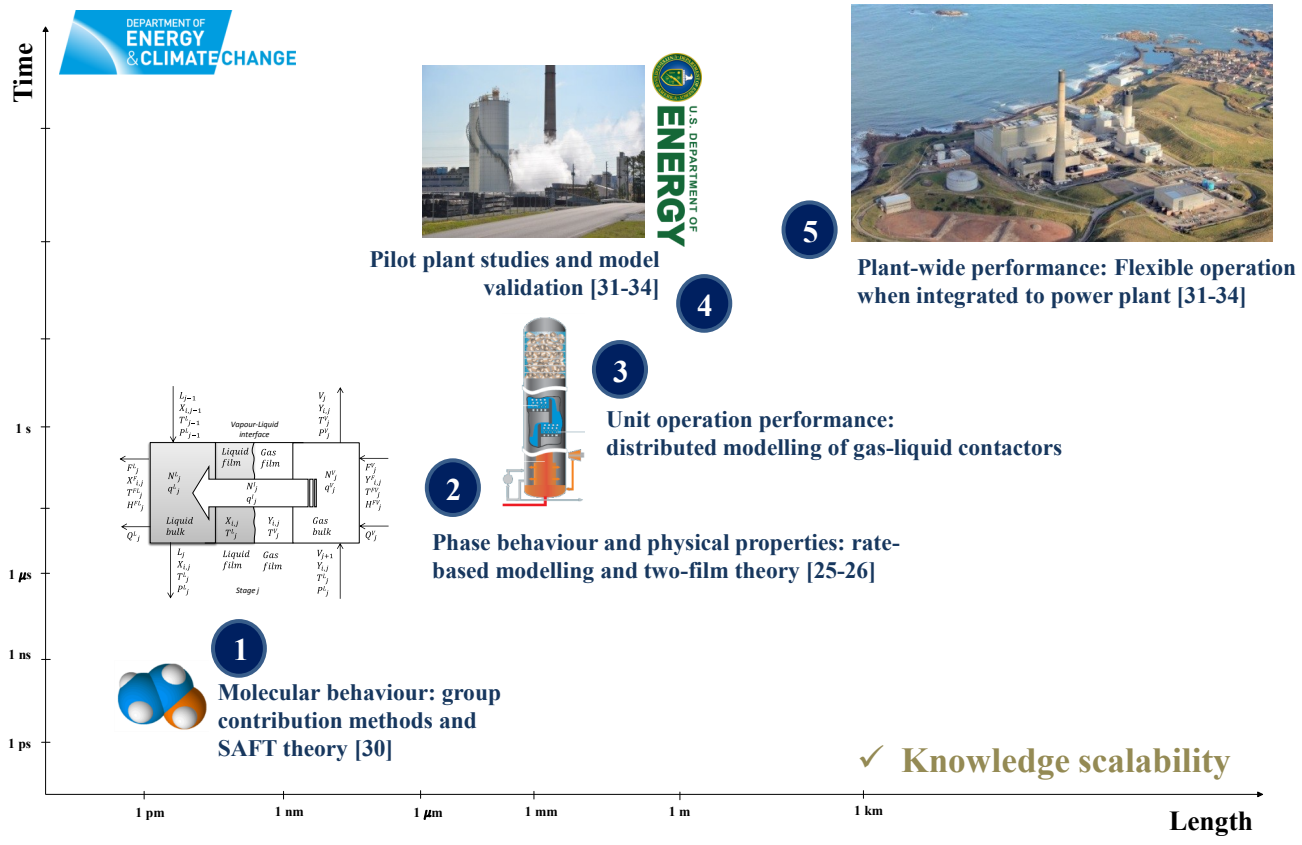

Figure 3. Carbon capture and storage from power plants is a multi-scale engineering challenge; while the economic and environmental footprints should be evaluated at plant-wide scales, the energetic performance depends on the intermolecular interactions between solvent and CO2 molecules.

