

Separation of Concern Capabilities of Information Model Candidates for Modular Plant System Engineering Lines

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ABSTRACT

Pharmaceutical and fine chemical industries face strong pressure to shorten time-to-market while maintaining compliance with complex regulatory frameworks. These conflicting demands require rapid process design, validation, and scale-up. Modular production plants standardized in VDI 2776 and VDI/VDE/NAMUR 2658 have emerged as a promising strategy to shorten engineering and validation efforts. The Product-Process-Resource (PPR) philosophy represents a key approach to efficient data management in modular plant engineering. It enables the separation of different flexibility dimensions into distinct, relevant aspects that can ideally be exchanged or modified independently. To realize this principle in practical applications, formalized information models and ontologies serve as a key enabler for structuring and managing semantic data. This work investigates several information models and ontologies for the process engineering domain regarding their suitability to support separation according to the dimensions defined by the PPR approach. As a metric for separability, coupling measures from Design Mapping Matrix (DMM) research are applied. This work provides the foundation for improving computer-aided engineering tools to efficiently handle modular processes while considering the reshaped information distribution.

Keywords: Process Design, Industry 4.0, AAS, DEXPI, Modular Plants

INTRODUCTION

The chemical and fine chemical industry has an increased need for shorter times to market [1]. One approach to address this challenge is the utilization of modular plants [2]. In this context, the chemical process is divided into sub-functions, each provided by a Process Equipment Assembly (PEA). PEAs may be engineered prior to or in parallel with process development. As detailed PEA engineering is performed independently by the manufacturer, process-specific requirements are reduced to selecting an appropriate PEA topology.

This approach results in a significant knowledge shift compared to traditional monolithic plants. In monolithic plants, most of the knowledge about the chemical process, its operating conditions, recipes, operation, and detailed plant engineering is centralized within a single organization, often supported by service providers [3]. In modular plants, this knowledge is distributed among different parties, each specialized in a specific domain. [4]

introduced a philosophy that represents this changed knowledge distribution and its functional implications as a key approach for efficient data management in modular plants. This philosophy is known as the Product-Process-Resource (PPR) model. Building on this concept, the model has since then been extended with additional requirements [5][4], [5], [6], [7].

Because the different domains represented in the PPR model must interact and exchange information, efficient and standardized information exchange is a key factor in realizing the advantages promised by the modular plant approach [8], [9]. For instance, VDI/VDE/NAMUR 2658 [10] introduced the Module Type Package (MTP) as a standardized, machine-readable exchange format that enables rapid integration of PEAs into the Process Orchestration Layer (POL) of a modular plant. The MTP was specifically designed to address a particular information exchange requirement.

In addition, further standards exist that were not specifically developed for modular plants but can

nevertheless contribute to the need for standardized, machine-readable information exchange. [11] demonstrated the application of the Data Exchange in the Process Industry (DEXPI Plant & Process) standard [12] in the context of modular plants. Furthermore, it showed that a piping and instrumentation diagram (P&ID) modeled using DEXPI Plant can be successfully transferred to an MTP representation [11]. Furthermore, [9] demonstrated that interlinked information between DEXPI Plant and On-toCAPE [13] can support modular plant design within the context of the PPR model.

This work aims to provide a structured overview of how existing information models contribute to defined requirements derived from the PPR model. The overview supports the future development of machine-readable information exchange throughout the engineering and operation of modular plants. To enable systematic mapping, only information models that provide a sufficiently high level of abstraction to allow allocation within the PPR model are considered. At the same time, the evaluated information models are required to offer a technical specification that is detailed enough to enable matching at the class level.

