AI in Process Industries – Current Status and Future Prospects

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The chemical industry is one of the key industrial sectors in Germany and at the same time one of the largest consumers of energy and raw materials. A successful energy transition and the development of a circular economy can only succeed if they are actively supported and shaped by the chemical industry – through the redesign of existing production processes and the exploration and implementation of new process routes. The challenge is to realize this transformation within a very short time and for many production processes, whereby a much larger number of process routes must be explored. Digital technologies are key to master this transformation towards more sustainability, climate, and environmental protection. The KEEN project aims to explore and leverage artificial intelligence (AI) opportunities in process industry. The newly developed AI methods are tested wherever possible in real working environments and production plants to prove the economic benefit, applicability, and reliability of the methods and technologies.

Keywords: Data handling, Engineering of plants and processes, Optimization of operations, Self-optimizing plants, Surrogate models

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1 Introduction

The publicly funded project KEEN (AI Incubator Labs in the Process Industry) started in early 2020 with the mission of exploring and leveraging methods of artificial intelligence (AI) in the process industries. It is part of the Federal Ministry for Economic Affairs and Climate Action (BMWK) program "Digital Technologies" [1], in particular of the "Innovation Competition Artificial Intelligence". The 26 funded projects [2] cover a broad range of industrial and societal fields, but KEEN is the only project that focused on the chemical and pharmaceutical industries, the third largest industrial sector in Germany [3]. There are also several EU-funded projects related to artificial intelligence in industrial applications [4]. AI4DI – Artificial Intelligence for Digitizing Industry deals with applications in many sectors, including food and beverage. Specifically targeting the process industries, a cluster of six projects related to plant automation has been funded in 2018–2023: CAPRI, COGNITWIN, COGNIPLANT, FACTLOG, HYPER-COC, and INEVITABLE. These projects focused on platforms and standardized workflows to develop digital twins that include machine learning models. The CSA (support action) AI-CUBE: "Artificial Intelligence and Big Data CSA for Process Industry Users, Business Development and Exploitation" pursued the goal to develop an "AI and Big Data roadmap for Europe's process industries" mainly based on

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interviews with managers and experts. The EU-funded s-X-AIPI project started in Mai 2022 and aims to study, build, trial and demonstrate in the asphalt, steel, aluminum, and pharmaceutical sectors an AI technology toolset for Europe's process industry. All large manufacturers in the chemical sector have pursued own activities, however with only very limited publicly available information on successes and failures. At ACHEMA 2022 [5], a competition was organized by INVITE on behalf of NAMUR called the "Innovation Challenge – Plant Service Robot" [6], where autonomous mobile robots competed to capture sensor images, take samples, or to perform safety patrols in chemical and pharmaceutical plants. The challenges were defined by five major companies from the chemical and pharmaceutical sector. Results are reported in [7] and [8].

The KEEN consortium consists of 20 partners, innovative plant owners/operators, technology providers, R&D institutions, and agile start-ups. The goal of the project is to combine real data, available domain know-how and AI methods across the life cycle of chemical plants for increasing their efficiency and sustainability and to demonstrate applications in real plants. This provides the basis of an evaluation of the potential and of the economic benefits of AI methods and tools in the process industries. The project addresses three main areas of plant and process engineering and operation: (1) modeling and simulation of processes, products, and plants; (2) engineering of plants and processes; (3) optimal operation of production plants, with the goal of self-optimizing plants.

The purpose of this paper is to give an overview of the outcomes of the KEEN project after three years of project work. It discusses the challenges of AI applications in the process industries, the results of several use cases with major learnings and achievements, as well as open issues and future directions. The realization that digitalization is needed for the survival of process industry was formulated in a compact way using 12 propositions as part of the 57. Tutzing-Symposium 2018 "100% Digital" [9]. Key statements are (1) the digital twin is the basis; (2) digitalization pays off by shortened time-to-market, raised flexibility and reduced cost; (3) leveraging the full potential of digitalization requires AI; (4) smart manufacturing eco systems unleash further potential; (5) digitalization requires a holistic view on processes.

AI methods are currently gaining new momentum and are predicted to be a game changer when combined with platform solutions [10]. It is expected that they pave the way for reduced development times, higher efficiency, and lower cost, e.g., due to reduced number of experiments needed in model development, fast simulations, improved operator advisory and control systems. Machine learning (ML), comprising techniques such as deep artificial neural networks, support vector machines, and Gaussian processes, is an essential element of AI methods. To apply machine learning, however, requires sufficiently large amounts of data which are suitable for model training. In the process industries, data is highly correlated, comes from different legacy systems, and correlation and causal dependencies are hard to distinguish due to the presence of recycle streams. Therefore, the deployment of AI in the process industries faces specific challenges. On the one hand, these challenges lie in the complexity and the diversity of the processes themselves, e.g., due to inherent characteristics of continuous or discontinuous operation or different degrees of interconnectedness. On the other hand, stringent requirements and standards regarding safety and environmental effects must be met at all times, while maintaining high levels of availability and reliability. The need to exclude risks that cannot be clearly assessed is a logical consequence of this situation. The introduction of new digital methods or technologies must therefore overcome a high hurdle to find acceptance. At the same time, it is undisputed that AI-based methods can make a valuable contribution in the future, especially in sensitive areas. These aspects are examined in more detail in the different applications that are discussed in this issue.

