Systems & Control Transactions

Original Research Article
Peer Reviewed Conference Proceeding
ESCAPE 36 - European Symposium on Computer Aided Process Engineering
Sheffield, UK. 21-24 June 2026

PSE PRESS

Automated workflow for the configuration of modular plants and HAZOP analysis by utilizing DEXPI P&ID

Mathias Schmitz[a*], Janis Weber[a], and Norbert Kockmann[a]

[a] TU Dortmund University, Department of Biochemical and Chemical Engineering, Dortmund, North Rhine-Westphalia, Germany
* Corresponding Author: mathias.schmitz@tu-dortmund.de.

ABSTRACT

The increasing adoption of modular plant concepts in process engineering requires new strategies for design and safety evaluation. Conventional hazard analysis methods, such as HAZOP are time-consuming and must be repeated whenever a configuration changes, which contradicts the flexibility that modularization aims to achieve. This work combines concepts from the modular HAZOP method and the preHAZOP method to enable an automated, early-stage safety assessment for modular plants based on P&IDs. A workflow is developed that generates a combined P&ID for a modular plant from individual module (PEA) P&IDs provided in DEXPI format and performs an adapted preHAZOP analysis on the resulting plant representation.A key motivation is that P&IDs are always created during plant or module design and already contain relevant piping information, which can be reused for automated module interconnection and plausibility checks. In the proposed workflow, standardized interfaces enable automatic connection generation and validation. The safety assessment is performed by rule-based deviation propagation on a DEXPI-based P&ID graph and can operate with, without, or alongside process data. The workflow outputs structured scenario tables and selected design consistency checks and is implemented as a Streamlit web application, validated on a modular example system.

Keywords: Modular plants, HAZOP, DEXPI, P&ID, Safety analysis

INTRODUCTION

Globalized markets and increasingly dynamic product demands require the process industry to react faster and design plants more flexibly. Modular plants address this need by enabling reuse of standardized units and faster (re-)configuration of production systems [1]. However, the benefits of modularization are constrained by the effort required for safety studies and approvals. Conventional HAZOP is systematic but resource-intensive; repeating a full HAZOP after each configuration change undermines modularity's speed advantage. This work therefore targets an automated workflow that supports early safety assessments and helps accelerate approval processes for modular plants.

In industrial practice, each module plant or plant section is documented in a P&ID diagram during its design phase. The P&ID is a core component in the design phase during detail engineering. Manufacturers commonly annotate piping with information such as identifiers and nominal diameters, and sometimes even material information [2, 3]. In the workflow of this contribution, such data are explicitly attached to module interfaces and exported with the P&ID, enabling automatic connection generation and interface checks when assembling modules into a plant.

To achieve the goals, this contribution combines two ideas: a modular safety approach (splitting safety knowledge into reusable module/equipment-related parts) and automated, data-driven scenario detection from machine-readable P&IDs (preHAZOP). A software tool is developed that merges multiple P&IDs of modules into one plant-level DEXPI P&ID and then runs an adapted preHAZOP analysis on the combined P&ID of the modular plant.

BACKGROUND

Modular plants

Modular plants decompose a process into process equipment assemblies (PEAs), each delivering a defined process function and equipped with own automation. This automation is done by the Module Type Package (MTP) which is comparable to a driver of peripheral devices for a computer. It encapsulates the automation interface of a PEA and supports orchestration by the Process Orchestration Layer (POL). MTP ensures the manufacturer independent compatibility between each PEA as well as to the POL. Each PEA is able to execute certain services to perform dedicated unit operations. Rearrangement of the PEAs allows to perform different processes without building a completely new plant for one new product.

While the modular concept and MTP are defined by the VDI/VDE/NAMUR 2658 [4] and 2776 [5] guidelines and different vendors are offering POLs or support to create MTP-files, there is no example of a safety assessment for the approval of a modular plant.