PRODUCT PROCESS RESOURCE MODEL

In [4] the authors describe the structure of a digital twin for the process industry from a user-oriented perspective. They identify several data models that play an important role throughout the lifecycle of a chemical process plant. The authors argue that a plant-independent description level is a prerequisite for the effective use of digital twins and for the efficient and effective design of new production methods and processes [4]. To address this, the digital twin is structured into partial models that can be created and maintained by different disciplines, departments, and organizations. Overall, the digital twin is subdivided into six models:

- **Product model:** Contains information about the intended product.
- **Process model:** Contains information about thermodynamic, chemical, physical, and control-engineering relationships.
- **Resource model:** Contains information about the mechanical functionality and operational attributes of the plant and equipment structure.
- **Transformation model:** Contains product-related information about requirements for process control as well as individual transformation and separation steps. It is derived by combining the product and process models.
- **Capabilities model:** Contains plant-related information about the capability of equipment to

perform specific process-engineering operations, including static and dynamic parameters. It is derived by combining the process and the resource models.

- **Operation model:** Contains information about optimized operating parameters and recipes to enable optimized production scenarios. It is derived by combining the transformation and capabilities models.

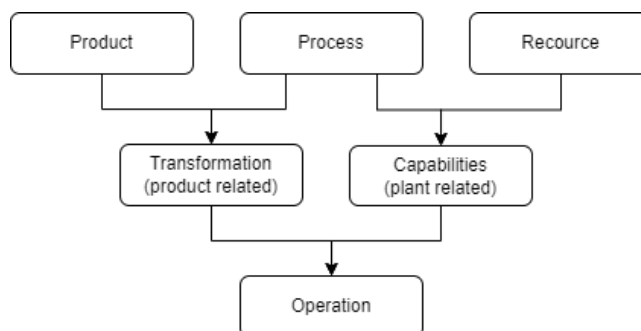


Figure 1. Visualization of the proposed Digital Twin structure according to the PPR-Model by [4].

In [5] several general challenges arising from this structure are highlighted, including:

- quality assurance and specification of simulation models,
- open and standardized interfaces,
- simulation and optimization algorithms that consider intellectual property (IP) issues, and
- model structuring and semantic description as key research and development challenges.

In the following section, requirements resulting from the different disciplines utilizing the model are summarized.

Product Model

The product model encompasses information related to the properties and specifications of chemical components and products. It contains component- and substance-specific properties, including physical properties of component mixtures and detailed product specifications [4] [5]. In addition, the product model incorporates specifications and data sheets [14] and provides information on product and component storability, safety- and transport-related requirements, as well as application and sales aspects [4].

Process Model

The process model contains information on thermodynamic, chemical, and physical engineering relationships, such as material transport coefficients and

reaction kinetics [4]. It further provides the information required for use in process simulation environments and includes the equations employed for process modeling and analysis [4], [5].

Resources Model

The resource model represents equipment-related information of the production system. It models attributes and characteristics of equipment, including properties specific to mobile equipment, and provides a structured description of equipment-related characteristics relevant for plant operation and engineering [4], [5]. In addition, the resource model includes a comprehensive list of equipment elements forming the plant structure [8].

Transformation Model

The transformation model contains equipment-independent information describing the production process. This includes laboratory measurement data, equipment-independent simulation models, and conceptual design knowledge related to the process [5], [8]. Furthermore, the transformation model captures key process characteristics such as residence times, throughputs, and risk potentials [4]. It also defines the capability requirements that must be fulfilled by the corresponding capabilities model [9].

Capabilities Model

The capabilities model describes plant-related information characterizing the ability of equipment to perform specific process-engineering operations. It includes stationary and dynamic parameters of a largely product-independent process plant, as well as capabilities resulting from the boundary conditions of the employed equipment [4]. In addition, the model captures material property parameters of the equipment and provides operational and behavioral information, including aspects of automation [5] [14]. Technical operating limits, such as maximum and minimum values for temperature, pressure, and viscosity, are also represented within the capabilities model [14].

Operation Model

The operation model addresses the execution and optimization of plant operation. It includes the modeling of recipes, as well as the monitoring and execution of operational procedures [15]. Furthermore, the model supports plant and PEA configuration and captures optimized process parameters to enable efficient and stable operation of the production system [4], [15].

