



**HAL**  
open science

## A multi-layered view of chemical and biochemical engineering

Rafiqul Gani, Jerzy Baldyga, Béatrice Biscans, Elisabetta Brunazzi, Jean-Claude Charpentier, Enrico Drioli, Hermann Feise, Andrew Furlong, Kevin M. van Geem, Jean-Charles de Hemptinne, et al.

► **To cite this version:**

Rafiqul Gani, Jerzy Baldyga, Béatrice Biscans, Elisabetta Brunazzi, Jean-Claude Charpentier, et al.. A multi-layered view of chemical and biochemical engineering. *Chemical Engineering Research and Design*, 2020, 155, pp.A133-A145. 10.1016/j.cherd.2020.01.008 . hal-02502429

**HAL Id: hal-02502429**

**<https://ifp.hal.science/hal-02502429>**

Submitted on 9 Mar 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1 **A multi-layered view of chemical and biochemical engineering**

2  
3 Rafiqul Gani\*  
4 PSE for SPEED Company, Skyttemosen 6, DK-3450 Allerød, Denmark  
5 and

6 Jerzy Bałdyga<sup>1</sup>, Béatrice Biscans<sup>2</sup>, Elisabetta Brunazzi<sup>3</sup>, Jean-Claude Charpentier<sup>4</sup>, Enrico Drioli<sup>5</sup>,  
7 Hermann Feise<sup>6</sup>, Andrew Furlong<sup>7</sup>, Kevin M Van Geem<sup>8</sup>, Jean-Charles de Hemptinne<sup>9</sup>, Antoon J. B. ten  
8 Kate<sup>10</sup>, Georgios M Kontogeorgis<sup>11</sup>, Flavio Manenti<sup>12</sup>, Guy B Marin<sup>8</sup>, Seyed Soheil Mansouri<sup>11</sup>, Patrick  
9 M. Piccione<sup>13</sup>, Ana Povoá<sup>14</sup>, Manuel Andres Rodrigo<sup>15</sup>, Bent Sarup<sup>16</sup>, Eva Sorensen<sup>17</sup>, Isuru A.  
10 Udugama<sup>11</sup>, John M. Woodley<sup>11</sup>

11

<sup>1</sup>Faculty of Chemical and Process Engineering, Warsaw University of Technology, ul. Waryńskiego 100 645  
Warsaw, Poland

<sup>2</sup>Crystallization Engineering and solid and particle processes, LGC -CNRS Université de Toulouse, France

<sup>3</sup>Department of Civil and Industrial Engineering, University of Pisa, Largo Lazzarino 2, 56122 Pisa, Italy

<sup>4</sup>Laboratoire Réactions et Génie des Procédés CNRS/ENSIC, Université de Lorraine, École Nationale  
Supérieure des Industries Chimiques, 1, rue Grandville B.P.20451 54001 Nancy Cedex France

<sup>5</sup>Institute on Membrane Technology (CNR-ITM), c/o University of Calabria, Via P. Bucci cubo 17/C, 87030  
Rende CS, Italy

<sup>6</sup>President, European Federation of Chemical Engineering, DECHEMA, Theodor-Heuss Alle, Frankfurt,  
Germany

<sup>7</sup>Cogent Content Ltd., 29 Hawthorne Drive, Thornton, Leicestershire, LE67 1AW, UK

<sup>8</sup>Laboratory for Chemical Technology (LCT), Department of Materials, Textiles and Chemical Engineering,  
Ghent University, Technologiepark 125, 9052 Ghent, Belgium

<sup>9</sup>IFP Energies nouvelles ; 1 et 4, avenue de Bois-Préau ; 92852 Rueil-Malmaison Cedex – France

<sup>10</sup>Nouryon RD&I, Zutphenseweg 10, 7418 AJ Deventer, Netherlands

<sup>11</sup>Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs  
Lyngby, Denmark.

<sup>12</sup>Politecnico di Milano, Dipartimento CMIC "Giulio Natta", Piazza Leonardo da Vinci 32, 20133 Milano,  
Italy

<sup>13</sup>Pharmaceutical R&D, F. Hoffmann-La Roche AG, Grenzacherstrasse 124, 4070 Basel, Switzerland

<sup>14</sup>Engineering and Management Department, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco  
Pais • 1049-001 Lisboa, Portugal

<sup>15</sup>Department of Chemical Engineering. Universidad de Castilla- La Mancha. Campus Universitario s/n.  
13071 Ciudad Real, Spain.

<sup>16</sup>Alfa Laval Copenhagen A/S, Maskinvej 5, DK-2860 Søborg, Denmark

<sup>17</sup>Department of Chemical Engineering, University College London, Torrington Place, London WC1E 7JE,  
UK

12

13 \* Corresponding author (rgani2018@gmail.com)

14

15

16

17 **Abstract**

18 The contents of this article are based on the results of discussions the corresponding author has had since  
19 2015 with the co-authors, who are members of academia and industry in Europe, on the scope and  
20 significance of chemical and biochemical engineering as a discipline. The result is a multi-layered view  
21 of chemical and biochemical engineering where the inner-layer deals with the fundamental principles  
22 and their application; the middle-layer deals with consolidation and expansion of the principles through  
23 a combination of science and engineering, leading to the development of sustainable technologies; and  
24 the outer-layer deals with integration of knowledge and collaboration with other disciplines to achieve a  
25 more sustainable society. Through this multi-layered view several important issues with respect to  
26 education, research and practice are highlighted together with current and future challenges and  
27 opportunities.

28  
29 **Introduction**

30 Industrial chemical technology revolutionized the modern world in the 20<sup>th</sup> Century, and now in  
31 combination with industrial biotechnology it is set to do the same in the 21<sup>st</sup> Century. Underpinning these  
32 developments is the discipline of chemical and biochemical engineering (C&BE). The discipline applies,  
33 among others, the fundamental principles of thermodynamics, reaction stoichiometry and kinetics,  
34 biochemistry and cell biology as well as transport phenomena together with the laws of conservation of  
35 mass, energy and momentum to create better materials, products and processes that are useful to society.  
36 In other words, at a technical level chemical and biochemical (C&B) engineers work with unit operations  
37 (be it at industrial scale, pilot scale, micro-scale or nano-scale) for the purposes of chemical and/or  
38 biochemical synthesis followed by downstream separations, which are all based on phenomena such as  
39 thermodynamics, reactions (chemical, biochemical, or thermal conversions), transport (mass, heat and  
40 momentum). In this way, C&B engineers solve problems related to synthesis, design, analysis,  
41 implementation, operation-control, optimization, etc., of chemical and biochemical processes needed to  
42 manufacture the products required by society. This implies that the scope and significance of C&BE is  
43 potentially enormous. In a given case, the scope is defined by the raw materials that can be converted to  
44 the desired products through the corresponding manufacturing processes where resources such as energy  
45 are consumed, water is used and the environment is affected. Nevertheless, the conversion of the  
46 resources to products is in all cases incomplete and therefore the issue of recycle and regeneration of  
47 resources becomes increasingly important and urgent (Negro et al., 2018). Over the past decades, as the  
48 demand for better and more versatile products and their corresponding flexible manufacturing processes  
49 has increased, so has the need for increased knowledge on related topics that is perhaps not well  
50 understood in the context of application of C&BE based technologies but are nevertheless very important.  
51 Moreover, society currently faces grand challenges like climate change, growing global population and  
52 resource limitations that require innovative solutions regarding the way products and services are  
53 provided. In this way, C&BE is also an evolving discipline.

54  
55 Historically, chemical engineering came into existence more than a century ago by synthesizing the

56 fundamental scientific disciplines of chemistry, physics and mathematics with mechanical engineering  
57 competences required for industrial processes and contributing, thereby, to the world's economic  
58 progress (Wei et al., 1979). Indeed, while chemical engineering has made enormous contributions as a  
59 discipline (and profession), it has also embraced rapid and dynamic technological changes and has  
60 frequently been at the center of emerging new developments (Butz and Tauscher, 2002). Today, perhaps  
61 more than at any other time in history, we face formidable challenges (Negro et al., 2018). But these  
62 challenges also represent unique opportunities such as exploring and exploiting new abundant resources  
63 (Wang and Krupnick, 2015); substituting and/or improving the exploitation of resources in current use  
64 (Christensen et al., 2008); delivering sustainable solutions related to energy (Chu and Majumdar, 2012),  
65 water (Gleick, 2016), environment (Allen et al., 2018) and food (Papargyropoulou et al., 2014);  
66 contributing to avoid danger and risk, for example, climate change (Monastersky, 2013) or accidents  
67 (Brunaud et al., 2019) and, optimizing the operation, distribution and safety of manufacturing processes  
68 (Grossmann, 2005).

69  
70 The objective of this paper is to present a multi-layered view of chemical & biochemical engineering,  
71 through which its scope and significance, as well as its future role can be better understood. This view  
72 highlights the important outcomes of chemical and biochemical engineering as a discipline as well as a  
73 profession. The inner core *fundamental* layer involves process-product related activities where  
74 application of the fundamental concepts of C&BE help to design, build and operate manufacturing  
75 processes that convert specific raw materials to desired products. The middle interface *consolidation*  
76 layer involves resources-efficiency related activities where improved understanding of the concepts and  
77 combination of science and engineering lead to the development of new technologies that when applied,  
78 lead to more sustainable engineering solutions. The outer *unifying* layer involves society-challenges  
79 related activities where industrial development helps to address challenges that when resolved would  
80 lead to a more sustainable society. Here, integration of knowledge, such as ideas, disciplines etc., play a  
81 major role. The main issues, challenges and opportunities at each level are discussed with respect to  
82 education, research and practice related to each layer.