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CO_2 removal solvent scrubber is the most promising technology for carbon capture, as this technology is an end-of-pipe treatment and has been in use since the 1930s for natural gas sweetening[21]. However, adaptation of this technology for post-combustion carbon capture is nontrivial as gas processing is significantly different from power generation in several aspects. Natural gas is often produced at an elevated pressure and does not contain any oxygen. Furthermore, in natural gas sweetening, a higher degree of CO_2 removal is required and the separated CO_2 is emitted to the atmosphere. Finally, gas processing is a relatively steady-state process. By comparison, post-combustion carbon removal is conducted at near atmosphere pressure and deep CO_2 separation is often uneconomic. In addition, power plants are subject to drastic variations in electricity demand and for the capture plant to remain integrated with the power plant, it should feature a high degree of flexibility. Nevertheless, integrated operation of carbon capture processes may not be realizable without considering the main operational characteristics of the upstream power plant. Power plants are subjects to drastic variations in the electricity demand. Examples of such variations include regular daily and hourly variations in the consumer demand or stochastic variations, for example due to extreme weather conditions or local events. It is expected that by the introduction of renewable energy resources the fluctuations in the electricity grid will also increase on the supply side, as some of these new resources such as solar or wind have intermittent generation characteristics. Thus, the fossil-based power plants are required to operate flexibly and balance the supply deficit . Therefore, commercialization of new CO_2 capture technologies strongly depends on their adaptability in order to remain integrated as the upstream power plant experiences variations in the electricity demand. Therefore, developing high fidelity models with predictive capabilities for the industrial-scale performances has been under scrutiny.

The idea is shown in Figure 3, which conforms to the notion of chemical supply chain proposed by Grossmann and Westerberg [22]. While the economic and environmental footprints should be evaluated at plant-wide scales, the energetic performance depends on the intermolecular interactions between solvent and CO_2 molecules. Therefore, underpinning energetic implications of the carbon capture and storage from power plants poses a multi-scale research question. The accurate modelling of the CO_2 scrubber systems requires thorough understanding of the underlying physical and chemical phenomena involved in absorption and desorption of CO_2 into and from the working solvent. The methods for modelling gas-liquid contactors can be broadly classified into equilibrium and rate-based models. Early-stage attempts for modelling gas-liquid separation processes were based on the assumption that at each separation stage, the exiting phases are in equilibrium conditions. In the absence of high-performance computers, these techniques were performed using graphical methods[23]. However, it was widely observed that for most industrial applications assuming equilibrium composition of the exiting phases results in unrealistic predictions. The first attempt to overcome this limitation was to consider an efficiency measure for each separation stage [24], which can be applied to calculate the actual number of stages from the theoretical number of stages. Application of empirical efficiency correlations has been promising for binary and close-boiling separation systems. However, for multicomponent systems, the efficiency of separation stages can vary from 5% for absorption systems with high viscosity, high molecular weight solvents to 120% in single-liquid-pass large-diameter distillation trays (or packed segments) because of the crossflow effect [24]. Due to difficulties associated with uncertainties in the stage efficiency method, intensive research was devoted to developing non-equilibrium models based on transport rates, which are also embedded in the simulation software tools [25, 26]. The rate-based models are founded on the two-film theory, as shown in Fig. 4. Here, phase equilibrium is assumed only at the interface of vapour and liquid phases. Unlike equilibrium-based models, the exiting vapour phase is superheated and the exiting liquid phase is subcooled and they have different temperatures. The exchanged mass and energy between phases depend on the driving forces, transport coefficients, and the interfacial area. Often, both convective and diffusive transport phenomena are involved and component-coupling effects should be considered [24]. Various empirical correlations for calculating the mass transfer coefficient are proposed by researchers for random and structured packing. Finally, the bulk liquid and gas phases may have different flow configurations such as plug or mixed flows.