SELECTED INFORMATION MODELS

The evaluated information models are selected based on the stated criteria. Specifically, the selected

models:

- provide a detailed and formally defined specification,
- exhibit a level of abstraction that allows concrete allocation to aspects of the PPR model,
- support technical implementation through machine-readable or formally specified structures, and
- classes are excluded that serve only internal or structural purposes of the model (e.g., datatype definitions), as these do not contribute directly to fulfilling PPR submodel requirements.

For example, the Asset Administration Shell (AAS) submodel *Handover Documentation* is capable of describing common document types and can therefore be applied across multiple PPR submodels. In contrast, the AAS submodel *Carbon Footprint* models calculation methods in a descriptive form (e.g., as strings) and can thus be concretely allocated to a specific PPR submodel, such as the *Product* submodel.

DEXPI Plant & DEXPI Process

DEXPI aims to provide a general method for data exchange, interoperability, and data integration covering all lifecycle phases of (petro-)chemical plants, from functional specification to operation. It seeks to avoid format conversions and data loss across CAE system boundaries, enable efficient project handover, reduce barriers between different CAE systems, support long-term storage in CAE-independent formats, and facilitate the coexistence of multiple engineering systems within an organization.[16]

The DEXPI Specification includes the DEXPI Plant and the DEXPI Process Model. DEXPI Plant represents plant engineering information and associated graphical representations e.g. Piping and Instrumentation Diagrams (P&ID). DEXPI Process represents chemical processes and associated graphical representations e.g. Block Flow Diagrams (BFD).

AAS Submodels

The Carbon Footprint submodel template supports the exchange of an asset's carbon footprint along the value chain to improve interoperability between stakeholders involved in documenting, evaluating, or optimizing environmental impacts. While it may contribute to initiatives such as the Digital Product Passport or Product Environmental Footprint. [17]

The Digital Nameplate submodel template provides interoperable asset nameplate information for Asset Administration Shells by defining standardized properties, ideally aligned with dictionaries such as ECLASS and the IEC Common Data Dictionary. It establishes a

standardized digital nameplate structure for process industry and factory automation equipment, while allowing application-specific extensions through supplementary submodel templates. [18]

The Functional Safety submodel defines a structured engineering data model for safety-relevant devices to support functional safety and reliability assessments in the design of safety control systems and related applications. Its intended benefits include reducing data-mapping effort, optimizing information exchange with engineering tools, supporting safety-oriented product selection, and enabling globally accessible, consistent product data independent of country, language, or culture. [19]

Module Type Package

The Module Type Package (MTP) provides a vendor-independent description interface for the automation interface of a Process Equipment Assembly (PEA). It includes descriptions of the human-machine interface (HMI), available services, procedures, and configuration parameters, as well as IP addresses and OPC UA nodes and their relations to data objects defined in VDI/VDE/NAMUR 2658 [10].

OntoCape

OntoCAPE is a large-scale ontology for the domain of Computer-Aided Process Engineering (CAPE), represented in a formal, machine-interpretable ontology language. It captures consensual process-engineering knowledge in a generic and reusable form, enabling knowledge sharing across software systems and supporting advanced engineering applications such as simulation model management, design data integration, electronic procurement, and mathematical modeling. [20]

Metadata4Ing Ontology

One of the main goals of the Metadata4Ing ontology is to enable documentation of data and material provenance in research processes. It is based on a generalized process model centered on the *processing step* class, in which data and material objects are represented as outputs, while methods, tools, and other contextual information are linked via dedicated classes, allowing complex research processes to be described through compositions of processing steps. [21]

METHODOLOGY

To achieve a transparent evaluation of various technically implemented standards with respect to an abstract philosophy representing general knowledge distribution, a multi-step methodology is applied. First, a literature review is conducted to identify suitable information models. This review focuses on standards that (i) provide a formal technical specification, (ii) exhibit an active

community or documented update history, and (iii) are sufficiently mature to support practical application.

To operationalize the PPR model, a second literature review is performed to identify requirements specific to the individual PPR submodels. Based on these requirements, a mapping matrix is constructed that relates each identified PPR submodel requirement to every specified class within the selected information models. This fine-grained level of detail enables a direct connection between the technical implementation of an information model and the abstract structure of the PPR model.

