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5 Process intensification and digital twin – the potential for the energy transition in process industries

Abstract: The work defines and discusses process intensification (PI) and digital twin (DT) as potential tools to accelerate the energy transition through their applications in the process industries. The PI technologies take advantage of innovative principles in equipment design and control to improve the physical process, while the DT offers the virtual model of the plant as an environment for production optimization. The effects of both tools on the energy transition are evaluated not only from the point of applications but also from the possibility of implementation and barriers in process industries. Although they are beneficial, the deployment of PI and DT requires not only infrastructure and capital investment but the knowledge and cooperation of different levels of plant personnel. Besides review of individual implementation, this work explores the concept of combining PI and DT which can make them the enabler of each other and bring a breakthrough in optimization of process design and control.

Keywords: digital twin; energy transition; process industry; process intensification.

5.1 Introduction

Over the course of the last years, the world has been facing many challenges at an unprecedented scale, from rapidly spreading diseases to devastating natural disasters which are tied to the global pollution and climate change. Significant transformations to cope with the new situation have happened in all aspects of society from working routine to energy usage and production methods. Therefore, sustainability and renewables are the target of the energy transition in terms of production, distribution and application. Process industries which are among the most intensive energy users require drastic changes to increase energy efficiency and reduce environmental impacts. Process systems engineering in combination with the digital transformation, known as Industry 4.0, brings the required tools such as process intensification (PI) and digital twin (DT) to transform the process industries.

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Even though there have been intensified processes since several decades, the concept of process intensification was firstly mentioned in the publication by Eastman Kodak in 1925 [1]. While the initial concept was the reduction in equipment- and plant size, it was proven that the scope of PI has been expanded far beyond the miniaturization hallmark [2]. The benefits of PI for energy production are not just smaller equipment and lower investment costs but also higher reaction rate, better product quality, reduced waste generation, improved process safety and reduced environmental burdens [3]. The advantages of PI can be found in different examples. The application of membrane reactors for biodiesel production improved the reaction rate and the purity of both biodiesel and glycerol by simultaneously removing the unreacted oil during the reaction. Without the oil impurity, the equipment and energy requirement for biodiesel purification were reduced, thus, lowering investment costs and environmental impacts [4]. In coating industry, acrylic and methacrylic monomers are widely used chemicals [5]. An economic analysis by Kiss (2018) showed that the cost of acrylate can be reduced by 43.5%, from 1350 EUR/t to 762 EUR/t, by using continuous processes with reactive distillation instead of batch processes [5]. With the development of new technologies, the potential energy saving of PI is increasing over the years. The report of Kim (2017) presents the data of energy saving by applying PI in the chemical and petrochemical industries for different countries and the world as in Figure 5.1 [6].

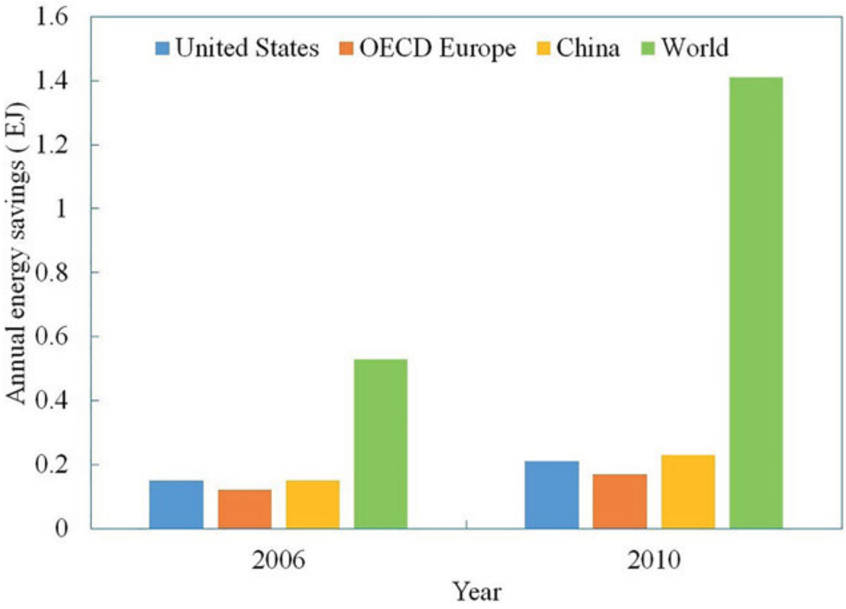

Figure 5.1: Annual energy saving of PI in the chemical and petrochemical industries (unit: EJ; 1 EJ = 1018 J) [6].

Digital twin is a fairly new concept compared to process intensification. It was introduced in a presentation of product lifecycle management by Michael Grieves at the University of Michigan in 2002 [7]. The DT was originally defined as a system including a physical object, a virtual replicant of that object and a link of data and information between physical and digital objects [7]. Since its introduction, the concept of DT has evolved rapidly and found its way into new applications and industries, for instance, supply chain management [8], shop floor management, prognostics, and health management of airplanes, monitoring and optimizing complex production processes [9]. Over the last ten years, the literature reported 46 DT definitions which combine the original concept with specific characterizations based on the applications [10]. Due to its ability to exchange data between the virtual models and physical objects, DT offers many benefits for a production process from real-time monitoring and analysis to intelligent update and management that can be applied in process design, maintenance and optimization [11]. Figure 5.2 illustrates the concept of DT for a production plant.