2 The KEEN Project and its Goals

According to McKinsey, there is significant potential of AI for process industries [11]. AI can be considered as a cognitive amplifier in different stages of process development and (fine) chemical production. KEEN was selected end of 2019 as part of BMWK program Digital Technologies – Innovation Competition "AI as a driver for economically relevant ecosystems". Fig. 1 shows how KEEN addresses the full scope of potential applications and enabling technologies in the process industries. White boxes indicate the already existing well developed toolbox consisting of process control, process identification, and mechanistic process models with the benefit for improved process design. KEEN supplements these by the green boxes, in particular a common data base, AI models and analysis as well as intelligent assistance systems.

KEEN has focused on three application areas of AI methods in the process industries: the support of the development of processes, the engineering phase of plant design and development, and the control, monitoring, and optimization of running processes (real-time application). In these areas, the hitherto unused potential was estimated to be the highest.

In the area of AI-based support for the development of processes and the engineering of plants, AI techniques have been investigated for the efficient and reliable description of thermodynamic properties of mixtures of substances. By these techniques, the modeling of unit operations and pieces of equipment for reaction and separation is improved by combining idealized balance equations, algorithms for calculating phase equilibria, and data-based model elements. AI-based modeling supports problem solution and may lead to new approaches. For example, the behavior in

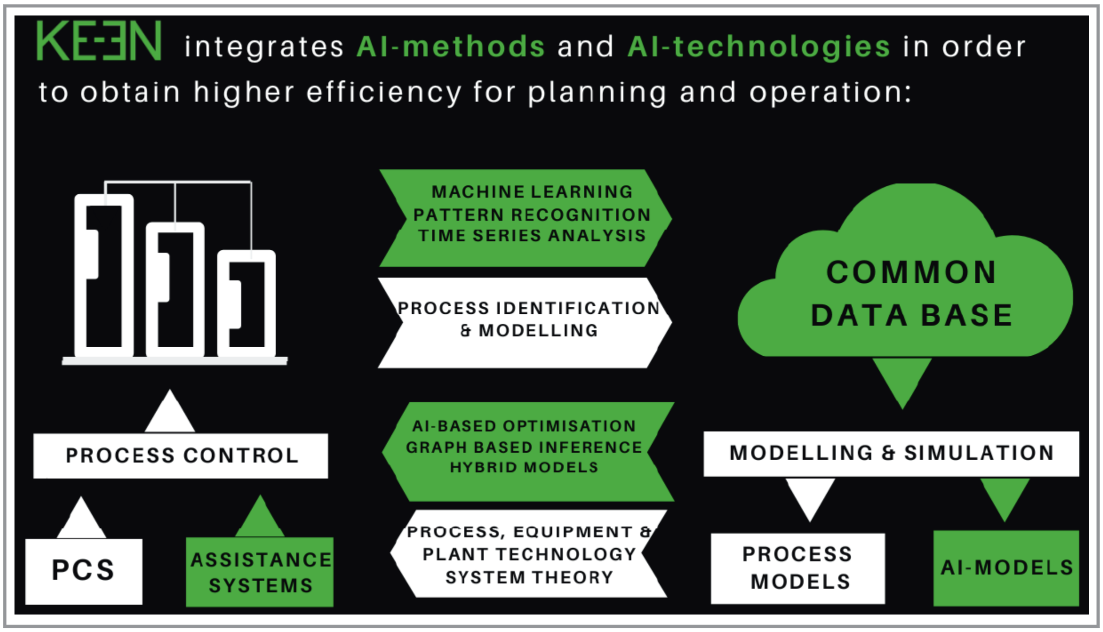

Figure 1. Structure of the KEEN project, as described in 2019.

extraction columns is analyzed both in experiment and simulation assisted by AI tools. Further, matrix completion methods are applied for adding missing information in substance's and their mixtures' properties computation. In AI-based engineering, support is provided for, e.g., HAZOP (hazard and operability) analysis, which is central for safety analysis, module selection, for optimizing the design of plants, as well as for supporting the transfer of laboratory results to simulation tools. For the support of the operation of complex processes, automatic performance evaluation is implemented in multi-purpose plants. It is based on MTP (modular type package)/DEXPI (data exchange in process industry, DEXPI P&ID specification, vers. 1.3, accessed November 28, 2022, https://dexpi.org/specifications/) and automatically links plant structure with operational data for rule based KPI (key performance indicators) evaluation.

Modularization in the process industry has been advocated for about 10 years [12] and is a driver for AI applications in the process industry due to the local intelligence in the individual module [13]. In addition to the hardware, planning documents and information for automation are available for a module [14, 15] They are described in semantic information models that can be interpreted by computers [16]. Due to standardization, modules can be captured in databases, selected, and interconnected with a high degree of automation. In KEEN, metadata standards and schemes for DEXPI/P&IDs (piping and instrumentation diagrams) as well as extraction and contextualization of data are proven in industrial pilot installations. The automatic, e.g., graph-based, analysis for DEXPI/P&IDs is key to provide a contextualized basis for, e.g., AI-based root cause analysis of anomalies.