83

#### 84 **The Multi-layered View**

85 The multi-layered view is shown in Figure 1, where three inter-connected layers are highlighted. The  
86 concept can be understood through the following logic; Horizontal - left: input of resources to the system,  
87 right: outcome in terms of conversion to products; Vertical - bottom: (intellectual) input from C&BE,  
88 top: impact on the system due to increased knowledge and available products. Layers – innermost: core  
89 topics defining the discipline, outermost: topics that define the contributions of C&BE to society.

90

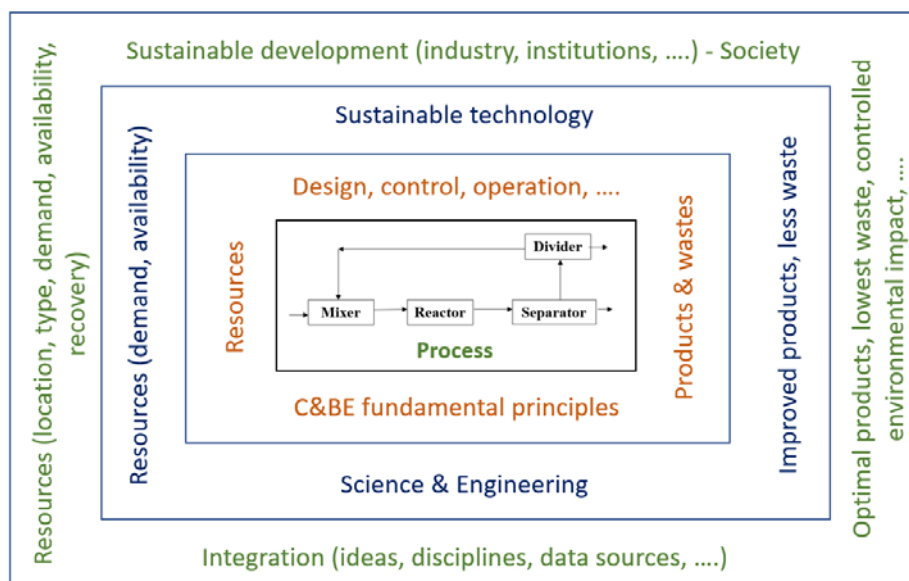


Figure 1: The multi-layered view of chemical and biochemical engineering (note: increasing details of the same resources (raw materials and utilities such as energy and water) are considered, moving from inner to outer layers).

In Figure 1, moving from left to right adds material, economic and societal value. That is, from resources (raw materials as well as utilities such as energy and water) higher valued products are obtained (inner-layer); considering demand and availability of these same resources, the products are further improved and the processes become more efficient (middle-layer); adding also considerations (for the same resources) such as resource location, type, recovery, etc., the optimal products with lowest wastes and controlled environmental impacts, etc., are obtained at various scales (plant, industrial parks, country, region, etc.). To obtain these incremental improvements, a better understanding of the concepts that lead to new technologies is needed. Moving from bottom to the top of the figure, input of knowledge leads to problem solutions. That is, fundamental knowledge of C&BE helps to design, build and operate the manufacturing process (inner-layer); combination of science and engineering gives a better understanding that leads to the development of sustainable technologies (middle-layer); integration of knowledge from different disciplines providing new ideas and data sources contribute to sustainable development of society (measured in terms of institutions, industry, ecology, etc.).

These layers are strongly interactive, that is, demand from the outer layers require increased know how from the inner layers to meet them. For example, as the need for structured products like food, detergents, cosmetics, etc., grows, as pointed out by Cordiner (2004) and Hill (2004), the numerous operational steps involved with the processing of these products provide opportunities as well as challenges to find better, more reliable and innovative alternatives (Zhang et al., 2016). First, however, the involved phenomena-microstructure-property-process relations need to be understood sufficiently through focused

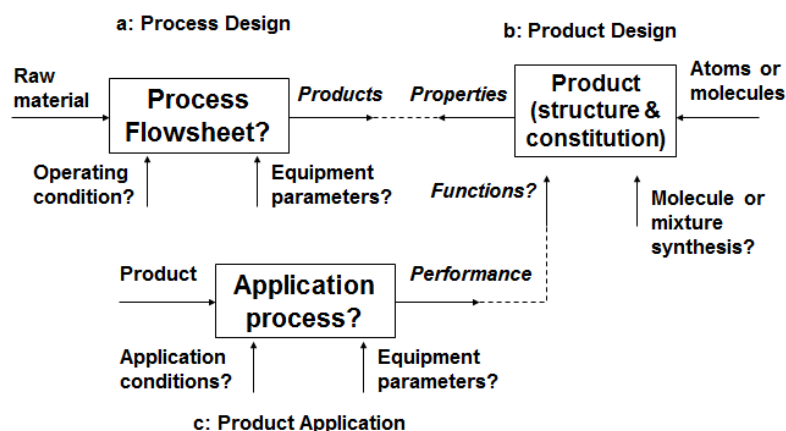
116 experimental work and subsequent experiment-based process analysis. The fundamental understanding  
117 gained together with experimental evidence could then be used to conceptualize and derive mathematical  
118 models for faster and more reliable process development. Also, as one moves from the inner layers to  
119 the outer, the scope and significance of the problems tackled, the solutions found and the knowledge  
120 required broadens. Therefore, the three layers together highlight aspects of incremental education,  
121 research and practice, as well as the impact on our society and on the global environment. Note that even  
122 though a topic or keyword is not listed in a specific layer, it does not mean they are not used in that layer.  
123 For example, the terms “resources” and “science & engineering” are listed in the core and middle layers,  
124 respectively, to highlight their key-roles in employing the fundamental principles as well as consolidation  
125 and expansion of the scope and significance of C&BE. Also, to find innovative solutions and to minimize  
126 the ecological impact and/or to maximize the societal benefits, even though resources such as energy,  
127 water, material, etc. are needed, human resources are also needed to develop technologies, methods,  
128 tools, etc., to design, construct and operate the processes and to distribute and/or supply the manufactured  
129 products. Similarly, the developments from the inner layers help to achieve sustainable industrial  
130 development and to educate-train the stake-holders by addressing the grand challenges through  
131 appropriate interdisciplinary and/or multidisciplinary approaches.

132

### 133 ***Inner core fundamental layer: processes and products***

134 At the fundamental level, C&BE involves the conversion of specific raw materials to desired chemicals-  
135 based products through appropriate processing routes while also utilizing resources such as energy,  
136 water, materials, man-power, etc. to achieve the desired objectives. However, successful development of  
137 a desired chemical or biochemical product requires an economically feasible manufacturing process and  
138 vice versa. For best success, both the product and the process should be optimal. To achieve this, the  
139 knowledge input is process engineering that may include aspects of chemical kinetics; transport  
140 phenomena; unit operations; process integration; control and many more. Adjacent areas such as organic  
141 chemistry, analytical sciences, biology, mechanical engineering must also be drawn on, as appropriate.  
142 The connection between the product and the process is highlighted through Figure 2 (Zhang et al., 2016),  
143 where in addition to the traditional product-process connection, the application of the product for  
144 performance evaluation is considered, for example, use of a solvent for solvent-based separation or use  
145 of a solvent for product delivery, for instance, in delivery of an insect repellent as a liquid lotion. Note  
146 that the objective of the process is to produce the product defined by its molecular structure (for single  
147 species products), purity, state, etc., while the objective of the product is to deliver its functions (product  
148 application). The objective of product design, in this case, is to identify the molecular structure (for single  
149 species products) with the desired properties.

150



151

152

153 Figure 2: Relationships between product-process design and product design-product application. The  
 154 dashed lines indicate the link between the design and application problems (Zhang et al., 2016).

155

156 ***Middle interface layer: science and engineering***

157 Raw materials and economically feasible processing routes are no longer sufficient to launch a successful  
 158 product-process. Use of resources such as energy and water need to be optimized together with efficient  
 159 management of raw materials supply-demand, economics, products distribution and environmental  
 160 impacts. Safety issues, both related to risk avoidance for plant workers as well as for the neighborhood,  
 161 is also of increasing concern. Innovative solutions for service provisions therefore need to be determined.  
 162 This requires additional knowledge in terms of the integration of science and engineering leading to the  
 163 development of innovative solution approaches to process integration and intensification as well as new  
 164 ways to manage supply chains and to monitor economic, ecological and societal impacts of  
 165 manufacturing processes and product use. The outcome could be sustainable technologies in terms of a  
 166 reduced ecological footprint together with greater societal benefits while maintaining profitability. The  
 167 inputs from fundamental sciences, the rational use of computational tools and focused experimental  
 168 validation need to play important roles at this level. The improved understanding of the phenomena at  
 169 all scales (including the core layer) need to be considered and integrated in order to be able to optimize  
 170 the production processes such that significantly improved innovative solutions are obtained, employing  
 171 new and more efficient unit operations. The combination of science and engineering in product-process  
 172 development needs to play a key role, where increasing scientific focus may lead to smaller equipment  
 173 sizes while increasing engineering focus may lead to larger scales of sustainable technologies. For  
 174 example, in the area of micro-structured products, the key to success is to first identify the desired end-  
 175 use properties of a micro-structured product at the small-scale, and subsequently to control product  
 176 quality and production efficiency by manipulating the microstructure formation at the process scale  
 177 leading not only to a novel product but also to less waste and lower energy consumption (Charpentier,  
 178 2003).