The generation and evaluation of the mapping matrices are performed automatically. The assessment of whether a given class contributes to a specific requirement is carried out manually using a binary (true/false) decision. To simplify the evaluation process, the assumption is made that if a superclass within an information model satisfies a requirement, all its' subordinate classes do so as well. The resulting matrices are then evaluated automatically. To account for differing numbers of classes across PPR submodels, the results are normalized accordingly. This normalization enables a comparative allocation of each standard to the respective PPR submodels.

The Python scripts used for generating and evaluating the matrices, as well as the completed matrices themselves, are provided in the accompanying GitHub repository <https://github.com/p2o-lab/-ESCAPE-36-Domain-Mapping-Matrices-supplementary-information>. Finally, the results are analyzed and discussed in detail.

DMM INTRODUCTION

To evaluate technically implemented classes against PPR submodel requirements, the Design Matrix Methodology (DMM) is adapted [22] [23]. To provide a structured overview of the suitability of the investigated information models for fulfilling PPR submodel requirements, a matrix-based evaluation is conducted for each combination of PPR submodel and information model.

In each matrix, the PPR submodel requirements are represented by the rows, while the classes of the respective information model form the columns. Each requirement-class combination is assigned a value of 0 if the class description does not contribute to fulfilling the requirement, or a value of 1 if it does. If no meaningful assignment is possible, the corresponding cell is left empty and excluded from the evaluation. This reflects the assumption that the implementation of a requirement does not necessitate the use of all available classes within an information model.

For each requirement, the assigned values are aggregated and normalized by the number of evaluated entries. This results in a representation in which, for each PPR submodel, a table is obtained where the rows

correspond to the requirements and the columns represent the normalized degree to which each information model satisfies the respective requirement. In the subsequent step, the mean value across all requirements of a PPR submodel is calculated. This yields a single value between 0 and 1 that describes the overall suitability of an information model to fulfill the requirements of that PPR submodel. A visualization is provided in Figure 2.

RESULTS

Figure 3 presents the outcome of the cross-dimensional coverage analysis as an overall heatmap. A higher value represents a better matching between the specification and the PPR-Submodel requirements. The rows correspond to the considered PPR-related concepts (Product, Process, Resource, Transformation, Capability, Operation), while the columns represent the analyzed standards and information models (OntoCAPE, AAS Carbon Footprint, DEXPI Process, MTP, DEXPI Plant, AAS Digital Nameplate, AAS Functional Safety, metadata ing classes). All values are normalized to the interval [0, 1] and express the relative degree to which a given model explicitly addresses a specific concept.

OntoCAPE achieves the highest overall coverage across all evaluated dimensions. In particular, strong scores are observed for Capability (1.000), as well as consistently high values for Product, Resource, and Operation (each 0.750) and Transformation (0.714). This indicates a broad and balanced semantic scope with respect to the PPR model.

The AAS Carbon Footprint submodel shows a pronounced focus on the Process dimension (1.000), with moderate coverage of Product and Transformation (0.500 each). All remaining dimensions exhibit negligible or zero coverage.

DEXPI Process demonstrates high alignment with Process (0.800) and Transformation (0.667). Product and Resource are only partially covered, while Capability and Operation are not explicitly represented.

The Module Type Package (MTP) model exhibits strong coverage for Capability (0.818) and Operation (0.750). Other PPR dimensions, including Product, Process, and Resource, are largely not addressed.

DEXPI Plant shows its highest relevance for Transformation (0.667) and Capability (0.600), with lower coverage for Operation (0.250). Product- and process-oriented aspects are only marginally represented.

The AAS Digital Nameplate submodel is strongly associated with Resource (1.000) and shows moderate relevance for Capability (0.400). All other dimensions show no explicit coverage.

The AAS Functional Safety submodel exhibits selective coverage, mainly for Capability (0.600) and Operation (0.250), while other PPR dimensions remain

unaddressed.