The area of process operations comprises solutions for the improved operation of plants, which provide support for plant operators for recognizing the state of a plant or adapting the mode of operation to meet the product specifications and to improve the energy and material efficiency and closed-loop applications. Applications in KEEN range from the detection of the state of plants using AI-based image processing, e.g., for crystallization and extraction processes and aerated tanks, over decision support for MDI production, batch distillation and ammonia plants, to advanced control solutions for bioreactors and distillation processes. In cross-cutting projects, use cases in KEEN have dealt with common process models, available benchmark data, and its preparation as well as interfaces, reference processes and business models. Hackathon events, trainings, and incubator labs open the AI challenges to a broader community, such that exploitation can be expected in the next years after the closure of the project.

3 Major Learnings and Existing Challenges

Tab. 1 provides an overview of the contributions from the KEEN project in this special issue. The table shows the challenges that were addressed. These are (1) data quality and availability, (2) the acceptance of automatic recommendations by the user/operator, (3) the reduction of model complexity of mechanistic approaches, (4) the reliability of models for closed-loop applications, and (5) the easiness and robustness to transfer models automatically between plants and applications. The contributions refer to different application areas. Cross Cutting include concepts for platforms and overarching results. Modeling & Engineering

Table 1. Scientific contributions in this issue with application areas and typical challenges.

KEEN Contribution	Application Area	Challenges				
		Data Quality & Availability	Acceptance	Model Complexity	Reliability	Transfer
Lammers et al., Linguistic Framing of AI [40]	Cross Cutting		x			
Sherpa et al., ProMetaS – a common metadata standard for process engineering and industry [41]	Cross Cutting	x				
Bortz et al., Real-Time Interactive Decision Support on Input-Output Data Sets in Chemical Process Engineering [42]	Modeling & Engineering		x			
Bortz et al., Predicting temperature-dependent activity coefficients at infinite dilution with and without physical knowledge [43]	Modeling & Engineering	x				
Klose et al., Automated Evaluation of KPIs based on DEXPI and MTP [44]	Modeling & Engineering			x		x
Neuendorf et al., Detecting crystals in suspensions: convolutional neural networks vs. a gravity-based approach for size distribution detection [45]	Modeling & Engineering	x				x
Neuendorf et al., A comparison of AI-evaluated experimental and simulated data on the behavior of a stirred DN32 solvent extraction column [46]	Modeling & Engineering	x	x		x	
Oeing et al., preHAZOP: Graph-based safety analysis for early integration into automated engineering workflows [47]	Modeling & Engineering			x	x	x
Oeing et al., Machine-readable plant topologies: open and smart P&IDs and their potential for future engineering [48]	Modeling & Engineering	x				x
Tolksdorf et al., Tool Chain to extract and contextualize process data for AI applications [49]	Modeling & Engineering	x				x
Bordas et al., Grey-box modeling of the molecular weight distribution in an industrial polycondensation reactor [50]	Operations	x		x	x	
Brand Rihm et al., Transfer learning of data-driven models from simulated to real batch distillation trajectories [51]	Operations	x		x	x	x
Ehlhardt et al., Application of Real-Time Optimisation with Modifier Adaptation to an industrial production process [52]	Operations			x	x	x
Elsheikh et al., Model Predictive Control of a Continuous Mother Liquor Distillation Column with Machine-Learning based Soft Sensors [53]	Operations	x		x	x	
Franks et al., Evaluating Methods for Time Series Anomaly Detection on the Tennessee Eastman Process [54]	Operations			x		
Gärtler et al., Machine Learning Approaches for Phase Identification Using Process Variables in Batch Processes [55]	Operations	x	x			x
Hubert et al., Production scheduling using Deep Reinforcement Learning [56]	Operations			x		
Khaydarov et al., Image-based Flow Regime Recognition in Aerated Stirred Tanks using Deep Learning and Transfer Learning [57]	Operations	x				x
Kloepper et al., Combining Active Learning and Learned Representations for Multivariate Time-series Classification in Industrial Applications [58]	Operations	x	x			
Winz et al., Dynamic Gray-Box Modeling of a Fermentation Process for Spore Production [59]	Operations	x		x	x	

gives missing links and workflow integration, addresses incubator labs, flow diagrams and conceptual process design. Operations ranges from timeseries analysis to control and optimization of plants. The key ideas and achievements of the application areas are summarized in the following sections.

3.1 Data Backbone

In many use cases, data were generated and analyzed, which are publicly available. The relevant metadata structure and content were setup and are described in the following.

3.1.1 Data Collection and Integration of AI-Based Solutions

AI applications need data. But the automation architecture of existing process plants has neither been optimized for extensive data collection nor for real-time AI applications. Currently, a significant overhead is required to adapt it to the needs of AI. To make the integration process into existing plants more efficient, novel hard- and software infrastructure concepts have been addressed in the project. Key aspects of the envisioned AI-enabling environment are solutions for a flexible data collection via wireless sensor hubs, real-time application of AI algorithms on edge devices, cloud access for storage and more. Prototypical realizations were implemented and successfully tested at laboratory process plants of the KEEN partners.

To understand and interpret both data and AI results, their context must be understood. Piping and instrumentation diagrams (P&IDs) provide such context information. With an automated P&ID import (using the DEXPI standard) structure information and topologies can be obtained and connected to measured data. A tool chain for this process was setup and evaluated with several use cases.

Several data standards (such as ISO, IEC, VDI, DIN) have been investigated and mapped by project partners to develop a normative blueprint to improve future data handling in process plants, which is needed for coming AI applications.