DEXPI P&ID

P&IDs are central documents throughout planning, construction, operation, and modification of process plants. They represent equipment, piping, valves, and instrumentation and control functions in a standardized way (e.g., via ISO/IEC-related standards), allowing consistent communication across disciplines. DEXPI e.V. is an initiative comprising various representatives from industry and academia who are working on common data exchange formats. The first implementations were carried out with the DEXPI Process Specification [6] and the DEXPI P&ID Specification [7]. In October 2025 were the DEXPI 2.0 Specification released which combines the Process Specification and P&ID Specification [8]. DEXPI is a standardized exchange format for P&IDs grounded in ISO 15926 concepts, typically realized as an XML-based schema that represents plant topology and attributes in a machine-readable form. While the DEXPI P&ID Specification relied on a Proteus-XML schema, DEXPI 2.0 uses a common XML format. The DEXPI format aligns with different international standards such as ISO 15926 [9]. The P&ID files in this work were created by using the software PlantEngineer from X-Visual Technologies GmbH.

Modular HAZOP

A HAZOP (Hazard and Operability) analysis identifies hazards and operability problems by systematically generating deviations from design intent using guidewords and parameters, then analyzing causes and consequences in an interdisciplinary team. The considered process is divided into functional units and their intended operation is described as a target function. While effective, the method is labor-intensive. Modular HAZOP extends HAZOP thinking to modular plants by structuring safety knowledge into module-oriented pieces and defining interfaces so results can be recombined for different plant configurations. For a modular plant the PEAs can be chosen as the functional units.

The ISSA (International Social Security Association) suggests seven guidewords in combination with parameters to form a deviation [10]. These guidewords are: no, more, less, as well as, partially, inversion, differently than. Three of them are considered in this work which are ‚no', ‚more' and ‚less'. The considered parameters in this work are temperature, flow and pressure. The combination of the other guidewords with the parameters is in certain cases not reasonable or brings up an open interpretation of the deviation case and should be discussed by a HAZOP team.

Klose [11] suggested in his doctoral thesis an approach to execute a HAZOP analysis for modular plants. He considered equipment-specific safety (mHAZOP) and process safety (pHAZOP) separately in the first place. This is because each PEA is built in a more generalized way and not tailored with a certain process in mind. The operator of the modular plant knows about the planned processes and can execute the p-HAZOP. Afterwards the m- and p-HAZOP are combined to check if the selected configuration of the PEAs is suitable for the process. Klose defined a PEA as a so-called HAZOP-ode which features one or more HAZOP-Interfaces to connect to other HAZOP-Nodes (PEAs) or the plants infrastructure. The different cases of deviations are applied to the HAZOP-Nodes. The HAZOP-Interfaces are relevant to transfer deviations from one HAZOP-Node to another one. [11-13]

preHAZOP

preHAZOP is a tool approach developed by Oeing et al. [14] that reads a DEXPI-P&ID and simulation results to build a graph model of the plant, enrich it with equipment, streams, and safeguards, and then detect typical HAZOP scenarios based on a machine-readable scenario database.

DEXPI P&IDs provide structured information about plant topology, equipment and connections. This topology is transformed into a directed graph (stored in GraphML) that becomes the basis for algorithmic searches of hazardous constellations. In addition, operating conditions are incorporated by mapping data from a process simulation onto the same graph.

Based on this combined model, preHAZOP detects potential scenarios using a scenario database that formalizes common HAZOP elements (guideword, parameter, cause and consequence) together with machine-checkable requirements expressed as graph patterns and attribute constraints. The tool is able to recognize functional and instrumentation-related structures by classifying valves and pipes, identifying measurement locations and control loops, and detecting the presence and assignment of protective devices such as relief paths, while also accounting for disabling configurations like isolating valves. The output is a structured list of scenario instances linked to specific equipment or sections of the plant, complemented by fields that indicate where automated assessment is insufficient and manual verification is needed (e.g., confirming design limits).

This contribution adopts the graph-centric idea but adapts the method to better fit modular plants, extend scenario generation, and support use cases without simulation data. The general workflow of the preHAZOP is presented in Fig. 1, where the added and adopted steps are outlined in blue.