Even though PI and DT have different approaches, they have the similar objective of making production process more efficient and can be combined for mutual improvement. The innovative designs of PI can be further optimized by integration with more precise and up-to-date data and information from the DT. Safdarnejad (2019) proposed a novel dynamic approach for PI application which utilized the data-driven modeling of the entire production plant [12]. The data-driven approach gave similar results while having advantages of less complexity and lower costs compared to traditional gradient-based methods [12]. The improved systems of PI can bring new

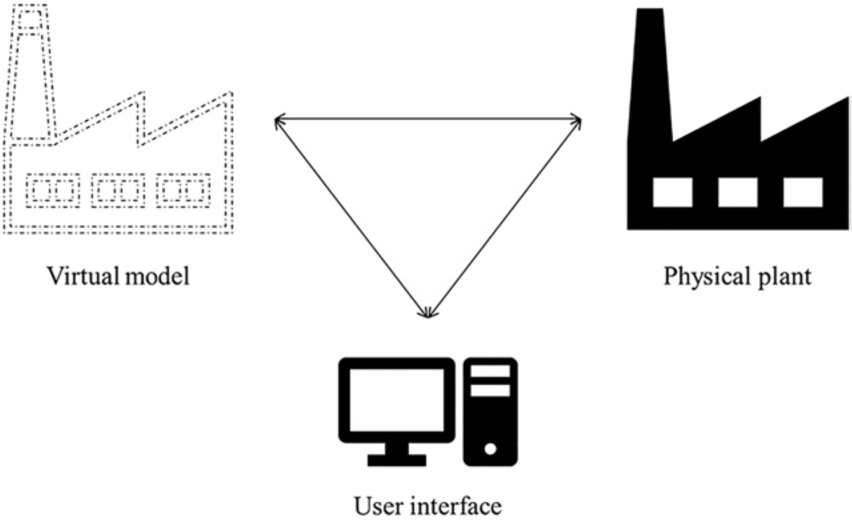

Figure 5.2: The data exchange between virtual model, physical plant and users in a DT system.

challenges for the data management and digital simulation of DT, thus, leading to improvement of sensory systems, new data processing methods and simulation programs. A combination of PI and DT will bring greater benefits in terms of production capacity, investment and operation costs, and environmental impacts for process industries which require more economic and sustainable production methods. This contribution provides a literature review of PI and DT applications and the state-of-art trends of combined concepts for the energy transition in the process industries. After the introduction in Section 5.1, more details and examples of technologies and applications relating to PI and DT in process industries are presented in Section 5.2 and 5.3. Section 5.4 discusses the benefits of combining PI and DT. Finally, Section 5.5 provides take-away messages of important topics and developments for future works.

5.2 Applications and effects of process intensification on energy transition

The European Roadmap for Process Intensification presents the potential of PI which can improve the energy efficiency in several industries as in Table 5.1 [13]. The long-term potentials of PI have attracted a lot of research interest with many reviews of recent developments and more than 12 books published since 2003 [14]. The applications of PI can be categorized as separation, reaction and separation–reaction-combined technologies.

5.2.1 Separation technologies

Distillation is the most popular separation technology in process industries, thus making it one of the best candidates for process intensification. The dividing wall column (DWC) is one of the most preferred PI technologies in commercial application [15]. Another potential PI technology based on distillation is the cyclic distillation which has been applied in industry since 2000 [16]. Other potential separation technologies are the pressure swing adsorption (PSA) and simulated moving bed (SMB)

Table 5.1: The energy efficiency increases (by percentage) over time by applying PI in different process industries [13].

	5–20 years	30–40 years
Petrochemicals	5%	20%
Pharmaceuticals	20%	50%
Food ingredients	25%	75%
Consumer foods	10–15%	30–40%

which can be intensified for process industries [15]. The potentials of PI separation technologies do not only reduce the costs, energy requirements and environmental impacts but also present very effective ways to improve product quality [15].

Since its first industrial application in 1985, the dividing wall column which is the integration of two conventional distillation columns into one shell, has more than 100 applications and will become a standard distillation tool in the near future [17]. When changing from traditional distillation columns to DWC, it offers smaller installation footprint and lower investment costs due to the reduced number of equipment units. The saving of operating costs and energy of DWC can be up to 50% as compared to conventional units [17]. Kiss et al. presented a reactive dividing-wall column design (Figure 5.3) in an industrial case study of AkzoNobel that provided up to 35% savings of investment costs and 15% savings of energy costs [18].

Besides DWC, the cyclic distillation is a potential intensified distillation process which was proposed by Cannon et al. [19]. The operation of cyclic distillation column can be described as a cycle of a vapor period (when the vapor flows upwards and the liquid is stationary) followed by a liquid period (the liquid flows down the column while the vapor is stopped) [19]. The implementation of cyclic distillation for ethanol

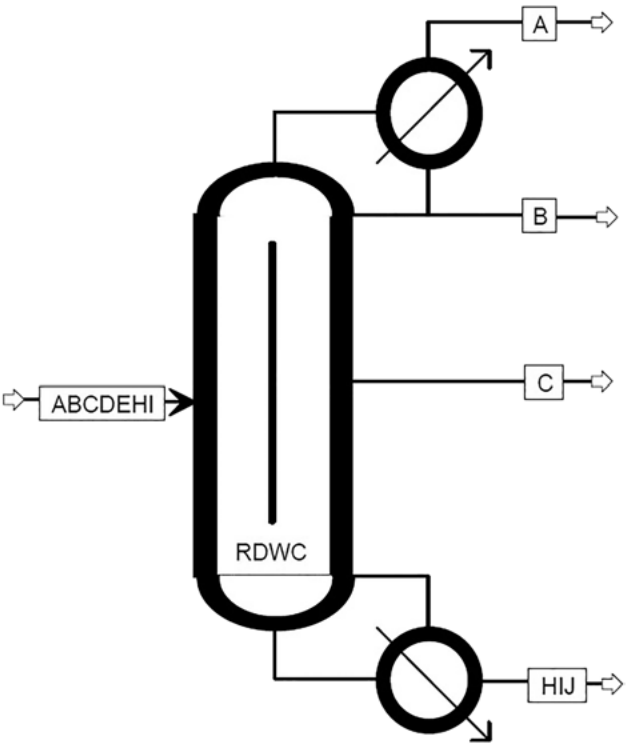

Figure 5.3: The illustration of the proposed reactive DWC [18].

production has been evaluated in Eastern Europe food industry with significant results [16]. The cyclic distillation columns requires 20–30% less energy and 1.5–2 times lower height than the traditional columns, thus greatly reducing the utility consumption and greenhouse gas emission [16].