3.1.2 Enabling Sharing of Data

Data collection in the process industry yields a variety of data types. To ensure that data sets are FAIR (Findable, Accessible, Interoperable, and Reusable) and suitable for machine learning, a platform for data exchange and a common metadata schema for describing process industry data were developed. Both developments were made in close cooperation between universities, software companies and the KEEN use case providers. In an iterative process, requirements were collected, implemented, tested, and evaluated.

ProMetaS, the Process Engineering/Industry Metadata Schema [41], defines various modular metadata categories (e.g., for plants, processes, or sensors) adhering to available metadata standards and extending it as needed (Fig. 2). Thus, it is possible to fully describe the provenance of data sets. ProMetaS is used to document the data on the KEEN data platform prototype (https://keen.zih.tu-dresden.de/), which is based on the open-source data repository *Dataverse*. Several KEEN uses cases already share their data there (e.g., DEXPI P&IDs or images for neural network training). The API of the platform makes it easy to directly access or ingest the data and the according metadata.

The German National Research Data Initiative (NFDI) is planning to create an infrastructure to make data accessible for research, and to connect data and people on a national and international level. The KEEN project cooperates especially with the NFDI4Cat consortium and plans to integrate the developments.

3.1.3 Data Curation and Quality

In the process industry a huge amount of data is created and collected every day. To give one example, at Air Liquide 3.5 billion data points are gathered daily across the company. AI is key to improve the ways that we leverage data to support the industry transformation. Data becomes a cornerstone but cannot generate value on its own. Besides the maturity of the algorithms and data quality, the success of AI applications relies on the three factors: people, technology, and governance. KEEN provides further training and education based on the experiences of the project; requirements have been identified and will result in offerings for academic and industrial customers to increase maturity level in the application of AI methods for process industries. All KEEN publications serve as input for further development; the incubator labs show AI application to a broader community along reference processes and will convince people for modern technology in process industries. KEEN provides benchmark data shared via the KEEN data platform based on industrial and academic input. Hackathon events, business model workshops and mirror committee discussions with the VCI have been organized, the whole KEEN project was accompanied by DECHEMA. Hackathon

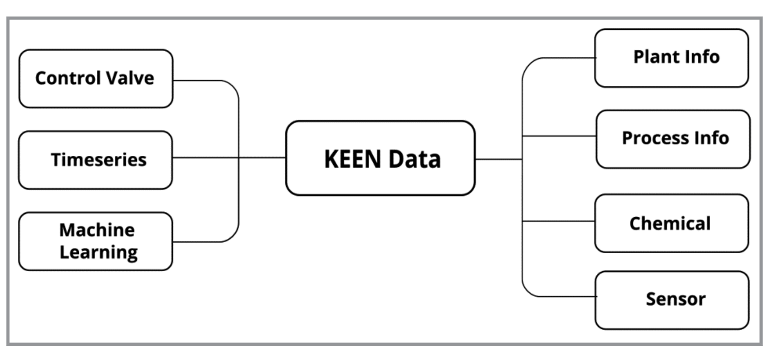

Figure 2. Categories of the ProMetaS metadata schema.

and workshops show that small teams, speed boats in agile management structures deliver most valuable and fast results.

3.2 Modeling & Simulation

The chemical industry extensively uses modeling and simulation methods, which describe and predict

I) the properties of substances and mixtures of substances,
II) kinetics, transport phenomena, and fluid dynamics,
III) unit operations and pieces of equipment to convert and separate substances,
IV) flow sheets of interconnected pieces of equipment,
V) dynamic phenomena, and
VI) logistic aspects with flow of materials, utilization of and competition for resources.

These prerequisites for successful process design have been addressed in KEEN from a modeling point of view. As far as the prediction of properties of substances and, especially of mixtures, is concerned, the available experimental data is usually scarce. Therefore, in the past, physically motivated approaches were in the focus that predict the properties of substances based on structural information, e.g., typical groups in the molecular structure, cf. [17]. Different model approaches exist, so that from a pattern recognition point of view, one may ask how many and which features are needed at all to describe the thermodynamic properties of all conceivable mixtures. Significant progress in this direction has been made by applying matrix completion methods to predicting activity coefficients of binary mixtures [18]. These methods rely on the assumption that both solvents and solutes can be described by a rather small set of independent features, which permits predictions on the binary behavior based on a very small set of training data. Within KEEN, these methods have been complemented with physical knowledge [18, 19] and were applied to different physical properties [20, 21]. In this special issue, matrix-completion is generalized to tensor completion techniques [43]. It is shown that this allows to systematically extract information on the dependence of mixture properties on a physical variable, e.g., temperature.

Once substance properties are known, the engineer may tackle the task of designing adequate processes to convert and separate the desired substances and mixtures. The combination of process simulation with experimental validation assisted by AI analysis multiphase flow phenomena is described in [46] for solvent extraction with population balances. One of the major advantages of virtual process design is the possibility to compare different scenarios: for a given process design, one may wish to compare different operating strategies according to certain KPIs, or one is interested in finding out the optimization potential of the current operating point. Typically, such comparisons are time-consuming and require quite some experience in handling process simulations. This motivated researchers in KEEN to employ machine learning methods to realize interactively what-if-comparisons in real time. Once a machine-learning surrogate model has been trained, the engineer can either change the values of process specifications or analyze the impact of this change on the KPIs of the process. Further, one may explore how far process KPIs can be improved and thereby obtain the corresponding process specifications. This is illustrated for a steam methane reforming process in [42].

