MOSAICmodeling PlantDesign - an integrated engineering solution based on intelligent data exchange

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Dedicated to my grandfather

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Abstract

Considering the volatile macro-economic environment aggravating competitiveness in the increasingly globalizing market the most important challenge facing industrial companies is to achieve an innovation lead with high quality and reliability with shortened innovation cycles. For the entire life cycle of chemical plants, several stakeholders, such as owners, operators, vendors, and contractors, are working together in one or more different trades and using several highly specialized software packages. Improving the interoperability between heterogeneous software tools applied in plant design offers an enormous potential for the improvement of workflows and in particular the availability of consistent and transparent plant data in digital form for the entire life cycle of a plant.

In this thesis, the concept and the implementation of the integrated engineering tool *PlantDesign* have been developed. *PlantDesign* is an assistant system for the automated design of Modular Process Units (MPUs) with a high level of detail with respect to constructions as they consist of equipment, close and internal piping, process measure and control technology, instrumentation, and steelwork. The prototypical implementation has been successfully implemented in the modeling and simulation environment MOSAICmodeling [MOSAICmodeling, 2019]. Output of the tool is source code for automated creation of 3D plant models that can be imported into different commercial 3D CAD tools. A novel source code converter framework has been developed to generate a source code generator in a higher programming language for different target formats. The 3D models of the MPUs generated using *PlantDesign* are so-called intelligent and transfer graphical as well as plant and process information into the 3D CAD tool. Beside this, *PlantDesign* enables different import and export data interfaces to heterogeneous CAE software tools applied within the plant design of process plants. The data interfaces enable (semi-)automatic data handover between tools applied in the different planning disciplines, e.g. process simulation and 2D CAD tools.

By using the integrated engineering tool *PlantDesign* in academic teaching and for an example process from industrial practice, it was successfully demonstrated that both the automation of planning processes in plant design and the transfer of data could be improved across disciplines.

Kurzfassung

In Anbetracht des volatilen makroökonomischen Umfelds, das die Wettbewerbsfähigkeit im zunehmend globalisierten Markt verschärft, besteht die wichtigste Herausforderung für Industrieunternehmen darin, eine Innovationsführung mit hoher Qualität und Zuverlässigkeit bei verkürzten Innovationszyklen zu erreichen. Für den gesamten Lebenszyklus von Chemieanlagen arbeiten mehrere Stakeholder wie Eigentümer, Betreiber, Lieferanten und Auftragnehmer in verschiedenen Gewerken und unter Nutzung vielfältiger hochspezialisierter Softwarepakete zusammen. Die Verbesserung der Interoperabilität zwischen heterogenen Softwarewerkzeugen im Anlagenbau sowie die Automatisierung von Planungsschritten bietet ein enormes Potenzial zur Verbesserung von Arbeitsabläufen und insbesondere zur verbesserten Verfügbarkeit konsistenter und transparenter Anlagendaten in digitaler Form für den gesamten Lebenszyklus einer Anlage.

In dieser Arbeit wurde das Konzept und die Implementierung des integrierten Engineering-Tools *PlantDesign* entwickelt. *PlantDesign* ist ein Assistenzsystem für die automatisierte Planung von modularen Prozesseinheiten (MPUs) mit hohem konstruktiven Detaillierungsgrad, die aus Apparaten, Nahverrohrung und internen Rohrleitungen, Mess-, Steuer- und Regelungstechnik, Instrumentierung und Stahlbau bestehen. Die prototypische Implementierung wurde erfolgreich in der Modellierungs- und Simulationsumgebung MOSAICmodeling [MOSAICmodeling, 2019] implementiert. Das Tool erzeugt Quellcode zur automatisierten Erstellung von 3D-Anlagenmodellen, die in verschiedene kommerzielle 3D-CAD-Tools importiert werden können. Ein neuartiges Source Code Converter Framework wurde entwickelt, um einen Source Code Generator in einer höheren Programmiersprache für verschiedene Zielformate zu generieren. Die mit *PlantDesign* erzeugten intelligenten 3D-Modelle der MPUs übertragen neben grafischen auch Anlagen- und Prozessinformationen in das 3D-CAD-Tool. Darüber hinaus ermöglicht *PlantDesign* verschiedene Import- und Exportschnittstellen zu heterogenen CAE-Softwaretools, die im Rahmen der Planung von Prozessanlagen eingesetzt werden. Die Datenschnittstellen ermöglichen die (semi-)automatische Datenübergabe zwischen den in den verschiedenen Disziplinen eingesetzten Werkzeugen, z.B. Prozesssimulations- und 2D-CAD-Werkzeuge.

Durch den Einsatz des integrierten Engineering-Tools *PlantDesign* in der akademischen Lehre und zur Auslegung eines Prozesses aus der industriellen Praxis konnte erfolgreich gezeigt werden, dass sowohl die Automatisierung von Planungsprozessen im Anlagenbau als auch die Datenübertragung gewerke-übergreifend verbessert werden kann.

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Nomenclature

Abbreviations

Abbreviations	Description
$1NF$	First normal form (relational database scheme)
$2D$	Two-dimensional
$2NF$	Second normal form (relational database scheme)
$3D$	Three-dimensional
$3NF$	Third normal form (relational database scheme)
$4NF$	Fourth normal form (relational database scheme)
$5NF$	Fifth normal form (relational database scheme)
$BCNF$	Boyce-Codd normal form (relational database scheme)
BFD	Block/Basic flow diagram
$BREP$	Boundary representation
CAD	Computer-aided design
CAE	Computer-aided engineering
CAM	Computer aided manufacturing
CAP	Computer-aided Plant Design, course at TU Berlin
$CAPE$	Compter-aided process engineering
$CAPEX$	Captital expenditure

CEN	European Committee for Standardization
CFIHOS	Capital Facilities Information HandOver Specification
CSG	Constructive solid geometry
DEXPI	Data exchange in process industries
Dir	Direct material balance
DLL	Dynamic link library
DMU	Digital mock-up
DWH	Datawarehouse
DXF	Drawing exchange format
E3D™	Everything3D (AVEVA)
ELN	Electronic lab notebook
ERP	Enterprise resource planning
FC	Flow control (sensor)
FEM	Finite element method
FI	Flow indicator (sensor)
FMI	Functional mock-up interface
GUI	Graphical user interface
H	Heating medium
HAZOP	Hazard and operability study
HETP	Height equivalent to a theoretical plate
IE&D	Integrated Engineering & Design (AVEVA)
IGES	Initial graphics exchange specification
Ind	Indirect material balance
IT	Information technology