The pressure swing adsorption is a gas separation technique based on the different adsorption forces between an adsorbent material and different components of a gas mixture [20]. It is a cyclic process of physical adsorption and desorption depending only on the gas pressure and the operating temperature [20]. PSA was mentioned in a patent in 1942 and developed widely in industry at the end of the 1960s and the beginning of the 1970s [21]. Main applications of PSA are in gas drying and purification, particularly in hydrogen production with several advantages such as high purity (up to 99.9% in case of hydrogen purification), less capital investment as well as lower energy requirement and operating costs compared to conventional technologies [22]. The twin-or multiple-bed pressure swing adsorption is popular PI choice to improve the capacity and energy-savings of gas production [23]. Marcinek et al. (2021) presented a PI study of the twin-bed PSA plant for nitrogen production with different operating strategies which can increase the productivity up to 23.9% [23].

In chromatography, the components of a mixture are separated by their adsorption and desorption at the surface of the adsorbents such as silica and alumina. One of the popular chromatographic separations in process industries is the simulated moving bed technology which was developed in 1961 by Broughton, Gerhold and Carson [24]. While the true moving bed technology requires the solid adsorbent to actually move in the opposite direction of the liquid, the operating principle of the SMB is the periodical shift in the position of inlet and out ports to create a similar effect of the counter-current flows as presented in Figure 5.4 [24]. The simulated moving bed reactor (SMBR) is a promising PI technology which found many applications in bio- and petrochemical industries [25]. For example, Shi et al. (2020) proposed a novel SMBR which used a homogeneous combination of catalyst and adsorbent to increase the yield of p-xylene about 25% and reduce the energy requirement by 19% [26].

5.2.2 Reaction technologies

The PI reaction technologies are usually called “green” chemical reactors because they bring green benefits for industrial processes such as reduced size by combination of several reactions, continuous process, improved safety and reaction rate, decrease of waste formation, etc. [28]. The industrial applications of PI reaction technologies are including spinning disc reactors (SDR), static mixer reactors (SMR), monolithic reactors and microreactors [28].

The principles of the spinning disc reactor have been developed in the 1920s and seen more application since the 1960s [29]. By generating a very thin film of liquid on the rotating surface with the centrifugal force, the SDR creates excellent heat-, mass- and

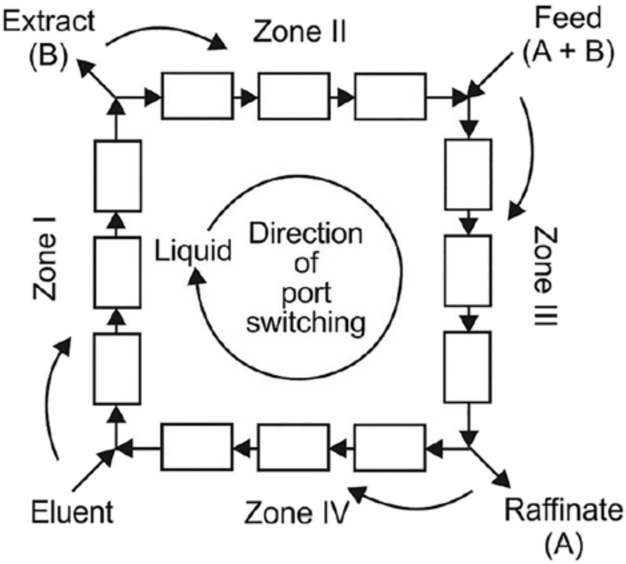

Figure 5.4: The illustration of a simulated moving bed [27].

momentum transfers between liquid and gas phases, and between the liquid and the disc surface [30]. Thus, the SDR is the ideal continuous reactor for fast reactions required gas–liquid contact and an intensive mixing environment [30]. In the processing industry, the SDR is a very high performance reactor which can improve the efficiency and economics of production processes [30]. For example, compared with traditional methods, the application of the SDR in pharmaceutical production can reduce the reaction time up to 99.97%, plant volume up to 99.21%, impurity level up to 93.33% and reaction temperature up to 6.83% [31]. An example of a large scale SDR which can be used for production up to 10 tons per day is shown in Figure 5.5 [32].

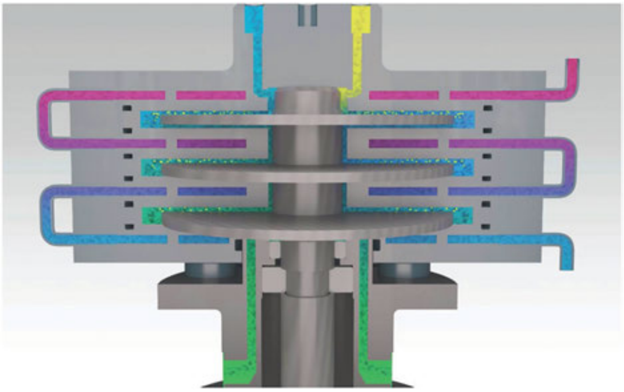

Figure 5.5: A cross section presentation of a spinning disc reactor by SPINID [32].

Although the forerunner of the static mixer reactor, a single element motionless gas mixer, was described in a patent in 1874, the reactor was not widely applied in the process industries until 100 years later [33]. The SMR has several advantages such as easily changed product types, continuous operation, smaller footprint, shorter residence time, lower equipment cost and energy requirement compared to the conventional continuous stirred tank reactor (CSTR) [33]. In a quantitative example presented by Bayer and Himmler (2005), a homogeneous mixture can be achieved with an SMR requiring only 1 kW power and 0.25 s residence time while a CSTR requires 10 kW and 1 h [34]. The continuous SMR process is commonly applied in fine chemical and polymerization plants with a 20%–25% better yield than the conventional batch type process [34].

The monolithic reactor was commonly applied for automotive exhaust gas treatment since the 1970s [35]. With a simple and robust design, the monolithic reactor is considered a potential PI replacement for the conventional packed bed reactor in catalytic gas–solid reactions [36]. The monolithic catalyst is a construction of multiple narrow straight parallel channels manufactured from ceramics or metallic components which create an ease passage for the reactant flow [37]. This design reduces the pressure drop and increases the specific surface area of the reactor, thus, improving the conversion rate per unit volume and heat and mass transfer efficiency [37]. Therefore, the monolithic reactor has smaller size and requires less energy than the conventional reactor with same capacity [37].