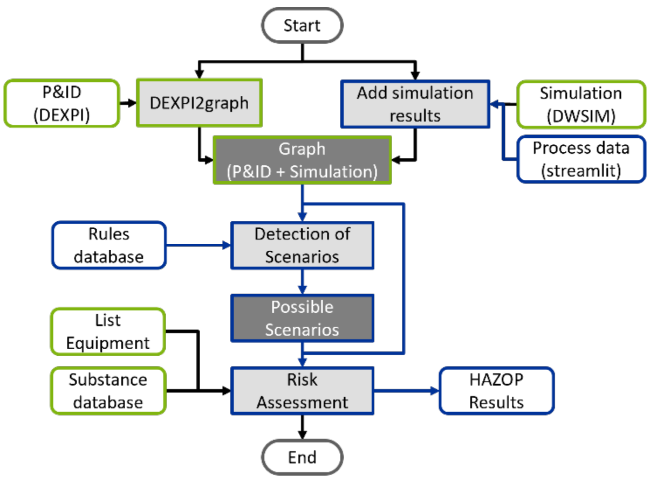

Figure 1. Suggested preHAZOP workflow. Blue marked steps are added or adapted from the original workflow.

METHODOLOGY

Laboratory set-up

The suggested workflow uses a modular reactor setup from the laboratory as an example for the P&ID flowsheets. The laboratory setup consists of four PEAs, which are shown in Fig. 2. These comprise a reactor PEA, two identical dosing units and a temperature PEA. The dosing units feed the two reactants via the temperature PEA into the reactor, where the reaction takes place before the product is discharged into another tank. The temperature PEA provides the required flow temperature for the reactants and also enables the temperature of the reactor to be controlled.

The Reactor-PEA is a continuous stirred tank reactor (CSTR) consisting of a vessel with a heating jacket, a stirrer with motor, three sensors to measure the level, the temperature and the conductivity of the substance filled in. The reactor has two inlets to feed educts inside of it and one outlet for the product with a controllable solenoid valve as well as an in- and outlet at the heating jacket.

The Dosing-PEA consists of a pump, a mass flowmeter and a storage tank. The Temperature-PEA is realized by a thermostat and is depicted here as a combination of a pump and a heater.

P&ID merge

In the workflow of Oeing [14] it was not necessary to consider multiple P&IDs. Since each PEA provides an own P&ID it is necessary to combine them to form the P&ID of the complete modular plant. To provide a user-friendly tool, the here presented workflow can executed by using a Streamlit application. Calling the python-file opens up a new tab in the user default browser, running the HMI. In the first step, the user is able to upload a DEXPI P&ID file or can select from already uploaded files.

For P&IDs of PEAs, correct and consistent interface definition is crucial. The PEA interfaces are defined as in- or outlets and are preceded by flanges. The flange objects store interface-related engineering constraints such as nominal diameter, design pressure, and temperature range.

Interface IDs follow a structured naming convention and are stored in attributes depending on whether an interface is an inlet, outlet, or bidirectional port. This convention allows the merging tool to automatically identify connection candidates, directions, and required adjustments.

Information about the PEA interfaces is extracted and listed to select how the different PEAs are connected with each other. When combining multiple DEXPI files, ID collisions must be avoided. The tool therefore prefixes each element ID with a PEA-specific shorthand and updates all references consistently across equipment, piping networks, and instrumentation functions. Simultaneously, it extracts geometric information (coordinates and extents) for PEA layout computation and stores interface coordinate data for later routing of inter-module connections. The individual P&IDs of the PEAs from the laboratory setup are shown in Fig. 2 as well as the combination of them to the complete modular setup.

To create a readable combined P&ID, PEAs must be arranged without overlaps and ideally with short connection lines. By using constraint programming in form of the CP-SAT-solver from the OR-Tools library and modeling each PEA as rectangle on the drawing sheet, enables to enforce certain rules. The first rule is that PEAs does not overlap and must keep a minimum distance. Secondly PEAs must remain within the sheet boundary and avoid the title block area. Lastly, an objective function minimizes the sum of Manhattan distances between connected interface points, discouraging small misalignments that would create unnecessary bends. This transforms a reasonable positioning into a reproducible optimization problem. The solver output is translated into shifts applied to all elements of each PEA P&ID so that the PEA internal structure remains intact while the plant-level arrangement changes. Fig. 3 shows the steps of the