179

180

181 ***Outer unifying layer: improved social benefits***

182 It is expected that within the next 20 years, the population on earth would stabilize to around 9 billion  
183 (Pereira et al., 2010); requiring 6-7 times increase of world GDP; which will require 5-6 times increase  
184 of existing production capacities for most commodities (steel, chemicals, lumber, etc.); 3.5 times increase  
185 in energy demand (7 times increase in electricity demand); very large increase in water demand. Costs  
186 related to CO<sub>2</sub> emissions are estimated to be 7 GTC/yr to 26 GTC/yr (Vooradi et al., 2018) together with  
187 concomitant increase in knowledge requirement. Therefore, in the outer layer, the grand challenges  
188 (<http://www.engineeringchallenges.org/challenges.aspx>) in terms of availability of resources and raw  
189 materials need to be reconciled with sustainable development of society  
190 (<https://sustainabledevelopment.un.org/>). An alternative way to meet the sustainable development goals  
191 is to focus on improving the quality of manufactured products (or related services), which as a result  
192 would drive down the need for quantity while also ensuring that society (the consumer) gets to at least  
193 maintain their current quality of life and comfort.

194  
195 To achieve this objective, a larger vision of the true needs of society with respect to the limited  
196 availability of resources needs to be implemented. With respect to C&BE, this requires integration of  
197 chemical and biochemical engineering know-how together with other disciplines (e. g., sociology, ethics,  
198 political sciences, economics) and with many of the main actors (such as decision makers and decision  
199 influencers) of society. Prausnitz (2007) has emphasized this aspect together with the special role of the  
200 human dimension in C&BE. The outcome is a set of optimal products generating minimum wastes and  
201 consuming less resources (raw material, energy, water, etc.) through more sustainable processes, that  
202 contributes to the education, training and practice of C&BE, and thereby, to sustainable development of  
203 society.

204  
205 ***Interaction between layers***

206 Referring to Figure 1, the application of C&BE and the associated challenges identify opportunities and  
207 help to set targets for improvements in education, training and practice. To achieve these targets, science  
208 and engineering needs to come together to develop techniques, methods and tools through which  
209 sustainable and innovative products-processes can be designed and/or developed in the middle layer.  
210 However, to develop the techniques of the middle layers, the available knowledge in the core layer in  
211 terms of theory, concept and data need to be enhanced. The movement is from the core layer to the outer  
212 layers with feedback towards the inner layers for adjustment and/or refocus of targets. For example,  
213 education gives the C&B engineer knowledge to practice and understand the fundamentals, which they  
214 employ for research in the middle layer to develop new techniques, which they employ in practice in the  
215 outer layer for the sustainable development of society. However, as the needs of society change, the  
216 fundamental concepts and the targets from the inner layers also need to be adjusted. Note also that  
217 education, research and practice may be applied at all layers, depending on the level or type of the  
218 institutions at which they are conducted. That is, the desires (targets) placed on C&BE on the outer layer  
219 for expected improved social benefits are related to the technical and economic constraints placed by the



220 middle layer as well as the understanding of the fundamental principles in the core inner-layer. This  
221 means all three layers are interconnected as any desire or constraints from the outer and/or middle layers  
222 respectively, could influence the scientific requirements placed on the inner layer while any development  
223 in the inner layer influences the outer layers and their ability to fulfil the constraints and/or desires.  
224

#### 225 *Education*

226 The key question in C&BE education is what skills, outcomes and knowledge are needed for the three  
227 cycle (BSc, MSc and PhD) education program in the subjects of C&BE. One option for the case of BSc  
228 and MSc degrees could be that the actions in the core layer of Figure 1 be linked to the core curriculum  
229 (for example, BSc), while the middle and outer layers could be linked to the advanced (related to the  
230 inner-core topics) and/or specialization topics not included in the inner-core (for example, an extended  
231 BSc or MSc). What is necessary is that C&BE students understand the basic concepts, scope and  
232 significance of the middle as well as the outer layers. One way to incorporate the additional knowledge  
233 from the outer layers into C&BE education is through design and/or evaluation projects, where concepts  
234 such as ethics, sustainability, sustainable development and/or circular economy are included. The PhD  
235 degree on the other hand is concerned with mainly research and development at all layers based on the  
236 knowledge gained at the BSc and MSc levels, posing of new problems, addressing of current challenges  
237 and/or exploring available opportunities. An important issue is the depth of knowledge gained at each  
238 layer. The outcomes of the BSc and MSc education are knowledge and understanding; engineering  
239 analysis; design and practice; investigations; transferrable skills; and ability to solve problems.  
240 Therefore, topics from the middle and outer layers of Figure 1 are needed as a complement to the core  
241 curriculum. In this regard, the use of virtual laboratories (or innovative pedagogies) to cope with the  
242 growing number of students, combined with a lack of adequate pilot-scale educational facilities is an  
243 alternative worth considering. The drivers for developing a virtual laboratory are highlighted in Figure  
244 3. Innovative pedagogical techniques that currently exist should be employed, both to motivate the  
245 younger generation that is keen on using new technologies as well as to benefit from a renewed content  
246 that addresses more explicitly their needs (adequate use of tools such as process simulators, data bases,  
247 social media, remote or distant learning, etc.).  
248

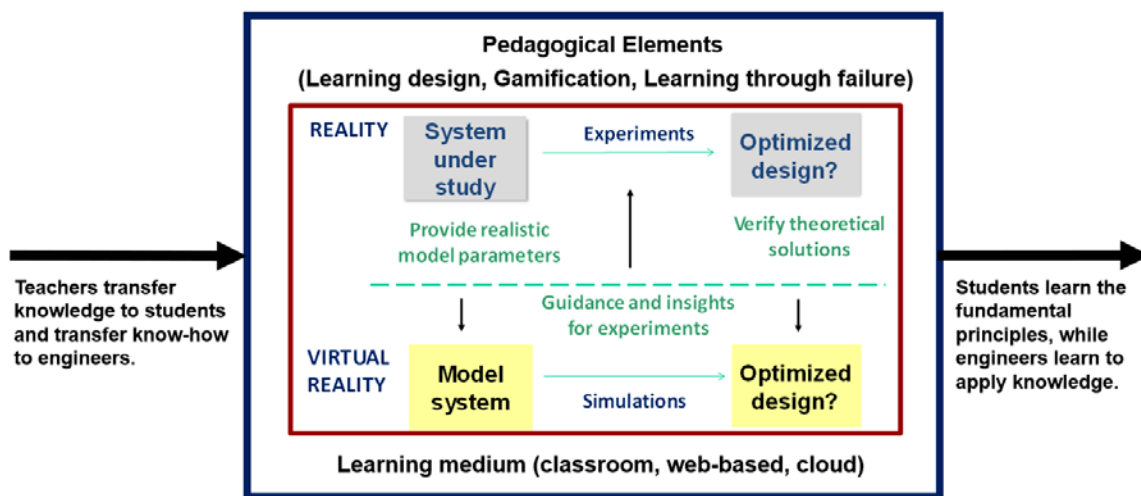


Figure 3: The drivers for developing a virtual laboratory

249  
250  
251

252 Another key issue is how to equip C&BE students to adapt to innovative technologies that may come  
253 from areas outside of the scope of C&BE. That is, how to widen the C&BE curriculum with non-  
254 traditional topics such as: life science related topics (biochemical engineering, molecular biology and  
255 genetic engineering; pharmaceutical engineering; biomedical engineering; product engineering; material  
256 engineering; environmental engineering); interdisciplinary fields (energy and fuel engineering;  
257 membrane science, aerosol, colloids and interface, organometallic chemistry; catalysis); and  
258 management related to advanced technology (operations management; change management; knowledge  
259 management) without sacrificing the core or fundamental topics from the inner layer? As the C&B  
260 engineers increase their knowledge and abilities, they are moving to the outer layers, gaining expertise  
261 in a wider range of disciplines. For example, they can increase their core competences in sciences related  
262 to separation; mixing of solids, gaseous and liquid materials; and transforming materials to more useful  
263 forms with the help of energy and/or catalysts, be they biogenic or non-biogenic. With this expertise the  
264 C&B engineers should be able to design and operate industrial plants and play an important supportive  
265 role in a wide range of other sectors, from manufacturing to mining and health care, for example.

266

267 With respect to non-technical skills C&B engineers need to develop skills in ethics, business, and  
268 administration that can help them, for example, in project management, budgeting, and economics. Also,  
269 ability to work as part of teams in multicultural and diverse environments needs to be developed.  
270 Adaptation is an important skill in a rapidly changing society and C&B engineers should have the ability  
271 to handle different situations as well as respond to emergencies, if necessary. In general, courses on  
272 process and plant design, combined with or without product design, are well suited to meet these types  
273 of learning objectives. Further enhancing of the fundamentals is very important, especially across the

274 different disciplines of chemical engineering as emphasized by Wu and Prausnitz (2019) on the particular  
275 role thermodynamics plays in connection to chemical engineering.