3.3 Smart Engineering Tools

The typical chemical process development starts from process synthesis on the base of the chemical reaction pathways and properties of mixtures, as described in the section before. The next step is the sizing of the equipment and detail engineering. For basic and detail engineering, the KEEN project explored various ways, in which artificial intelligence can support engineering and process development and help to minimize errors in the early engineering phases. An example is process design based on machine learning and process flow diagrams (PFD) together with consistency checks in piping and instrumentation diagrams (P&ID) using deep learning [22]. The combination of the model with optimization and its connection to a process simulator showed enormous potential in a feasibility study. Thus, the ML model serves as a basis for computer-supported process development [22]. Besides the specific application of AI to engineering data, the focus was also on using harmonized data as a basis to ensure the reusability of the models and to address a broad range of users from different fields [23, 44, 49]. Standardized P&IDs in DEXPI format are used as the data basis, which are available as graph-structured data. Graph learning algorithms such as graph neural networks (GNN) learn the existing patterns in these graphs. These patterns can then be used to check the consistency of new P&IDs and alert the user to potential errors in real time during the drawing process. Further, recurrent neural networks (RNN) can be used to predict subsequent components in P&IDs. The implementation of both approaches in the P&ID software Plant Engineer of the software vendor *X-Visual Technologies GmbH* proves the feasibility and demonstrates as a prototype the advantages of real-time, AI-assisted synthesis of P&IDs [24–26, 47, 48].

3.4 Operations

As stated above already, the activities within the KEEN project address both advisory systems for plant operators and plant engineers to detect anomalies and propose improvements and closed-loop systems, in which control actions are performed automatically. In both areas, it is critical that the developed AI-based solutions are reliable, i.e., do not lead to false alarms, wrong suggestions, or inefficient or even dangerous reactions of controllers.

Within KEEN, many applications have been considered in the domains of monitoring, advisory systems, and closed-loop control. Advisory systems should be easy to transfer from one plant to another, and must cope with different requirements, e.g., applications during startup and shut down vs. steady-state operation. Often, as not all interventions and events are recorded and annotated, the reasons for changes in the data are not explicitly visible. An interdisciplinary and experienced team is necessary for correct data interpretations due to the sensitivity of the results on the timeframe and boundary conditions. AI-supported modeling and simulation of both the dynamic behavior and the steady-state case is has been addressed in KEEN [27]. The contribution [54] compares time series analysis approaches for the example of the well-known Tennessee Eastman Process (TEP) benchmark example. Several machine learning approaches to tackle the problem of batch phase identification and labelling are compared in [55]. Time series classification, similarity-based clustering and change point detection work successfully on synthetic data, but their performance turned out to be lower on real world data. Active learning allows for a scalable trade-off between the number of required labels, the obtainable quality, and the involvement of human experts. The contribution [58] extends [55] with representation learning (RL). Here, a model first learns a latent space representation of the unlabeled data and then uses this to fine tune our classification model, which is trained on the labeled data (a smaller dataset). For validation, the Tennessee Eastman Process (simulated), a simulated batch production process, and data from a real-life batch production process are used.

Taking the human expert in the loop is one way to benefit from the fact that many physical relations are known in the process industries. Detailed physical simulation models are challenging to set up and require a high level of engineering expertise, but still are based on assumptions to represent the real situations. In [28], it could be shown that deep learning methods combined with contextual knowledge simplify the parameterization of complex models considerably. As mentioned above, in model-based operator support for optimal, e.g. energy efficient operation of processes, and even more in model-based closed-loop real-time operation, to establish dependability of models is a key issue.

Machine learning models have been used in several applications in KEEN to improve inaccurate models that are used for control and optimization or to reduce the complexity and computation time of mechanistic models. This can be achieved by purely data-based models which are trained based on simulation results from a state-of-the-art process simulator and then improved using measurements from the real plant as described in [51–53]. An alternative is to employ simplified mechanistic models and to train a parallel model that compensates the error of the simplified model [29]. The problem of using both purely data-based models and hybrid models is that it must be assured that the predictions of the data-based model element are only used when there has been enough training data in the region of the current model inputs. In [30], this problem is addressed by estimating the domain of validity of the data-based element based on a one-class support vector machine [31] and fading out the data-based component when the region where training data was available is left.

Another approach is to embed data-based sub-models into structured models that represent the basic energy and material balances, leading to grey-box models [32]. This has the advantage that the complexity of the data-based models is significantly smaller than that of the overall model and the validity of the data-based elements and the effect of errors in these can be controlled much better. The contributions [50] and [59] describe this modeling approach for two challenging examples from complex polymerizations and fermentation processes. Production scheduling is another activity in process operations where operator support can lead to large improvements of the productivity and of the energy consumption of production plants. The contribution [56] describes the application of reinforcement learning to this problem.

The monitoring of critical, but very often not directly measurable states of chemical processes such as concentrations or flow regimes is important to ensure the quality of the products and the efficiency of the process itself. Therefore, reliable information about relevant states must be extracted and good predictors must be identified. In an industrial use case, parameters from a multi-spectral capacitance measurement are used to predict the duration of various phases of a fermentation process by unsupervised ML. Flow regimes in aerated stirred tanks are in general good indicators for final quality and efficiency. Their image-based classification is analyzed in [57] using deep learning based on different pre-trained models to reduce data need.