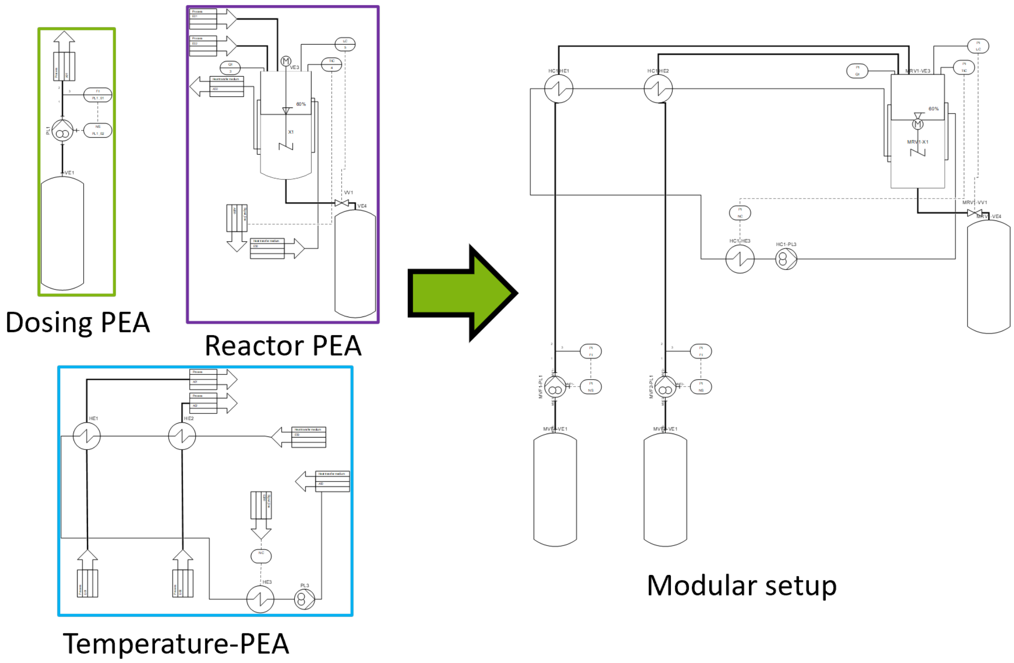

Figure 2. P&IDs of individual PEAs and combination to complete P&ID of the modular setup.

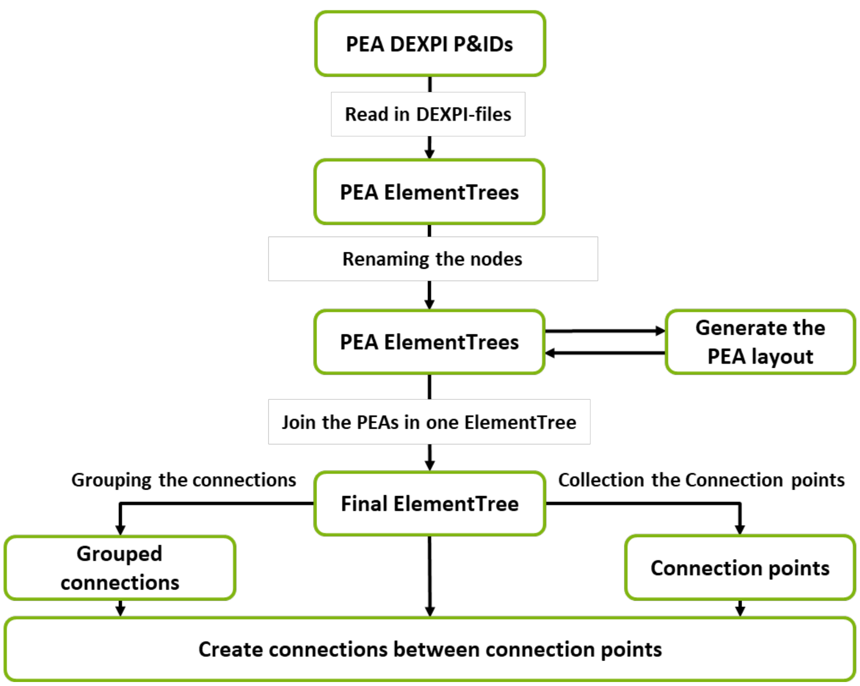

Figure 3. Procedure of reading out multiple PEA P&IDs and creating connections between their interfaces to create a combined P&ID.

programmed workflow to connect multiple P&IDs at their distinct interfaces.