276

### 277 *Research*

278 Research activities are needed in every layer. Scientific advances in the inner core topics could provide  
279 a better understanding of the underlying principles leading to increased availability of data, more reliable  
280 theory-models and therefore, the development of more flexible model-based methods and tools. This in  
281 turn could increase the scope and significance of C&BE. The objective of research activities in the outer  
282 layer is to understand the needs of the key societal stakeholders and to translate them to specific targets  
283 for development. In the middle and core layers, the objectives are to develop and apply techniques and  
284 technologies to realize the targets through appropriate combination of science and engineering, and new  
285 developments and understanding of the fundamental principles. That is, in the outer layer, the focus could  
286 mainly be on tackling the global challenges to ensure the sustainable survival of people (9+ billion) on  
287 earth with an acceptable standard of living by, for example, improving the standard of living and safety  
288 with minimal environmental and health impacts. Therefore, concepts such as sustainability, circular  
289 economy and resource recovery need to be integrated into product development, process design and  
290 retrofit activities, to name a few.

291

292 In the middle layer the established targets from the outer layer could result in the following  
293 developments/trends for technologies, which by no means is an exhaustive list, and also is not listed in  
294 terms of any priority:

- 295 • Use of industry 4.0 technologies of AI, machine learning and big data in improving  
296 manufacturing operations with the aim of reducing resource usage and improved production  
297 efficiencies (Venkatasubramanian, 2019). To this end concepts such as digital twins, hybrid-  
298 modeling techniques, novel sensors that are currently under development should receive more  
299 attention (Rosen et al., 2015). To achieve appropriate rather than indiscriminate application of  
300 data science, awareness of digital technologies amongst chemical engineers should be fostered;  
301 project activities should also be undertaken using conscious decisions to balance first principles  
302 and data driven methods (Piccione, 2019).
- 303 • Development of flexible and smart manufacturing technologies so that manufacturing plants can  
304 be “re-tooled” to produce multiple products and change production (Kang et al., 2016) as  
305 preferences and desires from the outer layer change. Concepts such as disposable reactors  
306 (Glindkamp et al., 2010), micro reactors (Rossetti and Compagnoni, 2016) as well as non-  
307 invasive measurement techniques such as image analysis (Forte et al. 2019) and tomography  
308 (Tapp et al., 2003) currently under development in the inner layer could enable this movement.
- 309 • Innovative and efficient processing through intensification that can significantly reduce the  
310 energy and resource demand are concepts that are already developed (Tian et al. 2019), but their  
311 industrial implementation need to increase. Process intensification is a promising technology that  
312 can lead the way towards more sustainable process alternatives.

- 313
- 314
- 315
- 316
- 317
- 318
- 319
- 320
- Better management of sources of energy in terms of harvesting, storing and using renewable sources of energy is necessary. Electrification by taking advantage of intermittent renewable energy sources, such as solar and wind; energy storage in the form of chemicals can contribute to balancing supply and demand if chemical processes could be run even periodically. In this context electricity storage in the form of chemical bonds (hydrogen, ammonia, methanol, and dimethyl-ether) is an opportunity and a challenge. Another option is to consider transformation of chemical and electrical energy not only for fuel cells but also for innovative alternatives such as redox flow batteries.

321

322 In the core layer, the constraints from the middle layer and desires (targets) of the outer layer require  
323 fundamental research results from the core layer, for example (not listed in any priority):

- 324
- 325
- 326
- 327
- 328
- 329
- 330
- 331
- 332
- 333
- 334
- 335
- 336
- 337
- 338
- 339
- 340
- 341
- 342
- 343
- 344
- 345
- 346
- Conversion of raw materials through chemical- and/or bio-catalysis using new synthesis paths, which can give important commodity chemicals at reduced energy and/or increased atom efficiency should always have high priority. For example, use of green electrons in electro-chemical conversion of water, CO<sub>2</sub>, and N<sub>2</sub> into fuels and base chemicals like hydrogen, carbon monoxide, methanol, di-Methyl-ether, light olefins and ammonia (Van Geem et al. 2019).
  - Separation principles that can discover new ways to separate chemicals from difficult separation problems at reduced and/or low energy consumption, high separation efficiency, minimal use of external separating agents that are energy intensive, and/or extract important new ingredients from plants or biomass should continue to attract attention of researchers. Combining more than one separation technique into hybrid operations where each technique performs at its highest efficiency is an option worth investigating.
  - Selection and design of functional materials that can have a reduced maintenance or replacement requirements, substitute the function of multiple materials and/or address any un-satisfied need of the outer layer (Cheng et al., 2011) are important for discovery of new processing routes and/or separation principles. Use of ionic liquids as environmentally acceptable separation agents and MOFs (Metal Organic Frameworks) and COFs (Covalent Organic Frameworks) for gas separations are alternatives worth investigating along with membranes.
  - Better understanding of the phenomena and the domain system involving complex chemical and biochemical systems is necessary to develop more comprehensive modelling of the process (Klatt and Marquardt, 2009) and the associated properties of chemicals and materials. Of particular interest are the modelling of properties of structured products, solids and polymers; multiphase operations with complex chemical systems, such as electrolytes; as well as the complexity of living systems and the difficulties in understanding them.

347

#### 348 *Practice*

349 Fundamentally, industry rewards and exemplifies the benefits of C&BE by translating the discipline to  
350 value – and offering interesting and challenging careers to motivated individuals who pursue employment  
351 in the field. The mechanism for such value creation is exemplified in the various layers of Figure 1,

352 starting with the outer layer: *identifying* which grand challenges it needs to address to *achieve* sustainable  
353 industrial development and thereby, improving circularity. Industry is ideally placed to do so by drawing  
354 on the skills from the inner layers, since it will have the economic and ecological insights and remit to  
355 ensure that important technologies are adopted in economically viable ways, thereby ensuring sustainable  
356 development. The combination of science and engineering to help develop commercially successful  
357 technology, in a sense, is the very definition of industry's remit, in addition to maintenance of its existing  
358 operations. To achieve this goal, at the innermost layer, skills such as handling of resources, feasibility  
359 of products, economic feasibility, etc., will need to be developed. In doing so, industry will of course  
360 link to both academic and government institutions to: a) set developmental challenges; b) identify  
361 collaboration opportunities to make efficient use of limited resources; c) encourage transfer technology;  
362 d) identify and share the capability challenges needed by practicing C&B engineers. It is also important  
363 to point out that in the next decades, increasing industry-industry partnerships are to be expected as well,  
364 especially in supply chain, mirroring the need for a greater set of organizational relationships within any  
365 company. The demand from the world's ever-growing population is towards more socially responsible  
366 corporations, which may be a factor that should be considered by the players from the industrial sectors.

367  
368 Table 1 lists forms of industrial practice in terms of what they do or use, what they need or consume and  
369 what they give to society or results. It can be noted that the different types of industrial practices are  
370 connected to each other. That is, the result (what they give) from one layer is used as input by another.  
371 The manufacturing companies will produce products that society needs using technologies developed by  
372 engineering companies and where equipment designed-developed by equipment companies are  
373 employed. Also engineering companies use tools developed by software companies as well as research  
374 results from academia. The services of consulting companies are needed by all other companies. The  
375 objective for all of them, however, should be to achieve sustainable development and/or circularity.

376  
377 Several routes could be followed in order to achieve the above objectives. C&BE subject to constraints  
378 (recycling and re-use of matter and energy, sustainable and safe processes, intelligent and personal  
379 products, full techno-commercial evaluations including real-world issues like tax laws, environmental,  
380 health and safety regulations) implies a top-down approach, which points to upstream scientific and  
381 technological developments. In a complementary way, a bottom-up research could also be considered  
382 for methodological and paradigm developments, in order to tackle the future challenges. Innovation will  
383 be the result from both approaches. To encourage diversity, gender issues must also be tackled.

384  
385  
386

387 Table 1: Forms of industrial practice and their activities

Practice form (type of company)	What they do or use	What they need or consume	What they give to society or results
Manufacturing	Apply production technologies	Resources (material, utility, human-power)	Manufactured products that society needs
Engineering	Use technics, methods, data	Resources (human-power)	Production technologies for manufacturing
Equipment	Design-develop production equipment	Resources (material, utility, human-power)	Equipment for manufacturing industry
Software	Develop knowledge (theory, concepts) based tools	Resources (human-power)	Tools with implemented methods and data
Consulting	Solve problems using the needed data, methods & tools to help apply-develop technologies	Resources (human-power), knowledge (theory, concepts, data)	Problem solutions (technology, methods, tools)

388

389

390

### Perspectives

391

The scope and significance of C&BE is enormous and it is not the objective of this article to provide a comprehensive list. However, perspectives on a few selected topics that we think have attracted current attention and could also be important in future are discussed briefly. It is important to note that the way in which industrial plants are built and operated in the C&BE sector is changing due to concepts such as disposable reactors and micro reactors (Roberge et al., 2008) allowing far more flexibility in the manufacturing process. Conversion of batch to continuous processing is steadily becoming more routine. Combining these concepts with the emerging fields of 3-D printing and functional materials allow for smart manufacturing practices to be established. Moreover, the influence of industry 4.0 (Kolberg and Zühlke, 2015), which encapsulates concepts of big data and artificial intelligence is changing the goal post of efficient process operations (Piccione, 2014). Figure 4 shows the engineering challenges in the next 10 years. According to this figure the relevance of various digital applications (model-based approaches) today and in 2025 are demonstrated with a score showing how they will become more important in the coming years (Keller, 2018). Specific activities to help bridge chemical engineering and data science are available (Piccione, 2019).