JAR	JAVA archive
LC	Level control (sensor)
LI	Level indicator (sensor)
LIMS	Laboratory information management system
MB	Mass balance
MPU	Modular process unit
N	Theoretical stage
Namur	User Assocation of Automation Technologies in Process Industries
NS	Number of theoretical stages
NURBS	Nonuniform rational B-spline
O/O	Owner/operator
OPCUA	Open Platform Communications Unified Architecture
OPEN	Open Process ENgineering Database
OPEX	Operational expenditure
OWL	Web ontology language
P	Packed column
P&ID	Piping and instrumentation diagram
PC	Presssure control (sensor)
PCA	POSC Caesar Association
PCS	Process control system
PDMS™	Plant Design Management System (AVEVA)
PFD	Process flow diagram
PI	Pressure indicator (sensor)
PIMS	Plant information management system

PML	Programmable macro language
PQM	Project Quality Management (Siemens)
QC	Quality control (sensor)
QI	Quality indicator (sensor)
RDL	Reference data library
SCDS	Simultaneous correction distillation, Chemcad distillation column model
SP	Service pack
SQL	Structured query language
STEP	Standard for the exchange of product model data
STL	Standard tessellation language
T	Tray column
TC	Temperature control (sensor)
TI	Temperature indicator (sensor)
TIA	Total Integrated Automation (Siemens)
URI	Uniform resource language
W3C	World Wide Web Consortium
XML	Extensible markup language

Greek Symbols

Symbol	Description	Engineering Unit
ν	Welding factor	$[-]$

Indizes

Symbol	Description	Max. Value
j	Theoretical separation stage	NS

Latin Symbols

Symbol	Description	Engineering Unit
$\dot{B}$	Bottom product flowrate	$[\frac{kg}{h}]$
$\dot{C}$	Cooling medium flowrate	$[\frac{kg}{h}]$
$\dot{D}$	Distillate product flowrate	$[\frac{kg}{h}]$
$\dot{F}$	Flowrate	$[\frac{kg}{h}]$
$\dot{H}$	Nominal head (pumps)	$[m]$
$\dot{L}$	Liquid flowrate	$[\frac{kg}{h}]$
$\dot{Q}$	Nominal capacity (pumps)	$[\frac{m^3}{h}]$
$\dot{R}$	Reflux flowrate	$[\frac{kg}{h}]$
$\dot{V}$	Vapor flowrate	$[\frac{kg}{h}]$
A	Area	$[m^2]$
c	Constant	$[-]$
D	Diameter	$[m]$
K	Factor wall thickness calculation	$[-]$
l	Length	$[m]$
n	Speed of rotation	$[\frac{1}{min}]$

p	Pressure	$[p]$
q	Thermal state of feed	$[-]$
R	Yield stength	$[\frac{N}{m^2}]$
S	Safety factor	$[-]$
x	Mole fraction liquid phase	$[\frac{mol}{mol}]$
y	Mole fraction vapor phase	$[\frac{mol}{mol}]$

Subscripts

Symbol	**Description**
bc	bubble cap (bubble cap tray)
col	Column
e	Elasticity (yield strength
$fall$	Falling
$feed$	Feed inlet nozzle
h	hole (sieve tray)
hm	Heating medium
i	inner, Index
max	maximal
$nominal$	Nominal
o	Reference state, outer
opt	Optimal
$start$	Starting value for iterative calculation
V	Vapor

v	valve (valve tray)
$vapBotIn$	Vapor bottom inlet nozzle

Superscripts

Symbol	**Description**
$'$	Refer to stripping section
B	Bottom product
bed	Packing bed (beween (re-)distributor)
D	Distillate product
f	Feed stage
HB	Heavy boiling component
LB	Low boiling component
rec	Rectifying section
str	Stripping section
tot	Total

1 Introduction

1.1 Problem definition and motivation

High production costs in highly developed industrialized countries, rapidly changing markets due to stagnation in traditional sales markets and rapid growth in emerging economies as well as growing competition due to the development of in-house production capacities in many industries make sustaining and, if possible, increasing competitiveness in the increasingly globalizing market the most important challenge facing companies [Vajna et al., 2009, p. 3]. The high prices caused by the high costs can only be enforced with products if companies can achieve a long-term innovation lead with high quality and reliability with shortened innovation cycles. Ongoing innovation usually entails higher complexity of the underlying products and manufacturing processes. Among other things, this includes process intensification, intelligent networking and integration of different areas and trades - especially information technology - but also an adapted structure for the execution of tasks in one's own company and with other companies, increasing scope of interdisciplinary teamwork - also across companies - as well as the introduction of new supporting technologies and methods.

Several stakeholders like owner operator (O/O), engineering, procurement and construction (EPC), supplier, vendor, and contractor companies are involved during the whole life cycle of industrial plants, especially during the planning phases. Thereby, a wide range of highly specialized computer-aided engineering (CAE) software tools are applied in the participating groups of the different disciplines and domains or even within the single working areas. It can be distinguished in homogeneous tools with the same functionality as well as heterogeneous software with different specialized functionalities. For both groups several tools of different vendors are on the market.
Improving the interoperability during the planning and the whole life-cycle of plants play a key role for digitalization in process industry. The challenges are well-known: Incompatible software and data formats complicate continuous and efficient planning, cause inconsistencies, are potential sources of errors, and cost valuable time.

The complex interaction between participating trades with respect to data handover during plant design is illustrated in the schematic overview in figure 1.1. Overlaps between the process and plant information of the individual trades must be considered with particular care, as any changes affect different work groups.