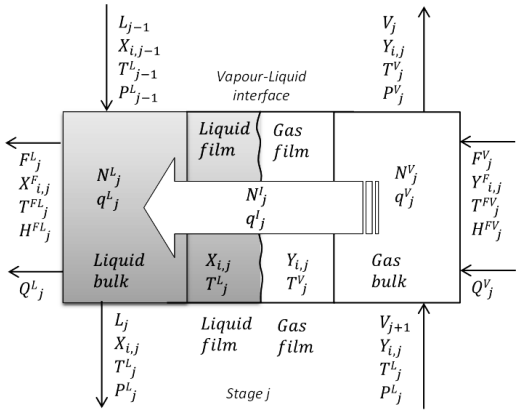

Figure 4. Two-film model used for modelling rate-based absorption and desorption of CO2 into and from solvent [31].

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Various thermodynamic models are proposed by researchers in order to describe the thermophysical properties of the CO_2-solvent mixture. These methods can be broadly categorized to non-rigorous and rigorous methods. In non-rigorous methods, equilibrium constants are considered for the involved reactions and are reconciled against experimental data. The major drawback of non-rigorous methods is the lack of precision for closing energy balances. In addition, the rigorous methods can be classified to (1) activity-based models (derived from Gibbs free energy), and (2) equation of state models (derived from Helmholtz free energy). A frequently used activity-based model is Electrolyte Non-random two-liquid model (E-NRTL) in which the activity coefficient expressions of the original NRTL model are modified, and certain constraints regarding local like-ion repulsion and electroneutrality are imposed. An alternative activity based model is the Extended UNIQUAC model where the original UNIQUAC model was modified to account for ionic interactions [27]. A limitation of the aforementioned activity-based models is that they only describe the liquid phase and a separate equation of state should be applied for modelling the vapour phase. Alternatively, researchers attempted to use equations of state which can consider the presence of ionic components. More recently, equations of state which are also capable of accommodating chemical equilibria, has been the focus of various research groups. Here, the treatment is based on statistical associating fluid theory (SAFT), in which the free Helmholtz energy is correlated to the intermolecular association between the molecule segments [28]:

$$\frac{A^{mix}}{NkT} = \frac{A^{IDEAL}}{NkT} + \frac{A^{MONO}}{NkT} + \frac{A^{CHAIN}}{NkT} + \frac{A^{ASSOC}}{NkT}$$

In the equation above, N refers to the number of molecules, k is the Boltzmann constant and T is the mixture temperature. On the right hand side, the first term represents the ideal Helmholtz free energy and the three other terms refer to the residual contributions due to monomer interactions, formation of chains, and intermolecular interaction between associating sites. Then, given the Helmholtz free energy of the mixture, A^{mix}, it is possible to calculate other mixture properties. The association contribution is based on thermodynamic perturbation theory (TPT)[29], where by using intermolecular potential models (e.g., square well with variable range) and by adjusting their parameters (well depth and range), it is possible to fully characterize the strength of the associating sites.