After placement, the tool creates inter-module piping segments between flange coordinates. This is done by collecting all interfaces and grouping them accordingly to their function as inlet or outlet. Before the connections are created, they are grouped together. Connections with identical start and end points are combined. This can result in a 1:1 connection between two points (single start to single end) as well as 1:n or n:1 links (multiple starts or ends). For the later one T-pieces are inserted and positioned between PEAs to avoid placing junctions inside PEA drawings. Additionally, a direction alignment is performed since individual interfaces can be defined as bidirectional. In Fig. 4 the procedure to create connections and inserting T-pieces if necessary is shown.

Before creating a connection, the tool compares flange attributes and records inconsistencies—for example mismatches in nominal diameter or minimum and maximum design pressure and temperature. This provides immediate feedback on interface compatibility and supports safer PEA coupling decisions early in engineering.

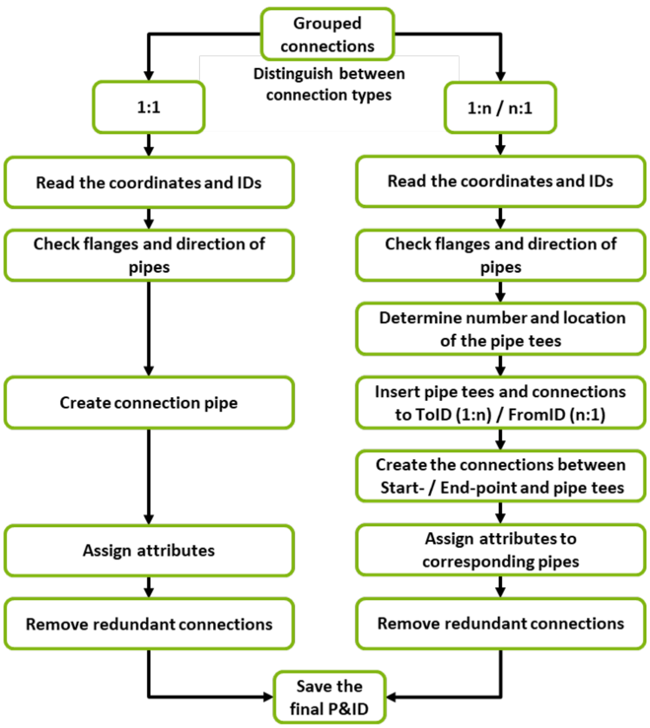

Figure 4. Procedure to check if its necessary to insert T-pieces between PEAs and how to connect them.

Adapted preHAZOP for modular plants

The original preHAZOP concept depends strongly on simulation data and a scenario database. For modular plants, simulation data may not exist when assessing a single PEA, or the final plant process may not yet be fixed. This work therefore adapts the preHAZOP so that scenario recognition remains possible without a simulation, while still benefiting from simulation or manually entered process data if available.

Instead of a purely pattern-based scenario search in a spreadsheet, this workflow implements a rule database organized by individual equipment classes in separated YAML-files. Within this rule base, different rule types are distinguished: rules that define local deviations as events originating at specific equipment, including frequency estimations and associated safeguards; rules that map these deviations to local consequences such as damage or leakage based on guideword–parameter combinations; rules that specify how deviations propagate forward or backward through the system depending on the type of piping; and rules that describe how equipment responds to deviations arriving from upstream or downstream, optionally depending on specifications such as the presence of a heating jacket, inertization, an agitator, or a control loop. This organization enables richer and more explicit logic than a flat table and aligns well with modular HAZOP thinking, because deviations can be generated locally within a PEA and then combined across PEA boundaries through propagation via the defined interfaces.