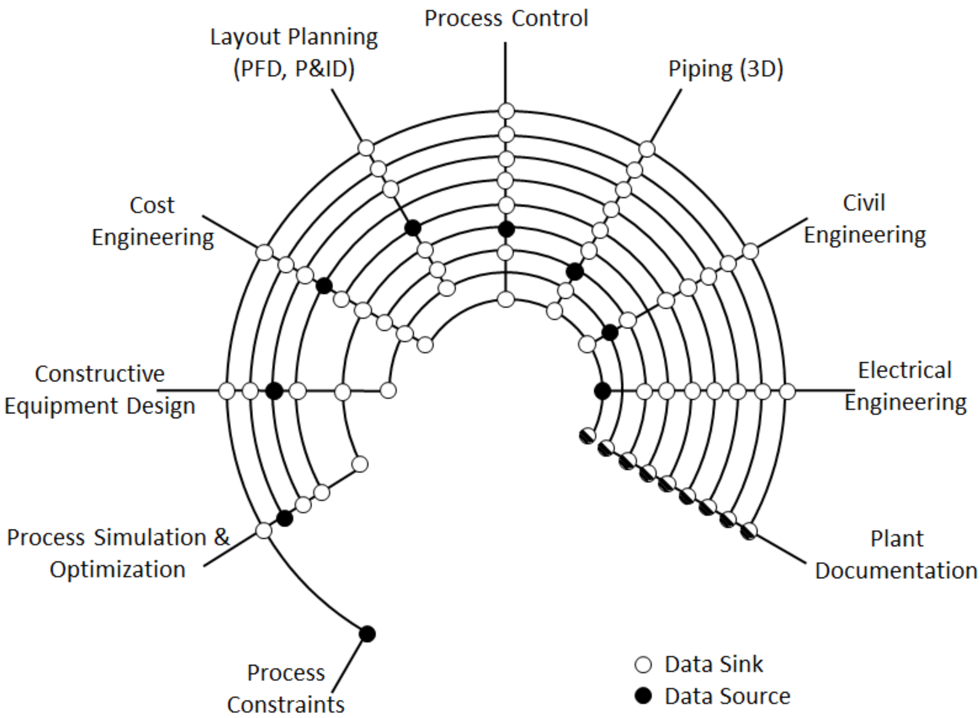


Figure 1.1: Trade-specific data exchange between tools applied in process industries [adapted from Fillinger, Bonart, et al., 2017]

The existing discrepancy in the current technological state of software interoperability represents a major deficiency for the process industry and leads to a variety of challenges. For the implementation of digitization in the process industry, in addition to the necessary international standardization efforts with regard to life cycle data models and data interfaces, adaptations of the business strategies of software companies and not least an extension of the training matrix of process engineers, especially regarding information technology and digitization strategies, are necessary. These points are reflecting needs and efforts of process industries, in current educational and research activities at the Academy as well as in developments in software companies.

1.2 Objective of the work

The efficiency of the planning procedure for (petro-)chemical plants is investigated from a process engineering point of view, possible improvements are suggested and a prototypical solution is implemented. Improving the interoperability of CAE tools applied in basic and detailed engineering as well as the automation of the generation of the detailed constructive design for modular unit operations are key elements of the suggested approach.
The design of process plants requires a high level of experience and engineering know-how and is time- and money consuming. One possibility for enhancing both is using a modular approach for the design of unit operations, especially for those, which are frequently installed in industrial processes. Furthermore, an increase of reusability of best-practice solutions and proven engineering know-how is achieved by using a modular plant concept. Plant modules related to the definition of [Hady, 2013, p. 43-50] in process engineering includes equipment (apparatus and machines), steel construction, foundations, close piping (piping and fittings), measurement, control and regulation technology used for the module-internal control loops. Repetitive, manual tasks during the workflow can be avoided or at least reduced and the more unique constructive design enables faster planning, also in related domains and subsequent planning steps, e.g. ERP or electrical planning. A concept and prototypical implementation for the automated constructive design of Modular Process Units is presented in this thesis.
Planning and operation of process plants benefits from the possibilities that modern software technologies offer. Numerous software tools are used, which are tailored for the specific needs of the various participating working groups. Hereby, the variety of software applications reflect the trade- and domain-specific division in process industries. The enhancements of the data exchange are requirement to achieve an optimal project workflow and an important part of the digitalization in process industries - not only within the planning procedure but also within the whole life cycle of plants. In this work, the heterogeneous data exchange between process simulation, 2D and 3D CAD environments applied in basic and detailed engineering phases are examined and evaluated.
Information collected during the engineering phase need to be continuously and consistently deployed in the entire life cycle. Prerequisite for an error-free and consistent data handover and data management during the life cycle are the digital processing of the data and interoperability of the software tools used, to avoid manual, error-prone data handover. These points are key elements to fulfill the requirements for the realization of digitalization in process industries and therefore they are of major importance for improving the whole planning procedure.

Up to now, a continuous and seamless data handover and communication between the different applied tools in process industries is not given and a lot of effort is spent in industrial companies as well as in industrial-driven consortiums to reach this goal. Furthermore, different developments are made in improving the interoperability within (software) vendor-specific eco-systems - but even in working groups within single companies' various tools including highly specialized in-house solutions are applied and an eco-system-independed approach for the linking of software is highly desired. First attempts are also made to achieve standardized data handover within different trades, but up to now only few up to no fully working solutions integrated in different tools are available.

1.3 Structure of the thesis

The state of the art in plant design, applied CAE tools as well as the current developments referring to data exchange between tools applied in the participating disciplines is given in chapter 2. The term of integrated engineering used in this thesis as well as in further engineering areas is introduced. Furthermore, life cycle data management and the challenges for digitalization are touched in this part.
In chapter 3 the prototypical implementation of the integrated engineering tool *PlantDesign* for the automated generation of 3D plant models for modular process units (MPUs) is explained. The development is shown for distillation columns and associated apparatus, whereby the detailed constructive design as well as the implementations are emphasized. Details of the general approach, data exchange interfaces to tools applied in different disciplines of the basic and detailed engineering and the generic source code converter framework for generation of different 3D CAD programming languages are given. The integration of *PlantDesign* into the classical engineering workflow is drafted. In conclusion, two case studies for applying the *PlantDesign* environment are presented, followed by an evaluation of the approach. The first case study is related to the application of *PlantDesign* in a course at TU Berlin, the second one demonstrates the application for the process design in an industrial case study in cooperation with a global chemical and pharmaceutical company.
Chapter 4 refers to the interoperability of CAE tools applied in the phases of basic and detailed engineering during the planning of process plants. Special attention will be paid to the possibilities of data exchange between 2D and 3D CAD tools and a successfully implemented prototypical data interface developed in cooperation with a software company developing 2D CAD environments in the field of process engineering will be introduced.

As a prerequisite for this heterogeneous data transfer an intelligent data model for data transfer in connection with 3D process models is presented, which has been developed in the context of this work. Finally, the constraints and limitations of the approach and the concept of a central data exchange model, which is based on the previous findings, are discussed. In chapter 5 a summary of the thesis as well as an outlook for future work is given.

2 Computer-aided plant design - State of the art in process industries and research

2.1 Integrated engineering in chemical process industries

The term *integrated engineering* is currently widely used in various areas of engineering - this section provides a brief overview of relevant application areas and the underlying meaning of the term followed by the definition used for this work.