The research and applications of microstructure devices such as microreactors, micro-heat exchangers and micromixers became more popular since the beginning of the 1990s [38]. The first industrial application of a microreactor was in 1935 in form of the falling-film microreactor for a gas–liquid reaction [15]. The potential of upscaling a microreactor has been demonstrated in a study relating the effect of oxygen addition on water–gas shift reaction by Neuberg et al. [39]. The results showed that the pilot scale microreactor retained the performance and efficiency of the laboratory scale reactor [39]. With advantages such as excellent heat and mass transfer, a continuous process with high conversion rate, easy control and compact size, the microreactor is a potential process intensification which saves a great amount of investment and energy for chemical and pharmaceutical industries that usually apply energy intensive reactions [40].

5.2.3 Reactive separation technologies

Reactive separation technology has several definitions from different authors [41]. One of the general concepts was presented in 1967 by Balashov [41]. The concept considers that the reactive separation technology is a development of several separation and reaction processes at the same time with the target of mutual intensification, efficiency improvement and reduction of process flow sheet [41]. A notable example of the

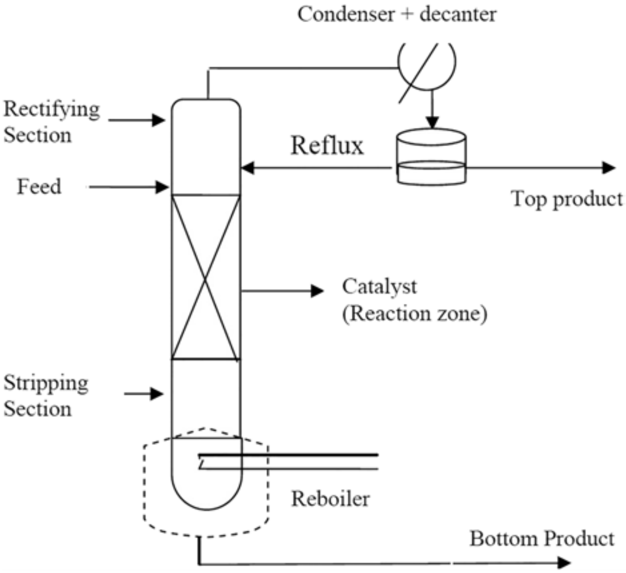

Figure 5.6: A schematic diagram of a reactive distillation column [43].

reactive separation technologies is the reactive distillation column as shown in Figure 5.6. Various strategies are applied to incorporate different separative functions into the reactor, which guarantee improvement of reaction rate and selectivity, and reduction in waste processing, equipment and energy cost [42]. A list of common reactive separation processes is given in Table 5.2.

The reactive distillation process to produce methyl acetate by Eastman Kodak is a well-known example of successful industrial reactive separation [28]. Methyl acetate is produced through the catalyzed esterification of acetic acid with methanol [28]. Due to the reversible nature of the reaction and its azeotrope products, the conventional methyl acetate production requires large amounts of reactants for high conversion rate and an energy intensive purification process to separate the products [28]. The Eastman process uses 80% less energy and only 20% investment cost of the conventional process by replacing an entire plant of reactors, distillation columns and liquid–liquid extraction with an RD column and two separation columns [28].

In conclusion, the application of PI technologies in industry is one of the key components in the EU energy transition strategy. Besides significant cost reductions, PI technologies offer great energy savings and environmental benefits for many industries, especially energy intensive ones such as chemical, oil and gas industries [28]. Dividing wall column, static mixer reactor, reactive distillation and reverse osmosis filtration are examples from many successes of PI technologies at industrial scale [28]. However, the application of PI technologies is not always going smoothly. When scaling up from laboratory to industrial level, there are several technical and non-

Table 5.2: Examples of reactive separation processes.

Process	Key features	Applications
Reactive distillation	Combination of separation and chemical reaction within a distillation apparatus where the production and removal of products are carried out simultaneously. Advantages: enhancing productivity and selectivity, consuming less energy and solvents while also keeping high efficiency of the reaction system. Disadvantages: limited application by operating constrains of both distillation and reaction, and more difficult control [44].	Synthesis of methyl acetate [42], biodiesel production [3], production of formic acid [45]
Reactive absorption	An equipment in which a selective absorption of gaseous species by liquid solutions is combined with simultaneous chemical reactions Advantages: improving the reaction conversion and the separation efficiency of absorption, capability to process gas mixtures, low thermal degradation of products. Disadvantage: higher capital investment and utility cost due to absorbent recovery units [41].	Production of nitric or sulfuric acid, treatment of industrial gases and elimination of CO_2, H_2S, ozone, and NO_x [41]
Reactive extraction	A single operating unit comprises liquid–liquid extraction and chemical reaction by adding a selective solvent to reaction zone. Advantages: higher yield and selectivity of reaction and liquid separation, lower waste generation, allowing extraction of difficult-to-separate products [41]. Disadvantages: loss of reactants because of emulsification, mixing and phase separation, technical and economic difficulties in the recovery of low concentration solutes, unsuitable for high viscous solutions [46].	Separation of carboxylic acids [47], production of renewable fuels [48]
Membrane reactors	Integration of a membrane separation into a reactor to overcome equilibrium limitations by continuously removal of reactants or products. Advantages: increasing reactor efficiency in term of productivity and purity of products, decreasing number of downstream processing units. Disadvantages: decline of production due to membrane fouling, lack of experience on equipment designing [49].	Production of biofuels, hydrogen and other basic chemical [50]

technical problems such as increasing fouling in membrane filtration, losing thermodynamics efficiency, new technologies being incompatible with existing infrastructure and the conservative of industrial management [28].