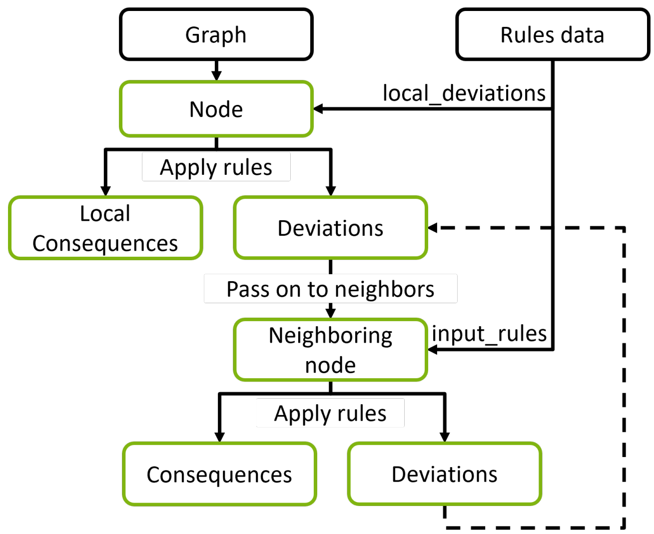

Figure 5. Workflow of applying the safety rules on the extracted graph.

The detection procedure follows two consecutive steps. First, the algorithm generates initial deviations at each node of the extracted graph based on the local deviation rules and records the corresponding local consequences immediately as scenario candidates. Second, these deviations are propagated through the graph using a queue-based mechanism. Whenever a deviation reaches another node, the engine checks the applicable input rules for that equipment, records any resulting consequences, and continues propagation if the defined propagation rules permit it. To keep the output manageable and to prevent an uncontrolled growth of near-identical scenarios, repeated events are filtered, for example when similar causes originate from the same equipment class at a node, and the propagation depth can be restricted, with a default limit of up to six nodes. The resulting scenarios are then stored in a structured, Excel-like table format consistent with modular HAZOP documentation, including deviation, cause, consequences with severity and frequency considerations, and safeguards that are either already present or recommended. Fig. 5

illustrates at which points the rules are applied in the procedure and how deviations are propagated to its neighbor nodes.

To support different stages of engineering maturity, the tool can handle process data in several ways. If simulation results are available, they can be imported in the same manner as in the original preHAZOP workflow. If no simulation file exists and operating conditions are determined manually, users can enter minimum and maximum operating pressure and temperature as well as relevant media, either as global default values or as equipment-specific overrides. If no process data are available at all, the scenario detection still runs, although parameter-based checks and media–material evaluation may be more limited. In addition to producing scenario lists, the adapted workflow performs two engineering checks that add practical value. Operating pressures and temperatures, whether derived from simulation or manual input, are compared against the design limits stored in the P&ID, so that exceedances and critical mismatches between neighboring equipment design limits can be documented as potential weak points during upset conditions. Furthermore, a media–material compatibility check is carried out using a dedicated database that flags problematic combinations with an A–D rating and can identify mechanisms such as catalytic decomposition, for example the incompatibility risk of hydrogen peroxide in contact with stainless steel. Any problematic combinations identified in this way are exported to support targeted follow-up in the subsequent engineering review.

Web Application Implementation

To make the workflow usable for engineers, the toolchain is implemented as a Streamlit web app with two separate tabs. In the first tab the user uploads PEA P&IDs, selects the PEAs, defines their interface connections via dropdowns populated from detected ports, specify attributes for connecting pipes, and export the configuration for reuse. The merged DEXPI P&ID and an interface mismatch report are returned.

In the second tab, the user runs the preHAZOP with the previously generated P&ID or is able to upload an older P&ID. Process data can be optionally entered either manually or in form of a simulation file. After running the analysis, the results can be downloaded as a table.

Validation

The workflow involving the simulation was tested by using a DWSIM simulation representing the lab set-up with a saponification reaction. In this reaction sodium hydroxide reacts with ethyl acetate to form sodium acetate and ethanol.

As a case for manual data input the oxidation of sodium thiosulfate with hydrogen peroxide is considered which serves as an example for a highly exothermic reaction [15, 16]. For 1 M sodium thiosulfate and 2.2 M hydrogen peroxide at 40 °C results in a temperature increase of 70 °C to 110 °C inside of the reactor. As a result, the HAZOP table shows that the process temperature exceeds the maximum operating temperature of the reactor. Additionally, the media and material compatibility check gives a message that hydrogen peroxide should not get contact with stainless steel.

The merging tool successfully combined multiple PEAs into a single P&ID without overlap and with short connection paths. The adapted preHAZOP detected meaningful scenarios both on the individual PEA level and on the combined plant level; when simulation data were available, the design-vs-operation checks identified a simulated design pressure exceedance (not necessarily representing the real lab setup, but validating the check mechanism). Media–material checks did not reveal issues for the lab media and materials considered.