In the field of process industries different software vendors are working intensively on an interdisciplinary software framework related to integrated engineering within their eco-systems.
Siemens defines integrated engineering as holistic engineering in «all phases of the product and plant life cycle characterized by a uniform engineering database and an open system architecture permit access to up-to-date data and information any time from anywhere in the world». Key elements of their definition and the related software portfolio are «consistent data management through standardized interfaces» (COMOS), «integration of all disciplines» (COMOS portfolio: Feed, P&ID, PipeSpec, EI&C, Isometrics, 3D integration, PQM), «shared engineering framework for all automation tasks» (TIA (Total Integrated Automation) Portal) and «comprehensive, scalable simulation for efficient commissioning» (SIMIT simulation framework). [Siemens, 2019a]
AVEVA's «Integrated Engineering & Design (IE&D) solution» is the core of their vision for «Lean Construction» to build up «high quality assets» using an integrated set of products (AVEVA portfolio: Bocad, Diagrams, E3D Insight, Electrical, Everything3D (E3D™), Instrumentation, Marine, P&ID). Important aspects of their digital asset approach are the «consistency across teams and disciplines» using «fully integrated applications and one central engineering information repository» as well as «complete compliance through accurate obligation, progress and completion reports» and «self-integrating software and interoperability with a wide range of third-party solutions». [AVEVA, 2019a] After the aquisition of SchneiderElectrics AVEVA's portfolio has been extended by the SimCentral simulation platform and the corresponding «unified life cycle engineering» approach. [AVEVA, 2019b]

Education and training programs as well as skill certification schemes in terms of «the modern job roles in integrated engineering» has been investigated by [Riel, Tichkiewitch, and Messnarz, 2009]. Here, the authors emphasize that «integrated engineering is characterized by a highly multidisciplinary approach to product development ... with the need to master several different engineering disciplines in order to get a sufficient understanding of a product service». It is pointed out that there is a «strong industry need for international training, qualification and certification» and a «lifelong learning concept of the ECQA» (European Certificates and Qualification Association) to improve the «engineer's system competence level».

In [Landgraf and Dubovy, 2013] the authors discuss the usage of «integrated solution» from a single software vendor in comparison to a «compilation of different software (best of breed)» in terms of software interoperability. The uniformity of the database of «monolithic solutions» is critically questioned and the existing heterogeneity of the software landscape in industries as well as the need for «revision-proof interfaces» have been pointed out. The authors (engineering service provider) rely on solutions for manufacturer-independent system integration using data interfaces called «adapters», which are developed on purpose during the planning.

In the field of mechanical engineering (tool and mould construction) Siemens presented (at ECO 2015) an integrated engineering approach to create a simulation model of the machine based on CAD data and to test the mechanical functionality and automation concept of a machine under real conditions during the development process. This enables to identify and eliminate planning errors, such as incorrectly dimensioned components, before the actual commissioning, and the machine development time can be reduced (by 30% in a pilot project). [Drescher, 2015]

Another related definition is «Integrated Computational Materials Engineering» (ICME), which is an approach to «design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales. » The key words are «Integrated», involving integrating models at multiple length scales (structural, macro, meso, micro, nano and electronic scale), and «Engineering», signifying industrial utility. [ICME, 2019]

For this work, integrated engineering refers to multi-disciplinary engineering tasks during the whole plant life cycle in process industries, whereby the focus is on heterogeneous software interoperability and the data handover between different software and disciplines to enable a consistent data management and an integrated planning workflow during the basic and detailed engineering phases.

2.2 Classical plant design - status quo in chemical engineering

Ensuring an adequate time-to-market at lowest possible cost and time requirements is of major importance for the economic success in chemical and pharmaceutical process technology. The plant life cycle typically consists of preliminary studies, basic and detailed engineering, manufacturing, construction and assembly, commissioning, operation and dismantling phases [Weber, 2014, DIN 28000-1, 2011] as shown in figure 2.1.
In addition, an overview of the most frequently used software tools during the various planning phases is shown on the right-hand side of the graphic. The tools relevant for this work (marked in blue) are described more in detail in section 2.3.

Subsequent to the analysis of profitability and feasibility of the project in the *feasibility study*, the *preliminary and strategic planning* focuses on the scope definition for the project, the requirement specification for the phases of the plant realization. Additionally search, evaluation and final selection of alternative process solutions in principle during the *pre-engineering or preliminary planning* and their design during *basic engineering* is performed. This phase is characterized as «provisional» or «preparatory», since it occurs before the binding investment decision.

The planning depth of *basic engineering* must enable the *approval planning*, the economic feasibility analysis of the plant investment and, if necessary, to start with the technical and implementation planning. The planning for permission or *authority documentation* includes the services in the development of legally binding, in due time permit application as well as the implementation of the permit procedure - technical basis for this is the results of the basic engineering. The cost estimation for the *capital expenditure* covers the determination of capital investment (CAPEX) including engineering costs, the operational costs (OPEX) and the provision of proof of economic viability.

Detailed engineering supplies documents ready for execution for the procurement and construction of the plant as well as for *commissioning* and *continuous operation*. Since the transition from *basic* to *detailed engineering* often involves fundamental changes in responsibilities, permissions and competencies, this interface is very concise and contains many sources of error and conflict potential.