405

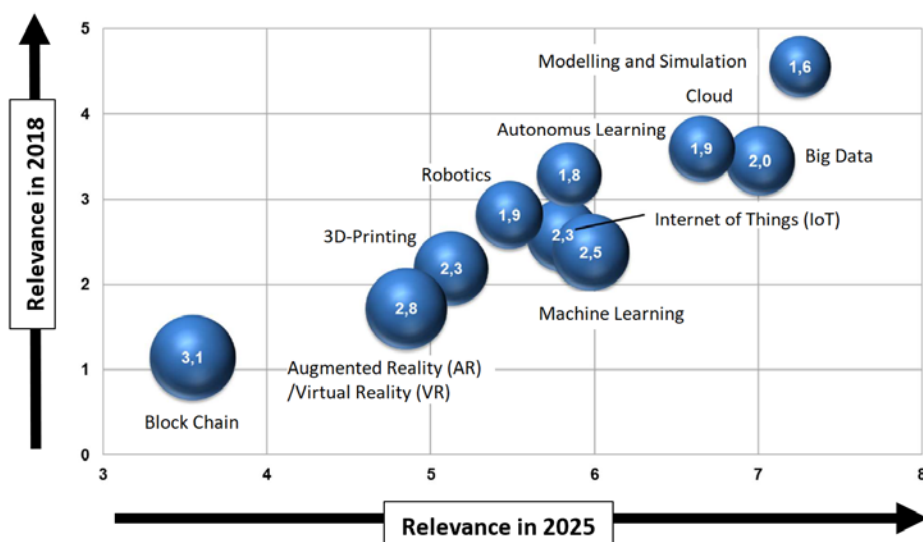


Figure 4: Industry 4.0 relevance in the next 10 years (Keller, 2018)

406  
407  
408

Likewise, digitalization has been an integral part of C&B development in the past decades be it the use of “digital” process controls as opposed to “pneumatic” controls; the development of process simulations; process synthesis and other tools in the domain of process systems engineering (PSE). These developments are now part of the standard set of “tools” that C&B engineers use routinely in their day-to-day work. With computing power still doubling roughly every few years, as predicted by Moore’s law (Schaller, 1997), the speed and reliability of PSE methods & tools continue to improve, allowing C&BE engineers to solve problems of increased complexity at higher fidelity in real time. In addition, Industry 4.0 and the big data concepts are becoming ever more prominent in the domain of C&BE. (Venkatasubramanian, 2019; Piccione, 2019).

418

The perspectives of C&BE are highlighted through the following two issues and their discussions in terms of opportunities and challenges.

421

422 ***Current scope & significance of C&BE***

423

424 *Products and their manufacturing processes (core)*

425 The main questions here (related to chemicals-based products) are what to make, when or why to make  
426 it and how to make it? The first two questions are related to the products and the last question is related  
427 to the associated process. Even though the chemicals-based products and their manufacturing processes  
428 are related, the education, research and practice do not always address the same issues. Using the  
429 classification of chemical products by Cussler & Moggrige (2001), Table 2 highlights the main reasons.  
430 It can be noted that until recently, most of the C&BE activities were focused on the production of  
431 commodity chemicals where process is the key. With the expansion of C&BE to molecular and functional

432 products and chemicals-based devices, the scope and significance of C&BE education, research and  
433 practice related to products and their sustainable processes have also increased.

434

435 Table 2: Types of chemicals-based products and their characteristics (adapted from Cussler &  
436 Moggridge, 2001)

Characteristics	Product types		
	Commodity-based	Molecule-based	Microstructure-based
Key issue	Cost	Speed	Function
Basis for success	Unit operations	Chemistry	Microstructure
Risk of failure	Feedstock	Discovery	Science

437

438

439 Other issues that could also play a major role in defining the scope and significance of C&BE are briefly  
440 highlighted below:

- 441 • The challenge is to design and develop novel and innovative chemical products of better quality  
442 and longer durability and the opportunity is the need for these products some of which can be  
443 developed through integrated experiment and model-based techniques, leading to reduction in time  
444 and cost in their development (Liu et al., 2019; Zhang et al., 2018).
- 445 • Interest in bio-based economy through new bio-catalytic processes converting biomass to valuable  
446 raw materials is increasing rapidly (van Dam et al., 2005). Direct biological production through  
447 genetically modified cells and protein engineered enzymes is showing promise, while, combined  
448 hybrid biochemical and chemical transformations continues to be attractive (Davy et al., 2017;  
449 Sanford et al., 2016; Woodley 2019).
- 450 • The separation and conversion of by-products needs to be strengthened, in particular, in bio-based  
451 productions with inspiration from traditional chemical engineering processes. Also, the  
452 introduction of intensified process designs and the introduction of separation technologies to  
453 capture secondary by-products of value which are currently discarded, need to be considered  
454 (Atasoy et al., 2018).

455

#### 456 *Resources (middle)*

457 The main questions to ask here are which resources to use, for what purpose and how sustainable are  
458 they? Not counting the manpower resources, as Figure 5 highlights, C&BE uses two types of resources  
459 – a) those that are converted to useful chemicals-based products through a specific processing route, for  
460 example, crude oil or biomass; and b) those that are needed to operate the processing routes, for example,  
461 energy (fossil fuel, solar, wind-power, etc.), water and material (metals, catalysts, solvents, etc.). Choice  
462 of the processing route and the form of resource are important issues (see below) that are the subject of  
463 much research, but not so much in education and practice. There is actually a third type of resources –  
464 the human resource, the development of which is related to education and their use is related to practice.

465



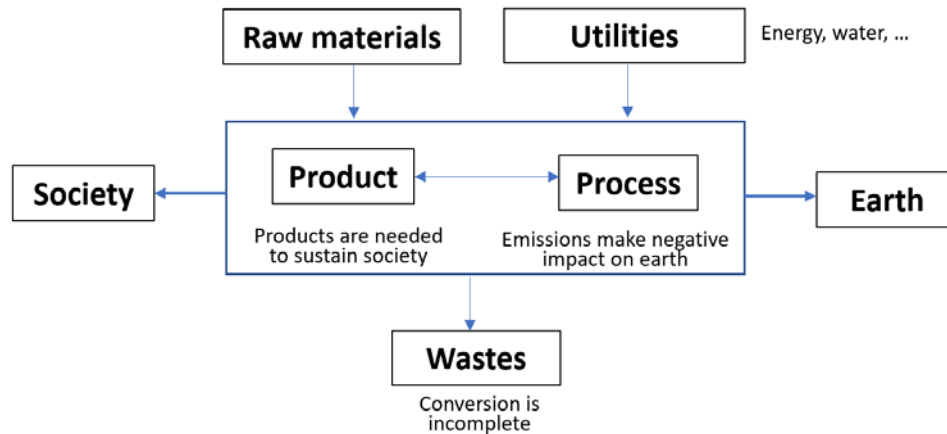


Figure 5: Use of resources by C&BE

466  
467  
468

Other issues that could also play a major role are briefly highlighted below:

470  
471  
472  
473  
474  
475  
476  
477  
478  
479  
480  
481  
482  
483  
484  
485  
486  
487  
488  
489  
490

- Fundamental transition from fossil to alternative sources of energy over the next decades through increased use of green energy sources and increased energy efficiency has started (Dresselhaus and Thomas, 2001). Moreover, the improvement of energy usage through a combination of renewable and non-renewable resources need to be further investigated (Agrawal et al. 2019) in particular the storage and management of energy. Since the global energy and mobility still rely on oil derivatives, the efficient usage of these resources through the introduction of hybrid technologies or the complete elimination of its use in some sectors (such as automobile industry) will allow the remaining resources to be stretched (Ediger et al., 2007).
- Even though competition for existing material and energy resources would remain, the supply chain issues related to water will need to be carefully monitored. The management of water resources through designing processes to be water efficient and recovery of water through recovery technologies implicitly as a part of the engineering process design (Glieck, 2016). Opportunities for environmentally efficient acquisition of materials such as rare earth metals and their efficient use, recovery and recycle needs to be investigated (Binnemans et al., 2013).
- The efficient cultivation of food and livestock, which enable the reduction of need for limited arable land available and the development of technologies to reduce the food waste through targeted application of process and materials technologies (Kummu et al., 2012). In parallel, analytics should play an increasing role in mapping occurrences of unwanted trace chemicals in our food and environment (for example, air and water) combined with their adverse health effects, which in turn, puts increasing demands on product formulation and their production process.

*Societal (outer)*

492  
493

Based on Figure 5, the following question could be asked – is C&BE addressing the challenges related to climate change, energy, water and food or is it adding to the problem? Surely, as the Barcelona

494 Declaration from 2017 (Negro et al., 2018) outlined, we all have the responsibility to address these  
495 challenges. Some notable developments are highlighted below:

496

- 497 • Strong demand for renewable energy sources and storage technology is an area of active interest  
498 to the society and must be addressed. This also means the adaptation of potential renewable energy  
499 technologies as well as storage technologies, which would benefit from government subsidies as  
500 well as support from the public, making their implementation easier.
- 501 • Health-care demands new advanced instrumentation and materials, and the push for a bottom-up  
502 approach for improved early diagnosis and treatment of disease (Aguado et al., 2018). This push  
503 can also be used in moving from a treatment oriented medical system to a predictive and precision-  
504 based early diagnostic system to allow the move towards prevention based medical systems. Here  
505 model-based approaches and data-driven tools developed within PSE discipline can facilitate  
506 future developments.
- 507 • Sustainable production and distribution of food and other products becomes very important (Validi  
508 et al., 2014), especially considering the steady increase of the human population and the scarcity  
509 of resources in general. This has knock-on effects on energy usage, water usage as well as land  
510 usage. To this end from a societal point of view the holistic and complete management of the Water  
511 – Energy - Food nexus as well as the efficient management of land usage would be important.