5.3 The effects of digital twin on the energy transition of the process industries

Digital twin has seen a wide range of researches and applications in many sectors, including but not limited to production, construction, aviation, education, automotive and meteorology with various scales from a single product to factories, cities and countries [51]. In the 2018 Tutzing Symposium of ProcessNet in Germany, DT was considered the foundation of digitalization and cooperation in process industries that can reduce production time, increase versatility and process efficiency [52]. Depending on its applications, the DT has different aspects and definitions [53]. The definition of DT for the applications in process industries is a set of virtual models which have a real-time connection with the physical production process and an ability of constant adaptation and update itself by getting real-time data from the physical process during its life cycle [53]. From this definition, the DT provides not just a digital replica but also abilities of control, prediction and optimization of the production process [53].

With the features as constantly updating and directly linking between the virtual model and the entire production line, one of notable DT applications in the process industries is production control. Novák et al. proposed a new production planning tool for production control by integrating a DT of a physical process into an automated planning system [54]. The real-time information of DT such as equipment states (ready, running, maintenance or failure), operating conditions (temperature, pressure), etc., enhances the speed, the flexibility and the adaptation of the production planning system [54]. The new planning tool is able to quickly reformulate a new plan in case of product change or technical failure, providing a global overview of the entire production line for further operating optimization [54].

Safety and risk management in process industries such as oil, gas and chemicals are usually considered of utmost importance [55]. The integration of DT into existing empirical process safety models can improve the process operation and safety [55]. Lee et al. proposed a concept of a “mega digital twin” model which linked different types of models with real-time data of a production process. The “mega digital twin” model was used to improve the performance of a process plant and give a depth safety and risk analysis through its entire life cycle, from design and construction to operation, maintenance, optimization and modifications, personnel development and environmental impact control [55].

Since 2018, the number of publications relating to applications of DT has increased, particularly in maintenance applications [56]. Because industrial process plants are usually enormous, complex and operating in high risk conditions, the maintenance is a crucial and costly operation to keep the plants running efficiently. The time-based or preventive maintenance which is generally based on operating experience or recommendation of equipment producers has been slowly replaced with condition-based or predictive maintenance [57]. The concept of predictive maintenance was introduced in 1975 to reduce maintenance costs by making decisions based on real-time assessments of the production process [58]. The DT is considered one of key enablers to achieve the transition from preventive to predictive maintenance by making the virtual models of equipment and production process more realistic [59]. With the constant updated models, the predictive maintenance becomes more accurate and adaptive through the life cycle of industrial process plants [59]. The integration of DT into the predictive maintenance model allows evaluation and prediction of the current- and after-maintenance states of the production process [56]. Optimized maintenance plans can reduce the operating costs, energy consumption and environmental impacts [59].

Process industries are highly susceptible to product market prices which fluctuate according to various factors including but not limited to seasonal changes, environmental policies, consumer demands and political issues. The integration of the DT into process models make them more adaptable to changes in the market due to the timely communication between the real process and the virtual model. The benefits of production optimization with the DT have been presented in several studies. The study of Min et al. presents an approach and a frame work for applying the DT in optimization of the production process in petrochemical industry which is a typical process industry(60). This study presents the DT based optimization experiment of MAYA, a Chinese refinery with capacity of multi-million tons (diesel, gasoline, LPG, propane, propylene, petroleum coke, oil slurry, naphtha,and sulphate MTBE) per year [60]. The case study results show an increase in the light oil daily yield of the refinery by 0.2–0.5% [60]. Shen et al. proposed a DT based optimization model in oil and gas industry [61]. The DT model provided a virtual environment which continuously connected the oil and gas supply capacity of oil wells with the working conditions and capacity of equipment [61]. The real time connection of different components in the production process allowed more precise prediction and control of the production capacity and energy requirements of refinery [61]. The proposed DT control model was applied to 35 oil wells which showed a reduction of daily average power consumption by 48.12 kWh and an increase of system efficiency from 11.02% to 16.43% [61].

Figure 5.7 presents search results from the website Scopus for keywords of “digital twin”, “process intensification”, combinations of “digital twin” or “process intensification” with “process industry” from 2012 to 2021. The number of publications relating to DT has increased significantly with 5860 papers. However, the applications of the DT in the process industries are still scarce and immature compared to other sectors [51]. There are several barriers for extensively applying the DT in process industries [51]. One of the main barriers can be identified as the high difficulty in application of the DT to the complexity of physical and chemical processes which are commonly used in process industries [51]. Another main barrier is the compatibility of existing industrial process plants which can be several decades old with new digital information and control systems [62]. With the exception of modern plants which are built with digital-ready designs, the investment costs for the DT in an existing plant can easily discourage most

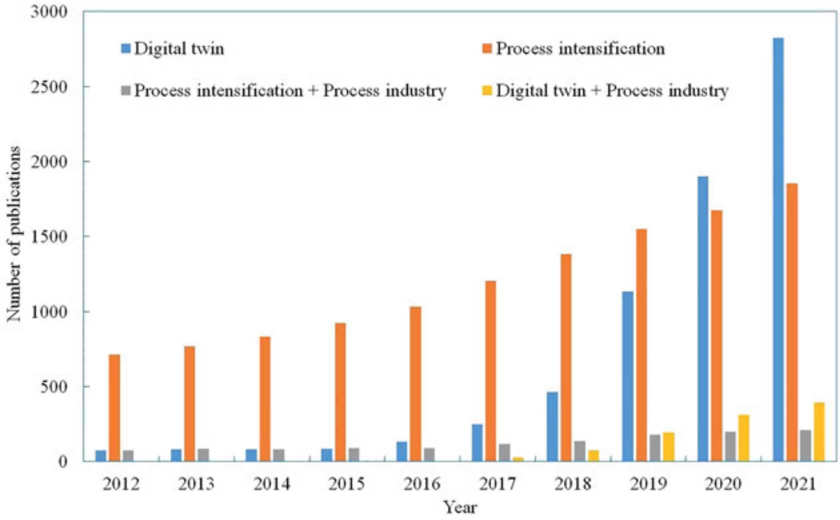

Figure 5.7: The number of publications relating to DT and PI over last 10 years.

of the plant management [62]. Therefore, the deployment methodologies of the DT are required to be innovative and adaptive with the situation of each process plant.