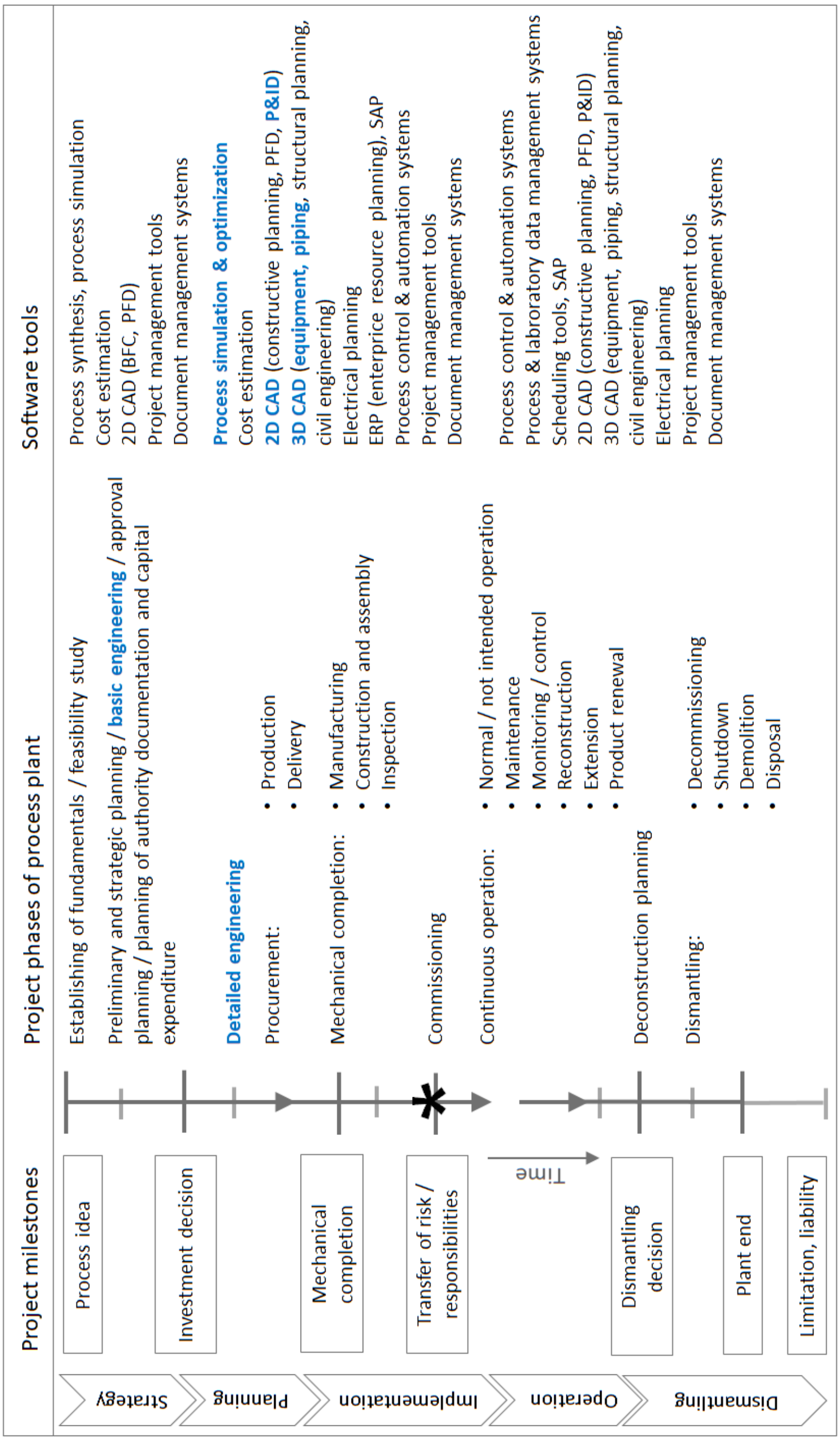


Figure 2.1: Life cycle and project phases of process plants and applied software [adapted from Weber, 2014; Wegener, 2003, p. 2; DIN 28000-1, 2011, p. 8-12]

Procurement comprises the preparation and realization of orders for supplies and services that are required for the realization of plants and, if necessary, for *commissioning*. The *construction* and *assembly phase* include the construction site handling from the opening of the construction site to the recording of *mechanical completion* and includes all work to be carried out on the construction site for the physical construction of the plant.

The *commissioning* is generally the last project planning phase and includes the services after the logging mechanical completion until the achievement of a contractual permanent operating condition after performance verification (if necessary after final acceptance of the contractual service). In the plant life cycle, the continuous operation of the plant follows, which also includes maintenance and conversion measures, expansions as well as production changes. Finally, the *plant shutdown*, including *decommissioning*, *dismantling* and *disposal* is the last phase in the life cycle. [Weber, 2014, p. 3-8; Wegener, 2003, p. 19-28]

The engineering offers a significant potential for savings and cost reductions [Wegener, 2003, p.27], despite the small proportion of $20 - 30\%$ of total costs over the entire life cycle [Schenk, 2012]. In this work, the focus is on improving the *basic* and *detailed engineering* planning phases highlighted in blue in figure 2.1.

2.3 CAPE- and CAE-software in basic & detailed engineering

CAE (Computer-aided engineering) comprises all variants of computer support for work processes in industry and technology, whereby CAPE (Computer-aided process engineering) is specifically tailored to the field of process engineering. According to [William, 2011, p. 1], «computer applications in chemical engineering range from methods that estimate chemical and physical properties through tools to develop and simulate efficient designs to methods of assessing the safety and environmental impact of the resulting processes». In the following paragraph a brief overview about common applications of process simulation and optimization as well as 2D and 3D CAD tools is given - advanced applications are not completely mentioned here.

2.3.1 Process simulation and optimization tools

Process simulators are established in chemical and process engineering since the 1960s and 1970s, with the advent of the first commercial series computers and the development of microprocessors. Nowadays the application for steady-state, pressure-driven or dynamic simulations or optimizations is manifold and extends over different length scales and levels of detail depending on the application:

- Modeling and simulation of processes by describing the conservation of mass, energy and momentum, the thermodynamic and reaction equilibria, the determination of material properties and operating as well as investment costs
- (Multivariant) optimization (under constraints) of the process design with respect to different objective functions (e.g. costs, thermodynamics, optimal design, process scheduling, transient process states)
- Process synthesis to assemble and arrange unit operations in an optimal way in order to fulfil the purpose of the process
- Computational Fluid Dynamics (CFD) to describe and solve fluid flow problems, mostly based on Navier-Stokes equations (e.g. simulation of mass and heat transfer phenomena, turbulence models)
- Engineering design (e.g. heat exchanger design, two-phase flows, heat transfer networks)

- Data-driven blackbox or greybox modeling to model the behavior of system output parameters depending on system input parameters (process data) with the help of functional relationships (e.g. using methods like neuronal networks)

- Data validation and reconciliation to correct measurement errors (due to measurement noise) in industrial processes

- Optimal experimental design

- Molecular simulations using a high level of physicality for e.g. prediction of physical properties based on the molecular properties

- Real-time optimization e.g. for model-based process control

Process simulators applied in process industries can be roughly divided into block-oriented flowsheeting environments using fixed coded, parametrizable models stored in program libraries and equation-oriented approaches, where the models are coded in a specific modeling language. It has to be mentioned that a strict separation of the approaches is not possible, since flowsheeting models are also based on equations. [Marquardt, 1992, p. 27] Commercial flowsheeting environments (e.g. Aspentech Aspen Plus, 2019, AVEVA, 2019d) are well suited for fast, plant-wide industrial production calculations, while equation-oriented approaches (Mathworks Matlab, 2019, MOSAICmodeling, 2019) provide greater flexibility in terms of modeling depth, but require more time for modeling and qualified personnel. Some environments (e.g. Process System Enterprise gPROMS, 2019, AVEVA, 2019e) enable a combination of both approaches. An overview of frequently applied process simulation and optimization environments applied in process industries is given in table A.1 in section A.1.1.

In this work prototypical data exchange interfaces to process simulation tools like Aspen Plus, MOSAICmodeling simulation and Chemcad are introduced. The main focus is on the automatic data import of process simulation information, which are the data basis for the whole plant design procedure.

2.3.2 CAD tools

According to [Kutz, 2006, p. 642] «Computer-aided design (CAD) uses the mathematical and graphic processing power of the computer to assist the engineer in the creation, modification, analysis, and display of designs».