Model predictive control (MPC) is the most successful advanced control approach that is applied in the chemical industry. Besides other aspects as a suitable instrumentation and well-tuned basic control layer of the process, the quality of the model is a key factor for the implementation of MPC solutions. For linear MPC, usually step-tests are performed, and a fixed linear model is fitted to these measurements. When the process behaves nonlinearly within the intended range of operation, first principles-based models must be developed and parameterized, which leads to a significant effort as a high fidelity of the model is required. The use of data-based and hybrid models is promising to reduce the modeling effort. In [53], a black-box model is fitted to simulation data and then improved based on measurements at the real plant.

The successful application requires:

- a good understanding of the physical, IT and mathematical aspects,
- a proper setup of the basic process control layer according to the process control pyramid,

- a good dynamic process model is required, and
- reliable data, e.g., obtained by performing step tests on the different variables of the process.

In [58], the performance of two MPC schemes using a data-based and a hybrid model, are compared when applied to a simulated industrial separation column. As knowledge of the concentration of the feed and the overhead product would improve control performance, a soft sensor estimating these missing measurements is added using artificial neural networks (ANN).

In [33] the domain of validity of the data-based element of the hybrid model is monitored and the contribution of this model is faded out when the domain of validity is left. This however may lead to a degradation of the performance, so the quality of the model is monitored online and is extended if the measurements show a good prediction accuracy. This approach is combined with the use of two ANN-based soft sensors for the unmeasured concentrations of the feed and of the product streams in [53].

3.5 Linguistic Analysis and Elements of Trustworthy AI

If we talk about AI, trust and acceptance are important conditions for the success of interaction, which can be induced, promoted, reinforced, and stabilized, but also compromised by certain linguistic patterns in communication. In [40], a psycholinguistic study is described, and its results presented. The subject matter was developed based on evaluations of KEEN internal communication against the premises of cognitive linguistic frame semantics. The study examined how the degree of trust in different fictional products is influenced by corresponding linguistic patterns – based on the DECIDING (kurzelinks.de/KEEN-DECIDING), CONTROL (kurzelinks.de/KEEN-CONTROL), and SUPPORTING (kurzelinks.de/KEEN-SUPPORTING) frames observed as characteristic in KEEN partners' communication – in product descriptions. The product type has the greatest influence on acceptance, while the expert or lay status of the participants has the least influence on evaluation. The level of confidence is rated higher by all groups when a product description is presented with the SUPPORTING frame than with the CONTROL or DECIDING frames. In a nutshell: If we talk about AI, we should, if possible, always talk about being supported in our decisions by AI. In a further step, recommendations for internal and external communication are derived from the results, which take account of focusing, perspectivization and the organization of the information structure of linguistic units. There is, for example, a significant difference in saying "The AI supports us", "We are supported by AI" or "We use AI as a supporting tool". Language structures are oriented towards agentivity to varying degrees, and possible features of animacy may be inhibited in reception, e.g., by comparisons ("as a tool").

3.6 Incubator Labs

Three incubator labs were set up in the KEEN project during the second and the third year based on the preliminary results from the work packages and use cases in Dortmund, Dresden, and Kaiserslautern. Typically, incubator labs are dealing with pre-seeding activities in the start-up phase to identify AI application fields and successful workflows.

The incubator lab at TU Dortmund University, Laboratory of Equipment Design (AD-Lab) focusses on smart equipment and smart engineering workflows for the process industry. Image recognition tools were combined with reinforcement learning and process control activities, e.g., avoiding flooding in the operation of distillation and solvent extraction columns [34, 35]. AI-assisted optical analysis of coalescing two-phase systems as well as rising droplets was used to determine fluid parameters such as density, viscosity and surface tension of a biphasic system [36, 37, 45]. The tools from smart engineering depend on a consistent data model, which is developed for research data in the NFDI initiative. Here, synergies were found for process simulation data as well as finite element and CFD models. This led to consulting activities for SME (small and mid-sized enterprises) and tech transfer projects. Furthermore, teaching and educating young students to work with AI tools is a major task, where the use cases from KEEN served as training material but also as starting point for further investigations. Together with the Laboratory of Process Automation Systems, Prof. Lucia, a machine learning course was set up and achieved high attendance by master students of Biochemical and Chemical Engineering. Further activities from students and research projects are discussed with and offered in the newly founded Competency Centre of Digital Production at TU Dortmund University, wherein the AD-Lab is a founding member and active with first consultations.

The Process-to-Order-Lab (P2O-Lab) at TU Dresden is going to follow a learning factory approach for the incubator lab. The focus of the incubator will be on enhancing data availability and accessibility by means of industry 4.0 solutions tailored to the actual challenges of the process industry. In order to guarantee a continuous improvement process, concepts in the area of modular plants, integrated engineering, life cycle accompanying digital companion technologies, added-value services, big data and smart analytics are developed, implemented, and validated, as well as represented in academic and industrial showcases.