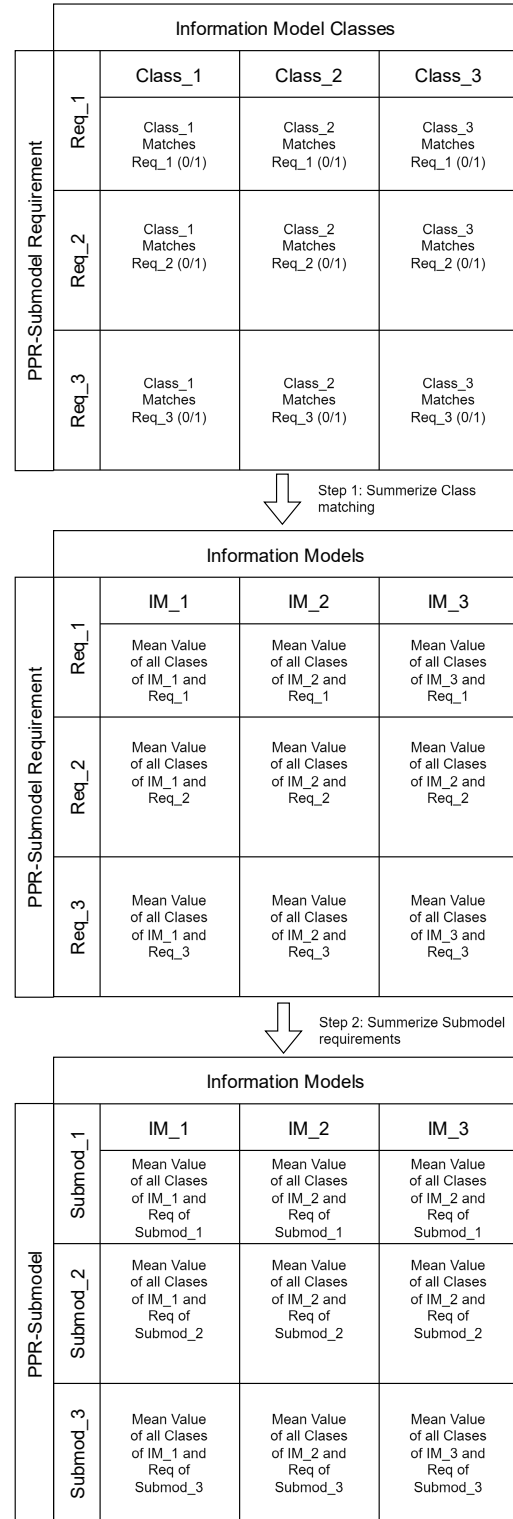


Figure 2. Description of the three step process to evaluate the information matching results. The corresponding data and code is available under <https://github.com/p2o-lab/-ESCAPE-36-Domain-Mapping-Matrices-supplementary-information>