2D CAD applications

2D CAD applications in process industries are typically used for the creation of drawings and flowcharts with different level of detail: block/basic flow diagram (BFD), Process Flow Diagrams (PFD) and Piping and Instrumentation Diagrams (P&IDs). They are important planning documents for the graphical representation of the process (within the site, the plant complex, the plant, the technical equipment) with respect to the interconnection of unit operations, energy and material flows, characteristic operating conditions, instrumentation including fittings and measurements, control structure, rough positions, piping, insulation and equipment information and identification tags [DIN 28000-3, 2009, p. 7-30].

3D CAD applications

In 3D modeling, geometric objects are built up and stored in a three-dimensional form and thus allow a realistic representation and better spatial understanding of the body. The 3D product model enables a reduction of created and to be managed planning documents since certain representation-related documents (e.g. section and view representations from different angles of view), document-related representations (technical drawings, parts lists, work plans, spare parts catalogues, assembly and operating instructions) and technical-visual representations (collision observation, explosion representations, installation and assembly instructions) can be (partially) automated derived.
3D CAD applications in process industry are typically used for the layout planning, constructive equipment design, electrical planning (e.g. laying of cable channels), buildings, and most important for piping. A complete representation of all plant components serve to increase planning reliability in the design of a plant, since plants and process information must be used in a coupled manner. This includes the determination of the optimal plant layout, since a complex plant has numerous possibilities to place it with all its components and to evaluate these layouts.

A key aspect for the application of 3D modeling in process industries is the early recognition and avoidance of functional and manufacturing problems and errors in downstream phases of the product development (constructive manufacturing and assembly, piping, prototype construction etc.), resulting in cost and time reduction as well as fewer optimization cycles in the product development and process design. In addition, the use of various intelligent functions for the design process itself, which are only possible and economical based on a 3D CAD system, e.g. parametric and feature-based modeling, partly already with the possibility of integrating rules for so-called knowledge-based design - this enables a quality assurance for the design process.
Furthermore, the 3D description of an object is a prerequisite for many other applications inside and outside the CAD system (CFD, FEM, virtual reality, rendering, 3D printing/fast prototyping etc.) and thus supports the creation of process chains in virtual product development. [Vajna et al., 2009, p. 170-175]

However, the advantage of the larger application range of 3D models is countered by a higher design effort, correspondingly extensive knowledge and practice with the modeling tools. [Vajna et al., 2009, p. 170-175] Easy access to all relevant data is of great importance, especially for the expansion, modernization, maintenance and turnaround of a plant. Hereby, difficult to access or distributed data drive up the effort and thus the costs. 85% of the costs in the life cycle of a plant are due to the handling of information, 75% of these costs being of a technical nature [Vajna et al., 2009, p. 17].

Geometric modeling in CAD applications

Referring to [Kutz, 2006, p. 648], the «Geometric modeling is one of the keystones of CAD systems. It uses mathematical descriptions of geometric elements to facilitate the representation and manipulation of graphical images on a computer display screen.».
In 2D modeling, geometric elements are drawn in one plane, predominantly in the form of sections and views of components or to generate volumes, which are created from two-dimensional geometric elements by certain operations from the 3D area (extrusion, sweeping, rotation, etc.), but also for the schematic representation of processes, designs and concepts. Lines, free-form curves (splines), circles/circular arcs and points are used, to which further attributes can be assigned, such as line thickness, line type (e.g. dashed, dotted) or color.
For 3D representations, there are four types of modeling approaches [Kutz, 2006, p. 649-651; Vajna et al., 2009, p. 175-179]:

- *Wireframe/edge modeling* is a skeletal description of the boundaries of a 3D object, consisting only of points, lines and curves (as in 2D modeling), without volume or surface information. Due to the minimal amount of data for the representation, edge models can be quickly displayed and moved on the screen indeed, but they are not unambiguous in their visual representation (difficult to clearly identify «front» and «back» as well as «inside» and «outside»). Since volume information is often prerequisite for operations like cuts through the body, cut edges, collisions checks, penetrations, cross-section or volume calculations, roundings, chamfers or shaded representations, pure edge models are only used in specific cases, e.g. as a basis for generating surfaces or volumes or as auxiliary geometry. Edge models are suitable for the representation of rotation-symmetric or plate-shaped components, e.g. for piping isometrics but it is also possible to get an edge model out of a surface or volume model only by changing the display mode.

- *Surface modeling* defines the surface or shell of a 3D object either with faceted surfaces (using a polygon mesh) or true curve surfaces (NURBS, nonuniform rational B-spline). NURBS is a surface defined by a series of weighted control points and one or more knot vectors, that can exactly represent a wide range of curves such as arcs and conics. Using NURBS enables a greater flexibility for controlling continuity and a precise modeling of nearly all kinds of surfaces more robustly than the polynomial-based curves used in earlier surface models. In extensive planar structures, orientation in the model is difficult (as with the edge models) - even if the information about «front» and «back» is given, the surface models lack information about «inside» and «outside». Surface models are used where surfaces of a product should have a complex shape which cannot be achieved by mere volume modeling (e.g. car bodies, aircraft fuselages, consumer goods) and an intuitive modification of the surface is desired. Surface models are applied for numerical control (NC) programs in computer-aided manufacturing (CAM) applications or for rapid prototyping systems.

- *Solid modeling* defines the surfaces of an object with additional attributes of volume and mass (if the material density is given). This allows image data to be used in calculating the physical properties of the final product. Solid modeling software uses constructive solid geometry (CSG) or boundary representation (B-rep) method for the representation. The CSG method uses Boolean operations (union, subtraction, intersection) on two sets of objects to define composite models, whereas B-rep is a representation of a solid model that defines an object in terms of its surface boundaries (faces, edges, and vertices). Volume models can be used for the majority of products in mechanical engineering.

Products which are built up from primitives or which are constructed in a production-oriented way (e.g. by using subtraction volumes such as bores) can be efficiently generated with volume modeling.

- *Hybrid solid modeling* allows the user to represent a part with a mixture of wireframe, surface modeling, and solid geometry.

Compared to 2D models, 3D models not only offer a much clearer and more complete object description in geometric terms. The usability for other work processes is extended, if additional information (e.g. for NC programming or finite element analysis) in the 3D models and passed on consistently. 3D Models allow a realistic description of future products and, moreover, form the basis of the basis for many simulation, animation and calculation methods. [Vajna et al., 2009, p. 159]

In this work the automatic generation of the constructive design of process units is introduced. Hereby, the solid modeling approach to build up 3D models is of major importance, especially for the development of the automatic parametric source code generation as well as the source code converter framework applied in the presented prototype.
Furthermore the data handover between different trades within the basic and detailed engineering using an integrated engineering appraoch is thematized. Beside the data import from process simulation tools also the data exchange between P&IDs and 3D plant models is examined and prototypical data exchange interfaces are developed. The standardized data exchange format for the exchange of data between P&IDs developed by the DEXPI initiative is taken into account and extended in the developed approach. Regarding the data exchange, the main focus lies on the transfer of process and plant related information.