The mission of the incubator lab at Fraunhofer ITWM in Kaiserslautern is to make scientific progress accessible for innovation that leads to a measurable benefit in industrial applications. Therefore, mathematical methods are employed to model, simulate, and optimize different processes covering both organization and technical challenges. Within KEEN, special emphasis was put on developing software prototypes that implement hybrid model approaches, i.e., combinations of both physical and data-driven methods. This has been done in the following contexts:

– Interactive analysis of time series, especially recognition of time intervals showing stationarity.
– Application of matrix-completion techniques to the prediction of thermodynamic properties of binary mixtures, enhanced by interactively considering meta-information like molecular weights, size of the molecule or substance classes.
– Comparison of different operating strategies of flowsheet models, based on a machine-learning based surrogate trained for a pre-sampled operating window.

For all three use cases, interactive software prototypes are available, have been tested and employed by industrial partners to realize the rather abstract goal of having AI that one can really touch, test and challenge. These pieces of software and the experience gained from the collaboration with the industrial partners forms a significant asset for the further exploitation strategy.

4 Open Issues and Future Directions

KEEN has delivered significant contributions to the application of AI-based technologies in process engineering and operation and increased the understanding of their potential and limitations. This understanding is important to improve quality and availability of data as well as machine recommendations for the user/operator. It was shown that matrix completion methods can enhance the prediction of thermodynamic properties significantly without additional experimental effort and that surrogate models can be used successfully in conceptual process design. Tools for data pretreatment and labelling have been developed to enable the use of ML methods, e.g., for the detection of anomalies. In particular, the use of hybrid models for the description of complex processes with the goal to reduce the modeling effort, increase the accuracy of the predictions and to be able to ensure the reliability of the predictions of the model has been investigated and successfully demonstrated in several applications. The list of ML tools investigated and presented here is not exhaustive and other examples can be found in textbooks such as the well-known book by Hastie, Tibshirani, and Friedman [38], or the monograph by Bishop [39]. The creativity of engineers and data scientists will find more applications and improvements by combination of process engineering and AI tools.

From a broader perspective, it is beyond controversary that industry is at the heart of major economic and climate challenges that require a fundamental review of production activities. The chemical and process industry must significantly reduce greenhouse gas emissions and CO_2 footprint. The industry commitment to SBTi (science-based target initiative) poses pressure on the sustainable transformation of the whole industry, particularly on the energy-intensive process industry. With classical product and material design, engineering, and operational technologies the timeline for target achievements cannot be met. Complex raw material properties (e.g., from circular economy value chains or renewable feedstocks) and strong variations in utility supply (e.g., from localized/decentralized renewable energies, increased couplings between different sectors) influence the economical operation and production and challenge the chemical industry in general. One can summarize that the competitive environment changes: in addition to time-to-market and cost pressure, shorter and more flexible product life cycles, there is an increasing need in taking the whole value chain and the sustainability objectives into account. This is accompanied by additional uncertainty and less planning security due to the current global crises. The value and supply chains must be considered from the beginning to ensure customer needs in the product development but also to ensure circular economy and sector coupling in a robust and resilient way. Value chains are complex. New products with less environmental impact require cradle-to-cradle concepts and the optimal interplay between the different partners along the value chain. Sustainable raw materials may also change efficient production processes and logistics.

Data and AI support this transformation with a wide range of opportunities across all aspects of process and plant design and operations ultimately leading to smart plants, which can manage their performance in an agile manner while reducing their carbon footprint. The urgency of climate change, digitalization, accelerated automation, and Industry 4.0 are transforming our activities in all our sectors. Harnessing data is essential to reach both business performance and sustainability objectives. Data science and AI are sources of value creation and represent a key lever to meet sustainability targets. By combining multiple data sources and using AI and ML, innovative solutions and opportunities for successful applications can be offered for a complex and volatile environment that were otherwise unimaginable. Fig. 3 shows a basic scheme of a chemical production site with potentially useful ML tools based on an AI-assisted engineering workflow.

Scope 2 of CO2e (CO_2 equivalent) emissions vary across raw material and energy supply. Smart engineering helps quantifying and optimizing this backpack. Smart operation reduces Scope 1 of CO2e that are directly controlled by the respective operator. The role of data management and information supply will be more important in tracking environmental impact in scope 1 to 3 emissions, with changing external logistic situation, market development and customer demand (scope 3 of CO2e emissions).

Digital technology will soon more and more overarch different phases of the lifecycle of chemical production plants from conceptual design to plant operations, maintenance and dismantling. Operation, management, and optimization of processes that are subject to strong variations and fluctuating boundary conditions will be handled in a more holistic manner. Digital technology provides the needed

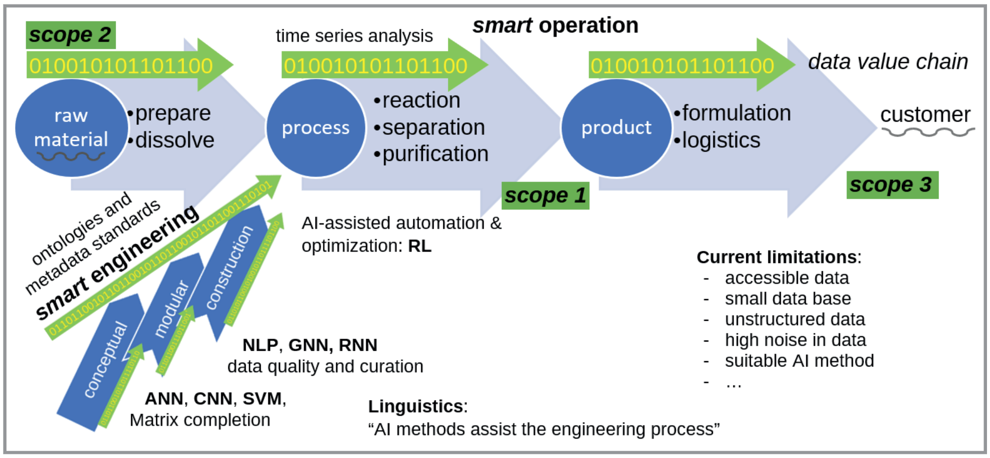

Figure 3. Value chain of chemical production with supporting digital and AI tools based on an AI-assisted engineering workflow.