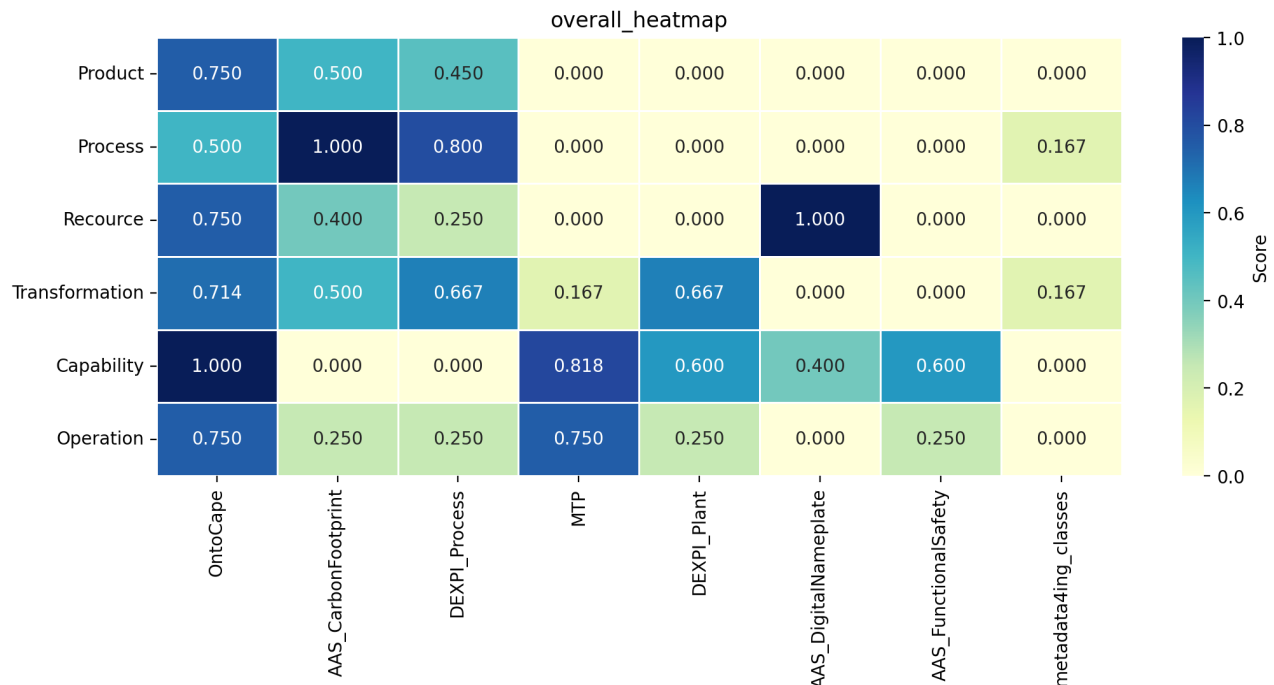


Figure 3. Heatmap of the cross dimensional analysis of the specified standards to the PPR-Model. A higher value represents a better matching between the specification and the PPR-Submodel requirements

Finally, the Metadata4ing classes show only minimal coverage, primarily for Process and Transformation (0.167 each), indicating a limited contribution to explicit PPR modeling.

DISCUSSION & OUTLOOK

The results highlight a clear differentiation between conceptually comprehensive ontologies and practically oriented engineering standards. OntoCAPE stands out with the most complete and balanced coverage across all PPR dimensions, underscoring its strength as a reference ontology from a semantic modeling perspective. However, this result must be interpreted with caution: OntoCAPE has not undergone a major specification update since 2009 and, to date, lacks documented large-scale industrial or production-level deployments. Its high scores therefore reflect conceptual expressiveness rather than validated applicability in current modular plant engineering practices.

In contrast, standards such as DEXPI, MTP, and the various AAS submodels exhibit narrower but more focused coverage profiles. DEXPI Process and DEXPI Plant emphasize process execution and plant structure, respectively, while MTP concentrates on capabilities and operations required for modular automation and orchestration. The AAS submodels further describe asset-centric, safety-related, or sustainability-related concerns. Although none of these standards individually achieve

comprehensive PPR coverage, they are actively maintained and have demonstrable relevance in industrial contexts.

The limited coverage of the Metadata4ing classes reinforce their role as generic framework and metadata structure rather than as domain-specific engineering model. They are well suited to complement other standards by providing traceability and documentation capabilities, but they cannot substitute detailed PPR semantics.

Overall, the analysis reveals a trade-off between semantic completeness and practical adoption. While OntoCAPE provides a rich conceptual foundation, its limited real-world uptake constrains its immediate applicability. Conversely, industrial standards offer pragmatic, implementation-ready solutions at the cost of reduced semantic breadth. These findings support the need for a combined modeling approach in modular plant engineering, in which actively used standards are combined for expressiveness, maintainability, and industrial relevance.

In the next steps, interfaces between the individual models can be evaluated according to their allocation within the PPR model, and the foundation for computer-aided tools suitable for the modular plant approach can be further substantiated.

ACKNOWLEDGEMENTS

Funded by the Federal Republic of Germany FKZ

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