The workflow demonstrates manual derivation and entry of operating parameters, including estimating the maximum adiabatic temperature rise for a strongly exothermic reaction. The merging workflow handled a larger number of PEAs, bidirectional interfaces, and multi-branch connections, including correct direction adjustments and T-piece insertion.

The adapted preHAZOP produced both intra-module and inter-module scenarios. Importantly, the additional checks detected a design-vs-operation temperature violation for a downstream pump (operating temperature exceeding the pump's max design temperature) and flagged a problematic media–material combination involving hydrogen peroxide and stainless steel (rated poor due to catalytic decomposition). These findings illustrate how the tool can surface concrete engineering issues early, even without detailed dynamic simulation.

SUMMARY AND CONCLUSION

This contribution builds up an the preHAZOP tool developed by Oeing et al. and adapts it for modular plants by incorporating modular safety concepts of Klose. The preHAZOP workflow is complemented with the option to combine multiple P&IDs into a complete P&ID of a plant and gives the opportunity to enter process parameters manually instead of relying on simulation files. It demonstrates that DEXPI P&IDs can serve as a practical, machine-readable backbone for two high-impact automation steps in modular plant engineering. Firstly, showing early safety assessment via graph-based, rule-driven scenario generation. Secondly, it provides a tool for rapid planning of different kinds of possible plant configurations by merging PEA P&IDs.

One of the main focuses in this work lies on the interfaces of the PEAs to connect the P&IDs with each other as well as compatibility checks between the PEAs.

Standardized connection points combined with manufacturer-provided piping attributes allow plausibility checks that are directly relevant for modular approval discussions (compatibility of design limits, nominal diameter, etc.). This helps in early phases of setting up a new plant configuration, to check if PEAs are allowed to be combined.

At the same time, limitations remain typical of knowledge-based safety automation: scenario quality depends on the completeness and correctness of rule databases, equipment classification, and available process data. The work therefore positions the tool as an accelerator for early-stage studies and as structured input for expert HAZOP teams—not as a full replacement for interdisciplinary review.

Several extensions for the preHAZOP can be proposed to improve the workflow further. The layout can be optimized by reducing line crossings, improving T-piece placement strategies and removing the current drawing-size limitation. Additionally, the rule database should be expanded to more equipment classes, guidewords, and better equipment sub-classification (e.g., distinguishing heaters vs. coolers). The media–material database could be enriched with concentration and temperature dependence. Towards an improved compatibility check, an implementation of ex-zone detection or check whether certain components are explosion-proof or not would be helpful.

Beneficial for the further automation of this workflow is the implementation of a connection to a chemical database to fetch safety relevant information of the used substances. Borgelt et al. has shown the implementation of such databases like the ChEBI, KEGG and PubChem [17].

Because DEXPI was updated during this work, the workflow should be adapted to the newer schema and—critically—support “clean” DEXPI files where properties are mapped into standard DEXPI attributes rather than vendor-specific attribute sets. This would improve interoperability with other authoring tools and strengthen the value of standardized P&ID data for safety automation.

A practical next step for usability is to leverage the HMI information contained in MTP files as a “preview” during plant configuration. Since PEAs in modular automation are already packaged with MTP-based interfaces, an automatically generated (or extracted) HMI view could guide users to select the correct connection points between PEAs more intuitively—reducing errors in manual interface selection and aligning the P&ID-based configuration step with the operational perspective of the PEA automation.

This work presents a coherent, implementable approach for accelerating modular plant safety assessments by reusing data already present in P&IDs. By merging PEA P&IDs (DEXPI) into a P&ID of a complete modular plant and applying an adapted, rule-based pre-HAZOP on a graph representation, the workflow enables systematic detection of deviation–cause–consequence chains across PEA boundaries and adds practical checks for design vs. operating limits and media–material compatibility. Implemented as a Streamlit web app and validated on modular examples, the workflow demonstrates how standardized engineering data can support faster, more reproducible early-stage safety assessments—an important step toward accelerating the approval of modular plants.