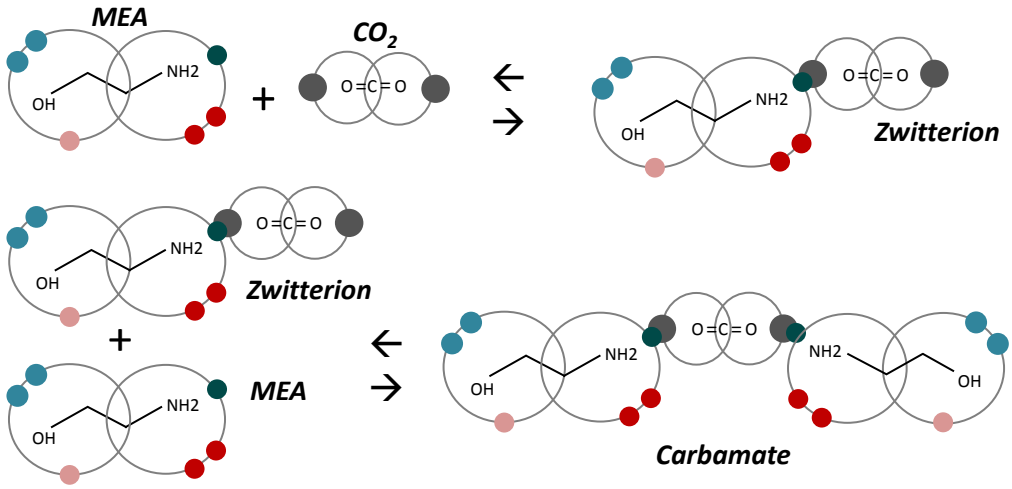

Fig. 5. Schematic representation of Carbamate formation [31]

The idea is shown in Fig. 5 for carbamate formation. Firstly, a molecule of CO_2 reacts with a molecule of monoethanolamine (MEA) to form an intermediate species called a zwitterion. Then, the zwitterion reacts with another MEA molecule to produce carbamate. However, in the new approach, the rate of reactions, the concentration of the intermediate zwitterion, and its thermophysical properties are not formulated directly. Instead, CO_2 and MEA are represented as associating molecule chains with two and six associating sites, respectively. Then, the concentration of CO_2 in association with two MEA molecules represents the actual CO_2 loading of the solvent at different temperatures and pressures. The combination of rate-based modelling and representation of chemical reactions using statistical associating fluid theory (SAFT) provides a consistent modelling approach. The justification is that for solvents such as MEA, the rate of reaction is significantly faster than the heat and mass transfer phenomena. Therefore, the knowledge of the rate of reactions at the gas-liquid interface is unnecessary and chemical equilibrium sufficiently describes the actual physical system behaviour.

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This modelling approach, which is now embedded in a software tool called gCCS [30], offers several advantages; firstly unlike activity-based models, the same equation of state is used to describe both liquid and vapour phases. Secondly, the chemical equilibria are treated at the same level as phase equilibria. Furthermore, the aforementioned approach establishes a connection between the chemical and physical behaviour of the mixture and the molecular structure of the involved materials. This is of particular importance to new solvents as the required information can be acquired from the available data for the molecular segments of associating sites from experimental data. Most of all, this approach results in significant model reduction because the speciation of intermediate ions is not included in the mathematical formulation and the uncertainties associated with their thermophysical parameters are disentangled from problem formulation. Such an abstract model with a high degree of predictability can be applied for optimization.

Recently, in a series of collaborative studies[31-34], we applied the aforementioned modelling techniques for commercialization of two novel solvents developed by Carbon Clean Solutions Limited (CCSL), for CO_2 capture from Natural Gas Combined Cycle (NGCC) and Pulverized Coal Power Plants (PCPP). The new solvents are of the class of amine-promoted buffer salt (APBS) solvents, and the aforementioned modelling approach consistently describes their behaviour. Nevertheless, power plants are subject to dramatic changes in the electricity demand and while the flowrate and composition of flue gas (i.e., capture plant feed) depends of the electricity power demand, the steam required for solvent regeneration imposes an additional burden to the power plant. Underpinning the true energetic performance of the whole integrated system requires studying the two-way interactions between the capture plan and power plant. The method of integrated process design and control (Figure 6) was applied in order to seamlessly integrate the carbon capture process with the upstream NGCC and PCPP processes. The results showed that it is possible to maximize overall energetic performance while ensuring process operability during various electricity load reduction scenarios.