2.3.3 Documentation in plant design

Documentation is of major importance during the entire life cycles of process plants. This is illustrated in figure 2.1 due to fact that data transfer from all participating disciplines lead into the documentation section. But here too, the heterogeneity and diversity of the documents and data storage systems quickly become apparent. An overview of plant documents during all life cycle phases mentioned in 2.1 is given in [DIN 28000-1, 2011, p. 13-18], the detailed content is described in [DIN 28000-2, 2011]. Special attention is paid to the creation of 2D process flowcharts, which are closer described in [DIN 28000-3, 2009, DIN 28000-4, 2014 and DIN 28000-5, 2015].

P&IDs in particular represent one of the most important planning documents for different involved trades.

The use of 3D plant models is becoming more and more important in the process industry due to the wide range of possible applications mentioned above - even if the creation and update process involve a higher effort. According to [Vajna et al., 2009, p. 21], a paradigm shift regarding product documentation from the 2D technical drawing to the often continuous three-dimensional product model has taken place («digital master»), but in many companies the P&ID is still the leading planning document for plant design.

For the sake of completeness, information management systems (e.g. Siemens COMOS, AVEVA NET) are mentioned as an important part of the plant documentation. They enable a central storage and administration of plant documents, but the effort to maintain and update the data and documents over different involved trades, to achieve a consistent as-built-status of the plant, is expensive. Interfaces to ERP (enterprise resource planning) systems (e.g. SAP) are typically available. Beside planning information also a huge amount of process data, experimental laboratory data or analytical data are available, which are typically stored in specific management systems (plant / laboratory information management system PIMS / LIMS, electronic lab notebooks ELN).

The mentioned systems are only a very rough overview to represent the complexity and heterogeneity of the data systems applied in industry. Typically, much more software environments and data storage systems for specific tasks are applied, which impedes a transparent and consistent data management - especially if changes occur. Due to the high complexity, the effort to replace the established paper-driven documentation due to a digital one is extensive and requires an improved interoperability among software to avoid manual, error-prone work steps. The opportunities, that digitization offers for process industries, are various, but the basis for a fully exploiting them needs to be established before.

The solution approach developed in this work offers the basic prerequisite for the automated creation and export of plant documents, in which the consistent availability of plant and process information is guaranteed by tool-spanning data interfaces.

2.4 Interoperability and plant life cycle of chemical plants

This section refers to the interoperability of engineering tools applied in plant design. The status quo with respect to data formats, standardization and recent developments are mentioned. The content of this section refers in parts to the following publications [Fillinger, Bonart, et al., 2017], [Fillinger, Esche, et al., 2019] and [Fillinger, Seyfang, et al., 2020 (submitted)].

2.4.1 Data types during the data exchange in process industry

This section deals with the characterization of data which is relevant for the exchange during the planning of industrial plants for the presented approach. In general, there is no universal definition of data, but various definitions for different existing specialist and application fields. The ISO 15926 defines data as the «representation of information in a formal manner suitable for communication, interpretation, or processing by human beings or computers» [ISO 15926-1, 2004], whereas information, related to [ISO 10303-42, 1994], are «facts, concepts or instructions».
From an IT perspective, data in general is a set of values of qualitative or quantitative variables in a specific format, i.e., structured, semi-structured, or unstructured, and with a specific physical location, i.e., *XML* file, relational database, etc. [Tolk and Jain, 2009, p. 45 ff]. Structured data is represented in a strict format and most commonly stored in relational databases or tables. However, not all data is collected and inserted in a structured way. In some applications, the collection of data is performed in an ad hoc manner before it is known how it will be stored and managed. This data may have a certain structure and some attributes may be shared among various entities, but not all information collected will have the identical structure and some attributes may exist only in a few entities. This type of data is known as semi-structured data and a widely known storage format is *XML*. If there is very limited indication of the type of data, the data is known as unstructured. [Elmasri and Navathe, 2011, p. 416-419]
Most often, the exchange of data must be accompanied by an exchange of the meaning of this data, which is called information exchange. Furthermore, an exchange of context, in which the information and data are valid, is required too, «since the meaning of data varies depending on the context in which it is used» [Tolk and Jain, 2009, p. 45].

Related to the transfer of specific information between tools, representing data has to be exchanged. For the 2D-3D data exchange framework, which is described more in detail in section 4.3.1, three types of data are identified: invariant, intermediate, and processed data. Invariant data does not change during the whole planning process, unless regular modifications during the planning occur. This kind of data has the same meaning within miscellaneous tools and is invariant during the planning process. For this reason, these data are transferred but not further processed or changed in the course of data transfer between different software applications.
Apart from these, intermediate data occur as kind of intermediate stage or result during the processing of (input) data. A direct, subsequent usage of intermediate data in further planning steps is not needed. Nevertheless, data transfer to other software is possible and sometimes useful regarding a better documentation of the engineering and the decision-making process. Improvements of long-term process modification, inspections and maintenance tasks regarding safety, engineering effort, and traceability can be achieved by providing these kinds of data.
Processed data are generated during the engineering process as a result of calculations or database queries (e.g. for manufacturer or standard data), which are depending on a set of input data. Processed data are typically created after data handover between different involved trades. Relating to figure 1.1, input data correspond to the transferred data from one discipline/trade (serving as data source) to another (serving as data sink). During trade-specific engineering, new data are generated and can be transferred to and used by other disciplines.

2.4.2 Data formats in plant design

This section refers to data formats for software used in plant design, especially for process simulation and CAD applications.

Data formats in process simulation

In the field of process simulation data files are usually proprietary and vendor-specific. Equation-oriented tools ordinarily are depending on the underlying programming language, commercial process simulation tools have vendor-specific formats, whereby the information is typically stored in different files. Some tools enable *XML* exports, but the structure is not standardized, but vendor-specific. Furthermore, there are several interfaces for the exchange of thermodynamic or physical property information, simulation models and numerical solvers, which are described more in detail in section 2.4.3.

CAD file formats

A large variety of data formats is available for CAD applications, which can be divided into *native file formats*, which are proprietary, vendor-specific formats, and *neutral file formats* or *standards*, which are created to encourage the interoperability (with respect to exchange graphical information) between CAD tools. Established formats for the exchange of 3D graphics are *STEP* (**ST**andard for the **E**xchange of **P**roduct model data, defined in the ISO 10303 standards), *IGES* (Initial Graphics Exchange Specification), *STL* (Standard Tessellation Language) and for 2D graphics the *DXF* (Drawing Exchange Format) file format from AutoCAD.