The DT approach for process industries is equally important as its applications. The method of DT application greatly depends on the size and state of the existing plant, the investment budget, the skills of operators and the available digital tools and data. Sierla et al. proposed a methodology of “semi-automatic generation of digital twins” for several decade old process plants or “brownfield process plants” where a large part of data was not available in digital format [62]. The method included nine steps to combine machine and human efforts in input and correction of data for setting up a DT model with reasonable investments [62]. Örs et al. presented an operational digital twin (ODT) focused on the optimization of plant operation and its generic development framework in chemical process industry [63]. The ODT was combined with artificial intelligence (AI) support to optimize the process model, schedule and control [63]. From the research, the application of AI-based ODT can improve the production flexibility and reduce the CO_2 emissions of chemical process plants [63]. Perno et al. systematically analysed the enablers and barriers and proposed a model for application of the DT in process industries [51]. The model connected the enabler with the right barrier to create a proper guidance of the DT deployment for process industry practitioners [51].

As its potential has been proven, the DT can play an important role in the energy transition of process industries. With the abilities of precise simulation and prediction, the DT can improve the design, control and maintenance plan from single equipment to entire processes. The application of DT through the lifecycle of industrial process plants increases production efficiency and reduces unnecessary costs and energy requirement.

5.4 The combination of PI and DT in process industries, a winning formula?

The barriers of PI applications in process industries can be overcome by connecting it to DT. The DT creates a virtual environment of the process plant where the PI strategies can be simulated, predicted and optimized with real-time data [64]. The effects of PI can be evaluated in the research and development phases, thus, saving the costs of prototypes and adjustments after physical implementation [64]. The analysis of a high quality DT model helps understand the chemical and physical limitations of the production process and improve PI designs [64]. With the knowledge from the DT, the need of many testing and pilot steps can be reduced during the scale-up while still ensuring the performance of PI equipment [64].

Due to the integration of two or more processes into a single equipment, operation and control are challenging issues of intensified processes [65]. With a real-time exchange between virtual model and real operating plant data, the DT is an advanced tool for control, simulation and optimization of the operating conditions of intensified equipment and production systems [65]. The high accurate simulation using the DT model allows process industry practitioners to optimize the operation and control of a PI system at the conceptual design stage [65].

López-Guajardo et al. have presented the concept of Process Intensification 4.0 which is the integration between PI, Industry 4.0 and Circular Chemistry [66]. The real-time data based simulation and prediction of the DT is identified as important tools to achieve the next generation of PI [66]. The PI 4.0 takes advantages of Industry 4.0 data-driven tools and algorithms to develop, improve and deploy innovative technologies and circular processes, thus, improving the viability of sustainable transitions in process industries [66].

The advances in PI allow the development of more sophisticated equipment and process designs, thus creating more complex physical and chemical systems. The challenges of understanding and describing high complex systems become the drive for developing advanced sensors, accurate and reliable simulation tools and updated modeling methods. These then lead to improve the depth, reliability and accuracy of the DT.

Figure 5.7 shows an upward trend in the number of PI and DT researches in process industries recently, leading to more attentions on the concept of integrating advanced computational and data-centric tools into process design, control and maintenance. Although the combination of PI and DT has been vaguely mentioned in a few publications, it is proven that process intensification can be evolved by integrating Industry

4.0 toolboxes, especially the digital twin model. Advances in process and equipment designs, intelligent technologies and big data management are applied to develop more flexible, environmentally friendly and efficient production processes.

5.5 Take-away message

The process intensification and the digital twin are potential tools to reduce the environmental impact of process industries. Besides economic benefits, they can increase the energy saving, enhance process safety and reduce unnecessary material consumption in production and equipment manufacturing. The concept of combining the PI and the DT can further improve their capabilities. The data based model and real-time data interaction of the DT and the physical process play important roles in the development of the next generation PI, which in turn has an impact on the sensory system, data management and simulation software. However, the applications of the PI and DT in process industries are not without difficulties such as lack of capital investment, insufficient skilled workforce, legacy equipment, conservative plant management, etc. Nonetheless, the deployment of PI, DT and their combination can accelerate the energy transition in process industries and the barriers can be overcome by identifying and communicating the solutions, combining different approaches and technologies, publishing new development in PI and DT openly and increasing public awareness of the impact of energy transition in process industries.

To conclude, there are important topics and future perspectives requiring our attention:

(1) The human-machine interface which gives access, details and explanation of DT knowledge to different level of industrial practitioners, from operator to supply chain manager, is a key to bring out all the knowledge of the DT. Finding a simple and effective communication method between user and virtual environment can be an important topic for DT developers.
(2) While various patented DT platforms have been developed by large companies such as IBM, Microsoft, General Electrics and Siemens [53], open-source software is a more economic option for implementing DT in small and medium size plants.
(3) The development of more effective methods to collect, process and communicate data are urgently needed because data availability is one of the key enablers for the implementation of PI and DT in process industries.
(4) In addition to DT, the combination of PI and different tools of Industrial 4.0 such as machine learning and data-driven simulation and modeling is crucial for developing more effective processes and a direction for the future chemical engineering.
(5) The energy transition in process industries requires a joint effort of different disciplines and management levels. A worldwide digital platform for sharing data and

knowledge of PI and DT can reduce costs and time of their development and application.

(6) Beyond the traditional process industries, the PI and DT can transform the production paradigm of other sectors such as renewable energy (solar, wind, biofuels, etc.), agriculture, and high-value biochemicals from microalgae. Therefore, studies to widen the applications of PI and DT are important in the long term strategy of energy transition.