512

### 513 ***Future scope & significance of C&BE***

514

#### 515 *Improvements of processes based on current needs*

516 Energy related issues will continue to dominate research and development with C&BE (Vooradi et al.  
517 (2018). New routes to fuels, fine chemicals and pharmaceuticals that are all based on ‘green’ feedstocks  
518 would contribute to tackling the grand challenges of energy, water, food and environment. Waste and its  
519 hazards would also be minimised. Therefore, there is a need for systematic identification of optimal  
520 processing pathways that lead to more sustainable production processes and supply chains (You et al.,  
521 2012). Achieve a state of clean, zero-waste producing processes in operation. The topics that could also  
522 play a major role are highlighted below:

523

- 524 • Intensification of chemical and biochemical processes will provide the means to develop novel  
525 more sustainable process alternatives (Stankiewicz and Yan 2019). However, issues related to  
526 design and control of such multi-functional unit operations need to be addressed at different levels  
527 of aggregation, i.e., phenomena, task and unit operations levels through systematic approaches that  
528 allow identification of novel intensified alternatives (Tula et al. 2019). Rapid developments in lab-  
529 on-a-chip technology could lead to (micro/nano) sensors and measuring devices as well as high-  
530 speed analysis methods for single cell genomics, transcriptomic, and proteomics.

- 531 • New reactor concepts, and designs controlling reactions in space and time will lead to increased  
532 productivity, reduced waste, lower environmental impact and lower cost of manufacturing (Hessel  
533 et al., 2013). In this essence, combining flow chemistry approaches with PSE methods and tools  
534 could lead to interesting new developments. In this combined mind-set, flow chemistry and  
535 microchemistry would allow developments in reaction engineering, while PSE methods and tools  
536 would reduce the time, cost and resources for experiments by systematically reducing the search  
537 space of alternatives to be tested through a model-based approach. The routine availability of  
538 continuous manufacturing approaches for many unit operations and their integration could lead to  
539 additional flexibility operational flexibility.
- 540 • Multi-scale modelling and optimization of phenomena from atomic scales into unit operations and  
541 supply chain management with side-by-side modelling and experimentation approaches need to  
542 play a leading role. In this context, for example, computational chemistry can be used to bring  
543 understanding at molecular level and assist in developing new products. This can be used to reliably  
544 develop new unit operation concepts for production and supply chains for distribution of such novel  
545 products. Thereby, reducing the experimental costs and efforts and leading towards a more rapid  
546 product development from concept to implementation. However, solving such problems requires  
547 development of innovative solution strategies in line with advances in computer science.

548

549 *Development of processes for future needs (products)*

550 Energy will continue to play an important role in the development of processes for the future. Energy  
551 demands and how they are supplied through sustainable conversion and storage technologies, such as the  
552 combination electrolyzers/fuel cells and new battery technologies with regard to large scale battery  
553 implementation to store renewable energy generated (for example, Redox flow batteries) will attract  
554 much attention, including the storage of large amounts of energy. The topics that could also play a major  
555 role are highlighted below:

- 556 • New catalysts and technologies for enabling high-efficiency materials production, for example the  
557 development of direct process pathway to convert hydrogen peroxide to propylene oxide  
558 technologies, which was in principle enabled through the development of a new catalyst and related  
559 process technologies. In addition, recent developments in electrified methane reforming for greener  
560 industrial hydrogen production seem to be very promising (Wismann et al., 2019). Smart material  
561 assembly through molecular control will be a critical enabler for this theme.
- 562 • Recovery/recycling of used product as precursor or source of raw material, which allows the  
563 realization of the zero-waste objective of circular economy (Geissdoerfer et al., 2017).  
564 Development of processes, approaching the ‘zero-waste’ target at minimum energy consumption  
565 (Straathof et al 2019). Use the concept of atomic economy in the development of new processes  
566 and in the re-design of existing technologies. Re- thinking processes based on the concept of  
567 circular economy, not only raw materials and products but also equipment and energy supply.
- 568 • Computational science to enable more developments of *in silico* techniques leading to “quality by  
569 understanding” of products and processes that rely on detailed, scalable quantitative descriptions.

570 In a related vein, sustainability requirements, especially with respect to environmental impact, keep  
571 increasing. It will be important to come up with frameworks that can be flexibly and quickly  
572 adapted in optimization methods.

- 573 • New manufacturing and associated field techniques will be required to realize the potential of  
574 personalized health care. Electrochemical technologies which avoids the use of reagents to oxidize  
575 or reduce a raw matter and change them by electricity, avoiding the formation of undesirable by-  
576 products and/or wastes. Nature inspired approach to reactor and catalysis engineering (Coppens  
577 2012) and more nature inspired chemical engineering leading to new design methodologies for  
578 sustainability (Trogadas and Coppens 2020) point to exciting new developments. A major  
579 challenge and opportunity here are to understand and learn from the living systems to develop these  
580 new and innovative design methodologies.

581

### 582 *Sustainable technologies*

583 Circular economy requires or is completely engaged and linked with circular engineering, especially to  
584 meet the societal grand challenges. In future, instead of using the concept of circular economy, it could  
585 be more relevant or appropriate to use the concept of the circular economy-engineering (especially in our  
586 case, the circular economy-C&BE).

587

588 The topics that could also play a major role are highlighted below:

- 589 • CO<sub>2</sub> management including capture, conversion, utilization and storage, new (catalytic)  
590 chemistries, which can be integrated with concepts such as CO<sub>2</sub> management. These concepts  
591 control the chemical reaction pathways at molecular level, aiming at 100% atom efficiency and  
592 zero waste. This could be aided by converting by products such as CO<sub>2</sub> into secondary products or,  
593 or by transforming it into carbonates with later deep storage to prevent its accumulation on the  
594 surface of earth, provided no adverse effects are caused by the deep storage.
- 595 • Feedstocks management, in particular, use of biological feedstocks through a combination of  
596 techniques - recycling of (communal) wastes and conversion of complex biomass feedstocks into  
597 chemicals, purification and desalination technologies for drinking water supply and recyclable  
598 construction materials (building, cars, etc.), to name a few, need to be studied (Clomburg et al  
599 2017; Sheldon 2014).
- 600 • Energy management, such as affordable, robust, sustainable-across-the-entire-lifecycle solar  
601 power as probably the only likely long-term sustainable energy source for humanity needs more  
602 attention. At the same time sustainable management of all energy sources for optimal demand-  
603 supply of energy should be incorporated with concepts such as circular economy, smart  
604 manufacturing and zero-emission.
- 605 • Water management, in particular, supply and distribution of water for different needs and  
606 applications, such as, water that is safe for drinking, water for washing-cleaning, water for  
607 industrial manufacturing, water for heating-cooling and many more, needs urgent attention. While  
608 there is an abundance of water on earth, this availability is not uniform geographically and requires

609 further processing before use. Therefore, new technologies for energy efficient water treatment,  
610 reduction of fresh water demand, etc., allowing better management of water resources are needed.

611

## 612 **Conclusions**

613

614 Because of their broad interdisciplinary knowledge and their key role in developing, operating and  
615 managing the industrial pillars of society as well as their professional link to many sectors, chemical and  
616 biochemical (C&B) engineers are in a pivotal position to help society shape a sustainable future. As  
617 professional experts and active responsible citizens, they can provide guidance, information and  
618 leadership to a society that has to meet the grand challenges of this century. Their expertise will be an  
619 essential contribution to the necessary interdisciplinary effort that includes all actors of society. C&B  
620 interdisciplinary and multidisciplinary engineers are in a pivotal position to help society shape a  
621 sustainable future with the zero-waste and minimum energy consumption objectives of circular economy.  
622 They will be engaged in the future, in the design of the factory of the future with the use of industry 4.0  
623 technologies to improve manufacturing operations by reducing resources and energy usage and improved  
624 production, thus leading to the design of sustainable technologies, that is, circular economy-engineering.

625

626 An important immediate activity is to define the grand challenges that society faces now, and hence to  
627 identify the main opportunities for C&BE. C&B engineers can exploit their services in education,  
628 industry or government to serve society – whether by finding sustainable (economic, social, ecologic)  
629 and/or technical solutions to the grand societal challenges; safeguarding the industrial economic base  
630 (products, processes, jobs) in competition with other regions and their geopolitical difference; or by  
631 promoting good engineering sense in the evaluation of new opportunities and challenges. By raising the  
632 recognition of the value engineers bring to society, young people will be motivated and encouraged to  
633 study and practice C&BE. Their conceptualization skills across many disciplines and ability to break  
634 problems down into unit operations and physicochemical processes will be sure to be value adding.