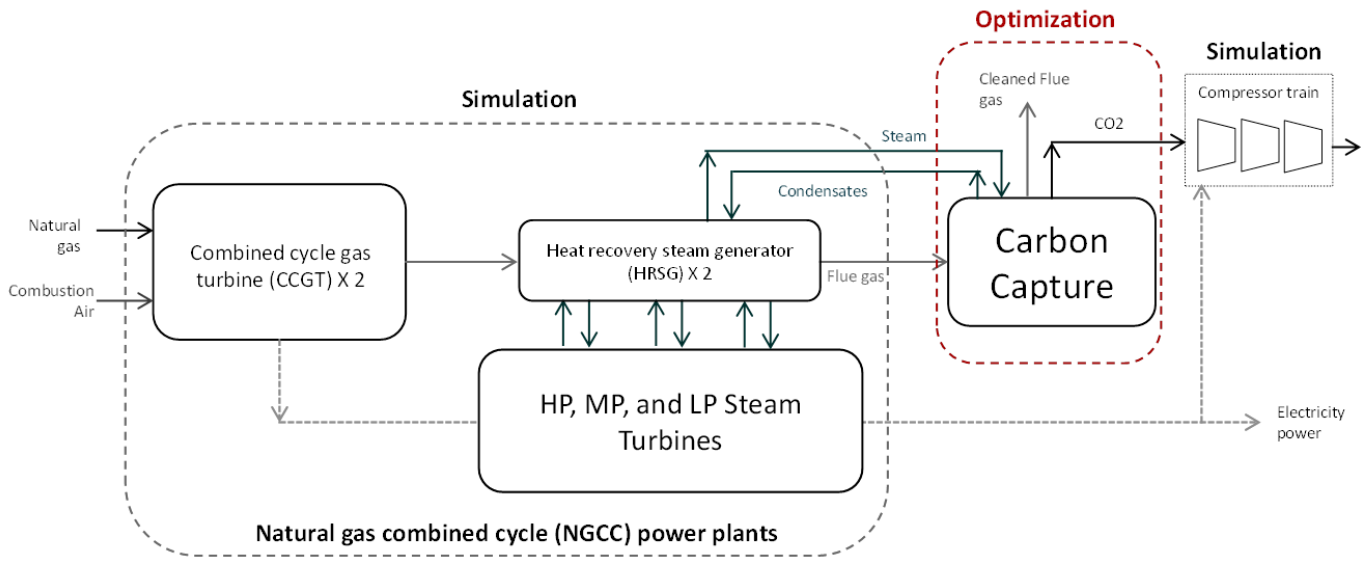

Figure 6. The proposed optimization framework for the problem of NGCC power plant retrofit and integration to the CO_2 capture and compression process [31]

While the "enabling" role of Computer Aided Engineering (CAE) is evident in all aforementioned examples, there is often a trade-off between the flexibility and customizability of the CAE software tools and the required modelling efforts. The idea is shown in Figure 6. At one extreme, it may be occasionally possible to construct the model using off-the-shelf libraries. The advantages of this approach include the ease of model development and access to the wealth of thermodynamic databanks. The limitation is that often new processes and materials may not conform to exiting models and data banks, or the associate software. For example in [9], the optimization capabilities of the simulator (Hysys) was further extended by linking the model to the MATLAB optimization toolbox. The dynamic optimization algorithm in [10], applies a steady-state model in order to initialize the dynamic model. Further customizability will require modelling the underlying equations which can be solved using Algebraic Modelling Languages (AMLs) or Differential Algebraic Equation (DAE) solvers. At the extreme, the modeller may need to develop tailor-made solution algorithms in order to solve larger problems faster.