DIGITAL SUPPLEMENTARY MATERIAL

A collection of the created and used files can be found here: https://repository.nfdi4cat.org/dataset.xhtml?persistentId=hdl:21.11165/4cat/86xp-e338 This includes: Python-files, YAML-files with rules, Excel-files containing results of the HAZOP analysis and DWSIM simulation file.

ACKNOWLEDGEMENTS

The authors thank the German Federal Ministry for Economic Affairs and Energy (BMWE) for funding this research (funding no. 03EN2100B).

Open access funding enabled and organized by Projekt DEAL.

AUTHOR IDENTIFIERS

Author ORCIDs:
Schmitz: 0009-0006-2883-1617
Kockmann: 0000-0002-8852-3812

REFERENCES

1. Klose A, Lorenz J, Bittorf L, Stark K, Hoernicke M, Stutz A, Weinhold H, Krink N, Welscher W, Eckert M, Unland S, Menschner A, Da Silva Santos P, Kockmann N, Urbas L. Orchestration of modular plants. atp 63:68-77 (2022). https://doi.org/10.17560/atp.v63i9.2599
2. Bindel T, Hofmann D. R&i-fließschema. Springer Fachmedien Wiesbaden (2016). https://doi.org/10.1007/978-3-658-15559-9
3. Baerns M, Behr A, Brehm A, Gmehling J, Hinrichsen K, Hofmann H, Kleiber M, N. Kockmann, Onken U, Palkovits R, Renken A, Vogt D, Technische Chemie. Wiley-VCH (2023)
4. Maurmaier ASM. Dezentralisierte kommunikationsarchitektur für direkte modul-modul-interaktion auf basis von standardisierten konstrukten der vdi/vde/namur 2658. Automation

2019 :343-360 (2019). https://doi.org/10.51202/9783181023518-343
5. Verein Deutscher Ingenieure, VDI 2776 Blatt 1. Process Engineering Plants - Modular Plants - Fundamentals and Planning Modular Plants, Düsseldorf (2020).
6. DEXPI e.V., DEXPI Process Specification 1.0 (2023) https://dexpi.org/static/process_model_1.0/index.html
7. DEXPI e.V., DEXPI P&ID Specification 1.4 (2024) https://dexpi.org/static/pid_specification_1.4/
8. DEXPI e.V., DEXPI Specification 2.0 (2025). https://gitlab.com/dexpi/Specification
9. ISO 15926-2, Industrial Automation Systems and Integration – Integration of Life-Cycle Data for Process Plants Including Oil and Gas Production Facilities – Part 2: Data Model, Beuth Verlag, (2013)
10. International Social Security Association, Das PAAG-/HAZOP-Verfahren und weitere praxisbewährte Methoden, Jedermann-Verlag GmbH (2020)
11. Klose A. Modulare HAZOP für flexible anlagen der prozessindustrie. VDI Verlag (2023). https://doi.org/10.51202/9783186479204
12. Pelzer F, Klose A, Miesner J, Schmauder M, Urbas L. Safety in modular process plants: demonstration of safety concepts. Elektrotech. Inftech. 138:462-468 (2021). https://doi.org/10.1007/s00502-021-00928-8
13. Klose A, Kessler F, Pelzer F, Rothhaupt M, Kostiuk D, Kabashi A, Forkel V, Urbas L. Representing causal structures in HAZOP studies. 2021 26th IEEE International Conference on Emerging Technologies and Factory Automation (ETFA) :1-4 (2021). https://doi.org/10.1109/etfa45728.2021.9613357
14. Oeing J, Holtermann T, Welscher W, Severins C, Vogel M, Kockmann N. Prehazop: graph?based safety analysis for early integration into automated engineering workflows. Chemie Ingenieur Technik 95:1083-1095 (2023). https://doi.org/10.1002/cite.202200222
15. Frede TA, Greive M, Kockmann N. Measuring kinetics in flow using isoperibolic flow calorimetry. Reactions 3:525-536 (2022). https://doi.org/10.3390/reactions3040035
16. Cohen W C, Spencer J L, Determination of Chemical Kinetics by Calorimetry. Chem. Eng. Prog., 58, 40–41 (1962)
17. Borgelt H, Kitel FG, Kockmann N. Ontology-based data pipeline for semantic reaction classification and research data management. Computers 14:311 (2025). https://doi.org/10.3390/computers14080311