information for close monitoring and optimization and thus to enable and reach transformation targets. AI methods can contribute to the efficient use of the ever-increasing amount of data that is generated and connected. However, there are still significant challenges that have to be overcome.

In many applications of AI and ML that have been investigated with the KEEN project, the lack of sufficiently rich data obtained from the observation of the processes themselves was the main challenge. Therefore, in many cases, classical process models were used to train ML models, which has the benefit of obtaining models that execute faster and do not exhibit convergence problems. On the other hand, the range of validity of the approximated models must be kept in mind as well as the assumptions behind the original models, and their transfer to similar problems is not necessarily possible. It has been shown in several examples that mechanistic models can be enriched by data-based models, either by training these models to predict and correct the model errors based on observations at the real plant or by embedding sub-models that represent certain model elements, e.g., reaction rates better than classical formulations. The combination of mechanistic and data-based models has the advantage that trust into the models is easier to establish than if purely data-based models are employed. However, this does not overcome the problem of the effort for model building, which often prevents advanced model-based techniques from being used.

A related issue is that of model adaptation. If models are trained using real data from the plants, it is obvious that new data that is collected during operation could and should be used to further improve the models. However, to guarantee the correct working of such adaptation mechanisms is by no means easy, as is illustrated by the fact that despite of huge research efforts over many decades, there are not too many applications of adaptive control. But only if continuous model improvement can be realized, at least in a supervised manner, data-based models will offer game-changing advantages over the classical mechanistic models.

5 Conclusion and Outlook

With increasing digitalization, both the quality and the utilization of the collected data is becoming more and more important in the process industry. The project KEEN has addressed three main areas of plant and process engineering and operation: (1) modeling and simulation of processes, products, and plants; (2) engineering of plants and processes; (3) optimal operation of production plants, with the goal of self-optimizing plants. The application in industrial reference processes and real plants show that hybrid approaches are the most promising to increase the accuracy and reliability of the predictions. Transfer learning and active learning approaches turn out to be suitable approaches to tackle the high cost of data acquisition and labeling, which is characteristic for the process industry. Despite all the progress in ICT frameworks, Industry 4.0 platforms, and IT/OT integration, data availability, data accessibility and data quality still are and will in the near future continue to be major hurdles for applied AI projects.

We hope that the articles in this special issue, which show in detail the results obtained for the different use cases and provide a deep dive into the current state of the art of AI applications in the process industry, are encouraging the readers to either get started themselves with implementations of such techniques in promising cases or continue the research on the open issues. The results of the uses cases show that AI techniques are becoming valuable tools for process engineers as well as plant operators. Techniques such as transfer learning, physics-informed neural networks, explainable AI, and knowledge management in general need further investigation to increase robustness, reliability, and transferability. A still wide-open field are methods for the design of a great user-experience for

AI-supported assistance systems that may help to reach the next level in making the process industries more efficient and sustainable.

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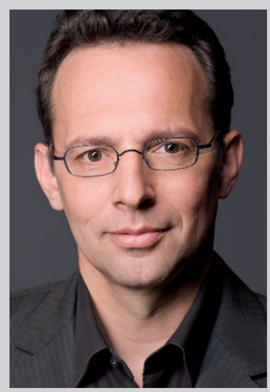

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Abbreviations

AD	Apparatedesign
AI	Artificial Intelligence
ANN	Artificial Neural Network
BMWK	German Ministry of Economic Affairs and Climate Action
CFD	Computational Fluid Dynamics
CO2e	CO2 equivalent
DEXPI	Data Exchange in Process Industry
DIN	Deutsche Industrie Norm
FAIR	Findable, Accessible, Interoperable, Reusable
GNN	Graph Neural Network
HAZOP	Hazard and Operational Analysis

ICT	Information and Communication Technology
IEC	International Electrotechnical Commission
ISO	International Standardization Organization
KEEN	AI Incubator Labs in the Process Industry
KI	Künstliche Intelligence (AI)
KPI	Key Performance Indicator
MDI	Methyl diisocyanate
ML	Machine Learning
MPC	Model Predictive Control
MTP	Modular Type Package
NFDI	Nationale Forschungsdateninfrastruktur
NFDI4Cat	NFDI für Katalyse und Prozesstechnik
PFD	Process Flow Diagram
P&ID	Pipe & Instrumentation Diagram
RNN	Recurrent Neural Network
SBTi	Science-based Target initiative
SME	Small and Medium Enterprises
SVM	Support Vector Machine
TEP	Tennessee Eastman Process
VCI	Verband der Chemischen Industrie
VDI	Verein Deutscher Ingenieure

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