References

1. Reay D, Ramshaw C, Harvey A. Chapter 1 - a brief history of process intensification. In: Reay D, Ramshaw C, Harvey A, editors. Process intensification, 2nd ed. Oxford: Butterworth-Heinemann; 2013:1–25 pp.
2. Zondervan E, Almeida-Rivera C, Camarda KV. 2. Performance products in a challenging environment. In: Product-driven process design: from molecule to enterprise. De Gruyter; 2020: 9–88 pp.
3. Kiss AA. Process intensification technologies for biodiesel production - reactive separation processes, 1st ed. Heidelberg, Germany: Springer, Cham; 2014:103 p. XV.
4. Dubé MA, Tremblay AY, Liu J. Biodiesel production using a membrane reactor. Bioresour Technol 2007;98:639–47.
5. Kiss AA. Novel catalytic reactive distillation processes for a sustainable chemical industry. Top Catal 2019;62:1132–48.
6. Kim Y-h, Park LK, Yiacoumi S, Tsouris C. Modular chemical process intensification: a review. Annu Rev Chem Biomol Eng 2017;8:359–80.
7. Grieves M, Vickers J. Digital twin: mitigating unpredictable, undesirable emergent behavior in complex systems. In: Kahlen FJFS, Alves A, editors. Transdisciplinary perspectives on complex systems. Heidelberg, Germany: Springer, Cham; 2017:85–113 pp.
8. Wang Y, Wang X, Liu A. Digital twin-driven supply chain planning. Procedia CIRP 2020;93:198–203.
9. Tao F, Zhang H, Liu A, Nee AYC. Digital twin in industry: state-of-the-art. IEEE Trans Ind Inf 2019;15: 2405–15.
10. VanDerHorn E, Mahadevan S. Digital twin: generalization, characterization and implementation. Decis Support Syst 2021;145:113524.
11. Cimino C, Negri E, Fumagalli L. Review of digital twin applications in manufacturing. Comput Ind 2019;113:103130.
12. Safdarnejad SM, Tuttle JF, Powell KM. Development of a roadmap for dynamic process intensification by using a dynamic, data-driven optimization approach. Chem Eng Process - Process Intensif 2019;140:100–13.
13. ERPI. European roadmap for process intensification. The Hague: Ministry of Economic Affairs; 2008. https://efce.info/efce_media/-p-531-EGOTEC-3ef8934e4edb103417aa50afced7096f.pdf.
14. Sitter S, Chen Q, Grossmann IE. An overview of process intensification methods. Curr Opin Chem Eng 2019;25:87–94.
15. Abdulrahman I, Máša V, Teng SY. Process intensification in the oil and gas industry: a technological framework. Chem Eng Process - Process Intensif 2021;159:108208.
16. Harmsen J, Verkerk M. 16 Intensified ethanol production by cyclic distillation. In: Process intensification: breakthrough in design, industrial innovation practices, and education. De Gruyter; 2020:176–87 pp.

17. Yildirim Ö, Kiss AA, Kenig EY. Dividing wall columns in chemical process industry: a review on current activities. Separ Purif Technol 2011;80:403–17.
18. Kiss AA, Pragt JJ, van Strien CJG. Reactive dividing-wall columns - defying equilibrium restrictions. Chem Prod Process Model 2009, https://doi.org/10.2202/1934-2659.1365.
19. Maleta VN, Kiss AA, Taran VM, Maleta BV. Understanding process intensification in cyclic distillation systems. Chem Eng Process: Process Intensif 2011;50:655–64.
20. Wiessner FG. Basics and industrial applications of pressure swing adsorption (PSA), the modern way to separate gas. Gas Separ Purif 1988;2:115–9.
21. Tondeur D, Wankat PC. Gas purification by pressure swing adsorption. Separ Purif Methods 1985; 14:157–212.
22. Fahim MA, Alsahhaf TA, Elkilani A. Chapter 11 - hydrogen production. In: Fahim MA, Alsahhaf TA, Elkilani A, editors. Fundamentals of petroleum refining. Amsterdam: Elsevier; 2010:285–302 pp.
23. Marcinek A, Guderian J, Bathen D. Process intensification of the high-purity nitrogen production in twin-bed pressure swing adsorption plants. Adsorption 2021;27:937–52.
24. Rodrigues AE, Pereira C, Minceva M, Pais LS, Ribeiro AM, Ribeiro A, et al. Chapter 1 - principles of simulated moving bed. In: Rodrigues AE, Pereira C, Minceva M, Pais LS, Ribeiro AM, Ribeiro A, et al., editors. Simulated moving bed technology. Oxford: Butterworth-Heinemann; 2015:1–30 pp.
25. Migliorini C, Fillinger M, Mazzotti M, Morbidelli M. Analysis of simulated moving-bed reactors. Chem Eng Sci 1999;54:2475–80.
26. Shi Q, Gonçalves JC, Ferreira AFP, Rodrigues AE. Simulated moving bed reactor for p-xylene production: modeling, simulation, and optimization. Chem Eng Sci 2020;225:115802.
27. Keil FJ. Process intensification. Rev Chem Eng 2018;34:135–200.
28. Kiss AA. Process intensification: industrial applications. In: Process Intensification in Chemical Engineering: Design Optimization and Control. Netherlands: Springer; 2016.
29. van der Schaaf J, Schouten JC. High-gravity and high-shear gas–liquid contactors for the chemical process industry. Curr Opin Chem Eng 2011;1:84–8.
30. Reay D, Ramshaw C, Harvey A. Chapter 5 - reactors. In: Reay D, Ramshaw C, Harvey A, editors. Process intensification, 2nd ed. Oxford: Butterworth-Heinemann; 2013:121–204 pp.
31. Reay D, Ramshaw C, Harvey A. Chapter 8 - application areas – petrochemicals and fine chemicals. In: Reay D, Ramshaw C, Harvey A, editors. Process intensification, 2nd ed. Oxford: Butterworth-Heinemann; 2013:259–321 pp.
32. Berg J. SPINID. Green Process Synth 2014;3:77–9.
33. Thakur RK, Vial C, Nigam KDP, Nauman EB, Djelveh G. Static mixers in the process industries—a review. Chem Eng Res Des 2003;81:787–826.
34. Bayer T, Himmler K. Mixing and organic chemistry. Chem Eng Technol 2005;28:285–9.
35. Hayes RE, Cornejo I. Multi-scale modelling of monolith reactors: a 30-year perspective from 1990 to 2020. Can J Chem Eng 2021;99:2589–606.
36. Zamaniyan A, Mortazavi Y, Khodadadi AA, Manafi H. Tube fitted bulk monolithic catalyst as novel structured reactor for gas–solid reactions. Appl Catal Gen 2010;385:214–23.
37. Baharudin L, Indera LAA, Watson MJ, Yip ACK. Process intensification in multifunctional reactors: a review of multi-functionality by catalytic structures, internals, operating modes, and unit integrations. Chem Eng Process - Process Intensif 2021;168:108561.
38. Schubert K, Brandner J, Fichtner M, Linder G, Schygulla U, Wenka A. Microstructure devices for applications in thermal and chemical process engineering. Microscale Thermophys Eng 2001;5: 17–39.
39. Neuberg S, Keller S, O'Connell M, Schürer J, Thiele R, Zapf R, et al. Effect of oxygen addition on the water–gas shift reaction over Pt/CeO2 catalysts in microchannels – results from catalyst testing and reactor performance in the kW scale. Int J Hydrogen Energy 2014;39:18120–7.