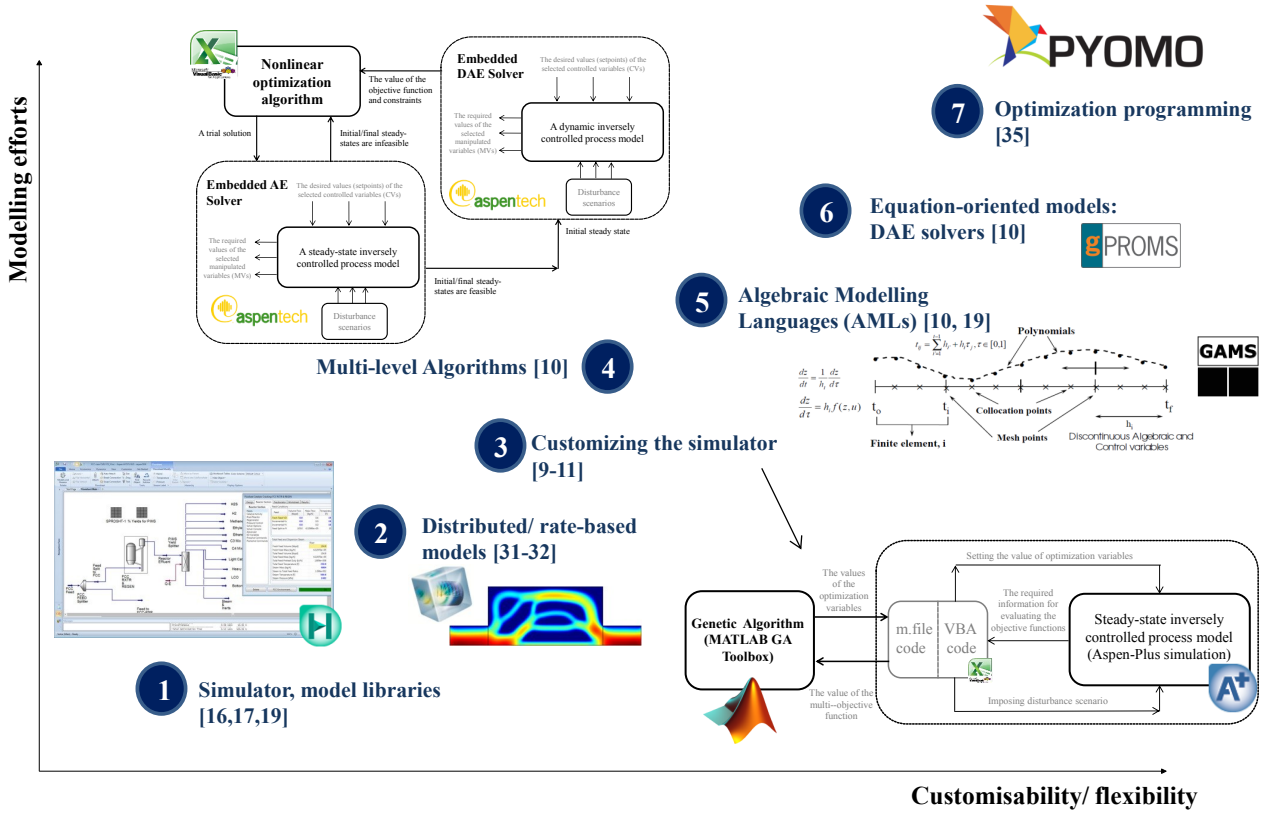

Figure 7. The trade-off between the customizability of computer-aided software tools and the required modelling efforts.

Summary

In this article, the impacts of Computer-Aided Engineering was illustrated using examples of design and operation of industrial processes with energy and environmental implications. It was shown that optimization programming enables considering different objectives and constraints systematically. Furthermore, it was discussed that underpinning economic and environmental footprints requires constructing whole-system analysis. Here, the role of Computer-aided Engineering tools is to embed the knowledge acquired in experimental set-ups and to scale-up for prediction of enterprise-wide and supply-chain performances. It was also illustrated that delivering economic and environmental impacts at the industrial scale may require multi-scale modelling and optimization. Computer-Aided Engineering enables integrated of different pieces of knowledge at various scales incorporated into models with high degrees of predictability and reasonable degree of complexity. As in future, climate changes and depleting resources require innovative solutions for energy security and environmental protection, it is expected that the Computer-Aided Engineer will have a more and more vibrant role in design and operation of industrial processes.

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