635

636 As experts in the management of mass flows, energy efficient operations as well as the management of  
637 supply chains and the interactions between man and nature the impact of C&B engineers should not be  
638 restricted to shaping a sustainable industrial system, but should reach far into planning and implementing  
639 future smart cities and regions as well as providing strong support to the health care of the future. They  
640 should be in a position to influence the decision makers as well as help make important decisions on  
641 issues such as education policy, research directions, environmental and safety regulations, resources  
642 management and many more. It should be noted that while techno-economic solutions can be found to  
643 make a desired product and its manufacturing process more sustainable, unless the decision makers  
644 restrict the demand or production rate, the product might still become unsustainable because of increased  
645 consumption and consequent depletion of resources.

646

647 Finally, we hope we have given a global view of C&BE, which the reader may interpret differently at  
648 specific geographical locations. We expect the educators and practitioners of C&BE to use the multi-  
649 layered view to find the balance of topics at each level that suits best their particular needs and  
650 background at their geographical location.

651  
652

## 653 **References**

654

- 655 Agrawal, R., 2019, Chemical Engineering for a Solar Economy, *Chemical Engineering Science* 210,  
656 115215. doi: 10.1016/j.ces.2019.115215
- 657 Aguado, B.A., Grim, J.C., Rosales, A.M., Watson-Capps, J.J., Anseth, K.S., 2018. Engineering  
658 precision biomaterials for personalized medicine. *Science Translational Medicine* 10, eaam8645.  
659 doi:10.1126/scitranslmed.aam8645
- 660 Allen, M.R., O.P. Dube, W. Solecki, F. Aragón-Durand, W. Cramer, S. Humphreys, M. Kainuma, J.  
661 Kala, N. Mahowald, Y. Mulugetta, R. Perez, M. Wairiu, and K. Zickfeld, 2018: Framing and  
662 Context. In: *Global Warming of 1.5°C. An IPCC Special Report on the impacts of global warming  
663 of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the  
664 context of strengthening the global response to the threat of climate change, sustainable  
665 development, and efforts to eradicate poverty* [Masson-Delmotte, V., P. Zhai, H.-O. Pörtner, D.  
666 Roberts, J. Skea, P.R. Shukla, A. Pirani, W. Moufouma-Okia, C. Péan, R. Pidcock, S. Connors,  
667 J.B.R. Matthews, Y. Chen, X. Zhou, M.I. Gomis, E. Lonnoy, T. Maycock, M. Tignor, and T.  
668 Waterfield (eds.)].  
669 [https://www.ipcc.ch/site/assets/uploads/sites/2/2019/05/SR15\\_Chapter1\\_Low\\_Res.pdf](https://www.ipcc.ch/site/assets/uploads/sites/2/2019/05/SR15_Chapter1_Low_Res.pdf)
- 670 Atasoy, M., Owusu-Agyeman, I., Plaza, E., Cetecioglu, Z., 2018. Bio-based volatile fatty acid  
671 production and recovery from waste streams: Current status and future challenges. *Bioresource  
672 Technology* 268, 773–786. doi:10.1016/j.biortech.2018.07.042
- 673 Binnemans, K., Jones, P.T., Blanpain, B., Van Gerven, T., Yang, Y., Walton, A., Buchert, M., 2013.  
674 Recycling of rare earths: a critical review. *Journal of Cleaner Production* 51, 1–22.  
675 doi:10.1016/j.jclepro.2012.12.037
- 676 Brunaud, B., Laínez-Aguirre, J.M., Pinto, J.M., Grossmann, I.E., 2019. Inventory policies and safety  
677 stock optimization for supply chain planning. *AIChE Journal* 65, 99–112. doi:10.1002/aic.16421
- 678 Butz, P., Tauscher, B., 2002. Emerging technologies: chemical aspects. *Food Research International*  
679 35, 279–284. doi:10.1016/S0963-9969(01)00197-1
- 680 Charpentier, J., 2003. The Future of Chemical Engineering in the Global Market Context : Market  
681 Demands versus Technology Offers. *Kem. Ind.* 52, 397–419.
- 682 Christensen, C.H., Rass-Hansen, J., Marsden, C.C., Taarning, E., Egeblad, K., 2008. The Renewable  
683 Chemicals Industry. *ChemSusChem* 1, 283–289. doi:10.1002/cssc.200700168
- 684 Chu, S., Majumdar, A., 2012. Opportunities and challenges for a sustainable energy future. *Nature* 488,

685 294–303. doi:10.1038/nature11475

686 Clomburg, J.M., Crumbley, A.M., Gonzalez, R., 2017. Industrial biomanufacturing: The future of  
687 chemical production. *Science* 355, aag0804. doi: 10.1126/science.aag0804

688 Cordiner, J.L., 2004. Challenges for the PSE community in formulations. *Computers & Chemical*  
689 *Engineering* 29, 83–92. doi:10.1016/j.compchemeng.2004.07.024

690 Coppens, M. O., 2012, A nature inspired approach to reactor and catalysis engineering, *Current*  
691 *Opinion in Chemical Engineering*, 1(3), 281-289.

692 Cussler, E.L., Moggridge, G.D., 2001. *Chemical Product Design*. USA: Cambridge University Press.

693 Davy, A.M., Kildegaard, H.F., Andersen, M.F., 2017. Cell factory engineering. *Cell Systems* 4, 262-  
694 275. doi: 10.1016/j.cels.2017.02.010

695 Dresselhaus, M.S., Thomas, I.L., 2001. Alternative energy technologies. *Nature* 414, 332–337.  
696 doi:10.1038/35104599

697 Ediger, V.Ş., Hoşgör, E., Sürmeli, A.N., Tatlıdil, H., 2007. Fossil fuel sustainability index: An  
698 application of resource management. *Energy Policy* 35, 2969–2977.  
699 doi:10.1016/j.enpol.2006.10.011

700 Forte, G., Albano, A., Simmons, M.J.H., Stitt, H.E., Brunazzi, E., Alberini, F., 2019. Assessing  
701 Blending of Non-Newtonian Fluids in Static Mixers by Planar Laser-Induced Fluorescence and  
702 Electrical Resistance Tomography. *Chemical Engineering and Technology*, 42(8), 1602-1610.

703 Geissdoerfer, M., Savaget, P., Bocken, N.M.P., Hultink, E.J., 2017. The Circular Economy – A new  
704 sustainability paradigm? *Journal of Cleaner Production* 143, 757–768.  
705 doi:10.1016/j.jclepro.2016.12.048

706 Gleick, P.H., 2016. Water strategies for the next administration. *Science*. doi:10.1126/science.aaj2221

707 Glindkamp, A., Riechers, D., Rehbock, C., Hitzmann, B., Scheper, T., Reardon, K.F., 2009. Sensors in  
708 Disposable Bioreactors Status and Trends. In: Eibl R., Eibl D. (eds) *Disposable Bioreactors.*  
709 *Advances in Biochemical Engineering / Biotechnology*, vol 115. Springer, Berlin, Heidelberg.  
710 doi:10.1007/10\_2009\_10

711 Grossmann, I., 2005. Enterprise-wide optimization: A new frontier in process systems engineering.  
712 *AIChE Journal* 51, 1846–1857. doi:10.1002/aic.10617

713 Hessel, V., Kralisch, D., Kockmann, N., Noël, T., Wang, Q., 2013. Novel Process Windows for  
714 Enabling, Accelerating, and Uplifting Flow Chemistry. *ChemSusChem* 6, 746–789.  
715 doi:10.1002/cssc.201200766

716 Hill, M., 2004. Product and process design for structured products. *AIChE Journal* 50, 1656–1661.  
717 doi:10.1002/aic.10293

718 <http://www.engineeringchallenges.org/challenges.aspx>

719 <https://sustainabledevelopment.un.org/>

720 Kang, H.S., Lee, J.Y., Choi, S., Kim, H., Park, J.H., Son, J.Y., Kim, B.H., Noh, S. Do, 2016. Smart  
721 manufacturing: Past research, present findings, and future directions. *International Journal of*