40. Yao X, Zhang Y, Du L, Liu J, Yao J. Review of the applications of microreactors. Renew Sustain Energy Rev 2015;47:519–39.
41. Alzate CAC, Sanchez MO, Pisarenko Y. Reactive separation for process intensification and sustainability, 1st ed. Boca Raton: CRC Press; 2019.
42. Krishna R. Reactive separations: more ways to skin a cat. Chem Eng Sci 2002;57:1491–504.
43. Sharma N, Singh K. Control of reactive distillation column: a review. Int J Chem React Eng 2010, https://doi.org/10.2202/1542-6580.2260.
44. Shah MR, Kiss AA, Zondervan E, de Haan AB. Evaluation of configuration alternatives for multi-product polyester synthesis by reactive distillation. Comput Chem Eng 2013;52:10.
45. Novita FJ, Lee H-Y, Lee M. Self-heat recuperative dividing wall column for enhancing the energy efficiency of the reactive distillation process in the formic acid production process. Chem Eng Process: Process Intensif 2015;97:144–52.
46. Wieszczycka K. Reactive extraction at liquid–liquid systems. Phys Sci Rev 2018, https://doi.org/10.1515/psr-2017-0141.
47. Djas M, Henczka M. Reactive extraction of carboxylic acids using organic solvents and supercritical fluids: a review. Separ Purif Technol 2018;201:106–19.
48. Mederos-Nieto FS, Santoyo-López AO, Hernández-Altamirano R, Mena-Cervantes VY, Trejo-Zárraga F, Centeno-Nolasco G, et al. Renewable fuels production from the hydrotreating over NiMo/γ-Al2O3 catalyst of castor oil methyl esters obtained by reactive extraction. Fuel 2021;285:119168.
49. Basile A, Falco MD, Centi G, Iaquaniello G. Membrane reactor engineering: applications for a greener process industry. West Sussex: John Wiley & Sons; 2016.
50. Basile A, Paola LD, Hai FI, Piemonte V. Membrane reactors for energy applications and basic chemical production. Amsterdam: Woodhead Publishing; 2015.
51. Perno M, Hvam L, Haug A. Implementation of digital twins in the process industry: a systematic literature review of enablers and barriers. Comput Ind 2022;134:103558.
52. Kockmann N. Digital methods and tools for chemical equipment and plants. React Chem Eng 2019;4:1522–9.
53. Semeraro C, Lezoche M, Panetto H, Dassisti M. Digital twin paradigm: a systematic literature review. Comput Ind 2021;130:103469.
54. Novák P, Vyskočil J, Wally B. The digital twin as a core component for industry 4.0 smart production planning. IFAC-PapersOnLine 2020;53:10803–9.
55. Lee J, Cameron I, Hassall M. Improving process safety: what roles for Digitalization and Industry 4.0? Process Saf Environ Protect 2019;132:325–39.
56. Errandonea I, Beltrán S, Arrizabalaga S. Digital Twin for maintenance: a literature review. Comput Ind 2020;123:103316.
57. Wen Y, Fashiar Rahman M, Xu H, Tseng TLB. Recent advances and trends of predictive maintenance from data-driven machine prognostics perspective. Measurement 2022;187:110276.
58. Ahmad R, Kamaruddin S. An overview of time-based and condition-based maintenance in industrial application. Comput Ind Eng 2012;63:135–49.
59. Damant L, Forsyth A, Farcas R, Voigtländer M, Singh S, Fan IS, editors, et al. Exploring the transition from preventive maintenance to predictive maintenance within ERP systems by utilising digital twins. Advances in Transdisciplinary Engineering. Amsterdam: IOS Press; 2021.
60. Min Q, Lu Y, Liu Z, Su C, Wang B. Machine learning based digital twin framework for production optimization in petrochemical industry. Int J Inf Manag 2019;49:502–19.
61. Shen F, Ren SS, Zhang XY, Luo HW, Feng CM. A digital twin-based approach for optimization and prediction of oil and gas production. Math Probl Eng 2021;2021:3062841.

62. Sierla S, Azangoo M, Rainio K, Papakonstantinou N, Fay A, Honkamaa P, et al. Roadmap to semi-automatic generation of digital twins for brownfield process plants. J Ind Inf Integrat 2021, https://doi.org/10.1016/j.jii.2021.100282.
63. Örs E, Schmidt R, Mighani M, Shalaby M, editors. A conceptual framework for AI-based operational digital twin in chemical process engineering. In: 2020 IEEE international conference on engineering, technology and innovation (ICE/ITMC), 2020, 15–17 June; 2020.
64. Aglave R, Nixon J, Lusty J. Using simulation and digitalization for modular process intensification. Chem Eng Prog 2019;2019:45.
65. Pistikopoulos EN, Tian Y, Bindlish R. Operability and control in process intensification and modular design: challenges and opportunities. AIChE J 2021;67:e17204.
66. López-Guajardo EA, Delgado-Licona F, Álvarez AJ, Nigam KDP, Montesinos-Castellanos A, Morales-Menendez R. Process intensification 4.0: a new approach for attaining new, sustainable and circular processes enabled by machine learning. Chem Eng Process - Process Intensif 2021. https://doi.org/10.1016/j.cep.2021.108671. In press.