- 722 Precision Engineering and Manufacturing-Green Technology 3, 111–128. doi:10.1007/s40684-  
723 016-0015-5
- 724 Klatt K-U, Marquardt W., 2009, Perspectives for process systems engineering – personal views from  
725 academia and industry. *Comput Chem Eng* 33, 536–50.
- 726 Keller, W. 2018. Berufe 4.0 – Wie Chemiker und Ingenieure in der digitalen Chemie arbeiten, Berufe  
727 4.0 – Ergebnisse, White Paper, VWC.  
728 [https://www.gdch.de/fileadmin/downloads/Netzwerk\\_und\\_Strukturen/Fachgruppen/Vereinigung\\_f  
729 uer\\_Chemie\\_und\\_Wirtschaft/whitepaper\\_initiative\\_berufe\\_4.0\\_2018.pdf](https://www.gdch.de/fileadmin/downloads/Netzwerk_und_Strukturen/Fachgruppen/Vereinigung_fuer_Chemie_und_Wirtschaft/whitepaper_initiative_berufe_4.0_2018.pdf)
- 730 Kolberg, D., Zühlke, D., 2015. Lean Automation enabled by Industry 4.0 Technologies, in: *IFAC-  
731 PapersOnLine* 48 (3), 1870-1875. doi:10.1016/j.ifacol.2015.06.359
- 732 Kummu, M., de Moel, H., Porkka, M., Siebert, S., Varis, O., Ward, P.J., 2012. Lost food, wasted  
733 resources: Global food supply chain losses and their impacts on freshwater, cropland, and fertiliser  
734 use. *Science of The Total Environment* 438, 477–489. doi:10.1016/j.scitotenv.2012.08.092
- 735 Liu, Q., Zhang, L., Liu, L., Du, J., Tula, A.K., Eden, M., Gani, R., 2019. OptCAMD: An optimization-  
736 based framework and tool for molecular and mixture product design. *Computers & Chemical  
737 Engineering* 124, 285–301. doi:10.1016/j.compchemeng.2019.01.006
- 738 Monastersky, R., 2013. Global carbon dioxide levels near worrisome milestone. *Nature* 497, 13–14.  
739 doi:10.1038/497013a
- 740 Negro, C., Garcia-Ochoa, F., Tanguy, P., Ferreira, G., Thibault, J., Yamamoto, S., Gani, R., 2018.  
741 Barcelona Declaration – 10th World Congress of Chemical Engineering, 1–5 October 2017.  
742 *Chemical Engineering Research and Design* 129, A1–A2. doi:10.1016/j.cherd.2017.12.035
- 743 Papargyropoulou, E., Lozano, R., K. Steinberger, J., Wright, N., Ujang, Z. Bin, 2014. The food waste  
744 hierarchy as a framework for the management of food surplus and food waste. *Journal of Cleaner  
745 Production*. doi:10.1016/j.jclepro.2014.04.020
- 746 Pereira, H.M., Leadley, P.W., Proenca, V., Alkemade, R., Scharlemann, J.P.W., Fernandez-Manjarres,  
747 J.F., Araujo, M.B., Balvanera, P., Biggs, R., Cheung, W.W.L., Chini, L., Cooper, H.D., Gilman,  
748 E.L., Guenette, S., Hurtt, G.C., Huntington, H.P., Mace, G.M., Oberdorff, T., Revenga, C.,  
749 Rodrigues, P., Scholes, R.J., Sumaila, U.R., Walpole, M., 2010. Scenarios for Global Biodiversity  
750 in the 21st Century. *Science* 330, 1496–1501. doi:10.1126/science.1196624
- 751 Pham, T.P.T., Kaushik, R., Parshetti, G.K., Mahmood, R., Balasubramanian, R., 2015. Food waste-to-  
752 energy conversion technologies: Current status and future directions. *Waste Management* 38, 399–  
753 408. doi:10.1016/j.wasman.2014.12.004
- 754 Piccione, P.M., 2014. Industrial Reflections on Modelling of Fine Chemicals and Seeds.  
755 *Process/Product Design, Chemical Engineering Research and Design* 34, 212–224.  
756 doi:10.1016/B978-0-444-63433-7.50022-5
- 757 Piccione, P.M., 2019, Realistic interplays between data science and chemical engineering in the first  
758 quarter of the 21st century: Facts and a vision, *Chemical Engineering Research and Design*, 147,  
759 668-675.
- 760 Prausnitz, J. M., 2007, Athena, Hercules and Nausica: Three dimensions of chemical engineering in the



761 twenty-first century. *Fluid Phase Equilibria*, 261(1-2), 3-17)

762 Roberge, D.M., Zimmermann, B., Rainone, F., Gottsponer, M., Eyholzer, M., Kockmann, N., 2008.  
763 Microreactor Technology and Continuous Processes in the Fine Chemical and Pharmaceutical  
764 Industry: Is the Revolution Underway? *Organic Process Research & Development* 12, 905–910.  
765 doi:10.1021/op8001273

766 Rosen, R., von Wichert, G., Lo, G., Bettenhausen, K.D., 2015. About The Importance of Autonomy  
767 and Digital Twins for the Future of Manufacturing. *IFAC-PapersOnLine* 48, 567–572.  
768 doi:10.1016/j.ifacol.2015.06.141

769 Rossetti, I. & Compagnoni, M. 2016 Chemical reaction engineering, process design and scale-up issues  
770 at the frontier of synthesis: Flow chemistry. *Chemical Engineering Journal* 17, 296, 56 - 70.

771 Sanford, K., Chotani, G., Danielsen, N., Zahn, J.A., 2016. Scaling up of renewable chemicals. *Current*  
772 *Opinion in Biotechnology* 38, 112-122. doi: 10.1016/j.copbio.2016.01.008

773 Schaller, R.R., 1997. Moore’s law: past, present and future. *IEEE Spectrum* 34, 52–59.  
774 doi:10.1109/6.591665

775 Sheldon, R.A., 2014. Creen and sustainable manufacture of chemicals from biomass: state of the art.  
776 *Green Chemistry* 16, 950-963. doi: 10.1039/c3gc41935e.

777 Stankiewicz, AI, Yan, P., 2019, The missing link unearthed: Materials and process intensification.  
778 *Industrial & Engineering Chemistry Research* 58 (22), 9212-9222. doi: 10.1021/acs.iecr.9b01479

779 Straathof, A.J.J., Wahl, S.A., Benjamin, K.R., Takors, R., Wierckx, N., Noorman, H., 2019. Grand  
780 research challenges for sustainable industrial biotechnology. *Trends in Biotechnology* 37, 1042-  
781 1050. doi: 10.1016/j.tibtech.2019.04.002.

782 Tapp, H. S., Peyton, A. J., Kemsley, E. K., Wilson, R. H., 2003, Chemical engineering applications of  
783 electrical process tomography, *Sensors and Actuators B: Chemical*, 92, 17-24

784 Tian Y, Demirel SE, Hasan MMF, Pistikopoulos EN. 2018, An overview of process systems  
785 engineering approaches for process intensification: State of the art. *Chemical Engineering &*  
786 *Processing: Process Intensification*. 133, 160-210. doi: 10.1016/j.cep.2018.07.014

787 Trogadas, P., Coppens, M. O, 2020, Chapter 2 - Nature-Inspired Chemical Engineering: A New  
788 Design Methodology for Sustainability, In: Szekely G., Livingston A. (eds) *Sustainable Nanoscale*  
789 *Engineering*, 19-31. doi: 10.1016/B978-0-12-814681-1.00002-3.

790 Tula, A.K, Eden, M. R., Gani, R., 2020, Computer-Aided Process Intensification: Challenges, Trends  
791 and Opportunities, *AIChE Journal*, 66, e16819. doi:10.1002/aic.16819.

792 Validi, S., Bhattacharya, A., Byrne, P.J., 2014. A case analysis of a sustainable food supply chain  
793 distribution system—A multi-objective approach. *International Journal of Production Economics*  
794 152, 71–87. doi:10.1016/j.ijpe.2014.02.003

795 van Dam, J.E.G., de Klerk-Engels, B., Struik, P.C., Rabbinge, R., 2005. Securing renewable resource  
796 supplies for changing market demands in a bio-based economy. *Industrial Crops and Products* 21,  
797 129–144. doi:10.1016/j.indcrop.2004.02.003

798 Van Geem, K. M, Galvita, V. V, Marin, G. B., 2019, Making chemicals with electricity, *Science*, 364

799 (6442), 734-735

800 Venkatasubramanian, V., 2019. The promise of artificial intelligence in chemical engineering: Is it  
801 here, finally? *AIChE Journal* 65, 466–478. doi:10.1002/aic.16489

802 Vooradi, R., Bertran, M.-O., Frauzem, R., Anne, S.B., Gani, R., 2018. Sustainable chemical processing  
803 and energy-carbon dioxide management: Review of challenges and opportunities. *Chemical*  
804 *Engineering Research and Design* 131, 440–464. doi:10.1016/j.cherd.2017.12.019

805 Wang, Z., Krupnick, A., 2015. A Retrospective Review of Shale Gas Development in the United  
806 States: What Led to the Boom? *Economics of Energy & Environmental Policy* 4 (1).  
807 doi:10.5547/2160-5890.4.1.zwan

808 Wei, J., Russel, T.W.F., Swartzlander, M.W., 1979. The structure of the chemical processing  
809 industries: function and economics. McGraw-Hill, New York.

810 Wismann, S.T., Engbæk, J.S., Vendelbo, S.B., Bendixen, F.B., Eriksen, W.L., Aasberg-Petersen, K.,  
811 Frandsen, C., Chorkendorff, I., Mortensen, P.M., 2019. Electrified methane reforming: A compact  
812 approach to greener industrial hydrogen production. *Science* 364, 756–759.  
813 doi:10.1126/science.aaw8775

814 Woodley, J.M., 2019. Accelerating the implementation of biocatalysis in industry. *Applied*  
815 *Microbiology and Biotechnology* 103, 4733-4739. doi: 10.1007/s00253-019-09796-x.

816 You, F., Tao, L., Graziano, D.J., Snyder, S.W., 2012. Optimal design of sustainable cellulosic biofuel  
817 supply chains: Multiobjective optimization coupled with life cycle assessment and input-output  
818 analysis. *AIChE Journal* 58, 1157–1180. doi:10.1002/aic.12637

819 Zhang, L., Babi, D.K., Gani, R., 2016. New Vistas in Chemical Product and Process Design. *Annual*  
820 *Review of Chemical and Biomolecular Engineering* 7, 557–582. doi:10.1146/annurev-  
821 chembioeng-080615-034439

822 Zhang, L., Fung, K.Y., Wibowo, C., Gani, R., 2018. Advances in chemical product design. *Reviews in*  
823 *Chemical Engineering* 34, 319–340. doi:10.1515/revce-2016-0067

824 Wu J., Prausnitz, J. M., 2019., 110<sup>th</sup> Anniversary: Molecular Thermodynamics – An Endless Frontier  
825 *IECR*, 58, 9707-9708

826