The *STL* file format is widely used in 3D printing, scanning, additive manufacturing, rapid prototyping and some CAM (Computer aided manufacturing) applications. It was developed by 3D-Systems Inc. [*3D Systems* 2019] and first published and used in 1989. This file format represents a 3D model in a triangular mesh, which can lead to distortion of shape elements, so that a direct conversion of curved form elements is not possible. Furthermore, the format includes no parametric data of the 3D object and therefore, is not suitable for plant models.

The neutral, manufacturer-independent data format *IGES* has been developed in the 80s and 90s in the USA by an industry association [IGES, 1983]. 3D objects are modeled based on individual surfaces (elements), but the file is not storing information about the relationship elements have within the assembly. This leads to problems in converting *IGES* data due to incorrectly recognized surfaces or mismatching boundary curves - so the format is not applied for exchanging CAD designs anymore.

Most promising candidate for the exchange of 3D CAD models is the also manufacturer-independent and standardized *STEP* file format [Anderl and Trippner, 2000], which is used in almost all areas such as architecture, construction, engineering, mechanical engineering. It is currently probably the most common format for exchanging CAD data, but an application in the exchange of 3D process plants requires an extension for the transfer of processing data without loss of information. In [Jandeleit and Strohmeier, 2000, p. 128], the authors pointed out that «increasingly more CADsystems have relatively efficient STEP processors for the exchange of different geometrical models; but the exchange of non-geometrical information of a product model is still impossible or only possible to a limited extent. In addition, the information relevant for construction provided by the different (STEP) product models is generally not detailed enough for integrated engineering.».

Moreover, a subsequent processing or changing of the 3D model after data transfer into another CAD environment is strongly limited - as with the other formats mentioned.

General aspects related to data exchange

Ideally, only noncommercial and non-vendor-specific, i.e., non-proprietary, standardized data exchange formats are employed for inner- or interdisciplinary data exchange. For commercial solutions, support of legacy formats cannot be ensured, implementations heavily depend on the internal software architecture, strategies, and bilateral agreements of software vendors, since consistency of data transfer cannot be independently verified. However, the extent to which information can be transferred using standardized data exchange formats heavily varies with each standard and not all standards are readily or even fully adopted by software vendors.

The prototypical solution presented in this work includes the development of a data exchange model for 3D plant models based on the standarized data exchange format for P&IDs published by the DEXPI initiative. The data exchange between 2D and 3D CAD models is perfomed based on the standard for P&IDs and the extended 3D data model developed in this work. Furthermore and in absence of suitable standardized data formats, proprietary data exchange interfaces based on the vendor-specific *XML* formats are implemented for the import of simulation information from commercial and in-house process simulation tools.

2.4.3 Interoperability and plant life cycle - current developments

Various initiatives are working on easing the data transfer between tools belonging to the same disciplines/trades, e.g., DEXPI for P&ID's [Temmen et al., 2016], CFIHOS for asset management in the process industries and handover between operators, manufacturers, contractors, and suppliers [CFIHOS, 2019], and CO-LaN for interoperability between process simulators [CO-LaN, 2019]. In addition, a number of initiatives have been started to allow for interdisciplinary data exchange, e.g., between P&ID and asset management in a DEXPI-CFIHOS cooperation, interchange between computer-aided engineering tools and process control systems [Namur NE 159, 2018], or P&ID and process control systems by the Namur initiative [NAMUR, 2019].

The data integration part of the ENPRO initiative has successfully developed a method for data integration of process simulation and P&IDs [Wiedau et al., 2016]. The levels of maturity of these standardization and data exchange initiatives and their respective specifications vary greatly. For some, implementations in commercial software are already available, for others, first prototypes exist but with rather limited capabilities regarding the information that can already be transferred.

At the moment, there is no metric available to estimate and quantify whether the combination of these standardization efforts will lead to an overall increase in the ease of interdisciplinary data transfer throughout the plant life cycle and, hence, ensure the consistency of all data associated with a plant.

Data Exchange Between P&ID CAD Tools

The DEXPI initiative [DEXPI Initiative, 2019] is a joint initiative by representatives of the German chemical industry, such as BASF SE, Bayer AG, Evonik Technology & Infrastructure GmbH, and Covestro AG. Recently, Equinor (formerly Statoil) joined as another industrial partner. Together with several software vendors and partners in research they work on data exchange in the process industry with a current focus on P&ID as the most important document of a chemical plant. DEXPI has issued a P&ID specification [POSC Caesar Association, 2017], which is based on the Proteus P&ID schema [Proteus Schema, 2016]. Important elements of the DEXPI specification for P&IDs are the basis in ISO 15926 and the according separation into model structure in part 2 [ISO 15926-2, 2003] and reference data in part 4 [ISO 15926-4, 2007] as well as the use of an *XML* schema in accordance to part 7 [ISO 15926-7, 2011] or web ontology language (OWL) referring to part 8 [ISO 15926-8, 2011]. With its basis in ISO 15926, a high degree of compatibility to other standards also derived thereof should be feasible. But even though ISO 15926 refers directly to process industries, the given attribute definitions are very general and need to be further extended and implemented for the special requirements of the process industries to turn it into a usable standard.
The main constraint for applicability lies in the extension of the reference data library (RDL), which currently only defines 19 attributes in ISO 15926-4 [ISO 15926-4, 2007] and needs to be extended for each implementation. Some import and export functionality according to the DEXPI specification has already been implemented by most major vendors of P&ID software.

However, currently, the functionality is rather limited in the amount of transferred data and few complex examples are successfully exported and imported between different tools from software vendors participating in DEXPI [DEXPI Initiative, 2018].

Data Exchange Between 3D CAD Tools

While the use of P&ID is rather limited to the process industry, 3D CAD tools are a lot more widely used from design of buildings to ships and automotive industries. Hence, a number of data exchange formats is already available with differing objectives and functionalities, as discussed in section 2.4.2.

As already mentioned, STEP is probably the most common exchange format for CAD data. The application protocol 221 of [ISO/TR 10303-221, 2007] is designed for «functional data and schematic representation of process plants». STEP data can be received in various formats, among them *XML* as specified by [ISO/TR 10303-21, 1994] (STEP file) or [ISO/TR 10303-28, 2007] (STEP-*XML*). In both cases, the actual data is contained in accordance with the EXPRESS data modeling language from [ISO/TR 10303-11, 2004]. The STEP format is currently supported by most vendors of 3D CAD tools and STEP files can be reliably exchanged between most tools. STEP enables the handling of different representation methods, e.g., CSG and BREP, but a further processing of the 3D model is not possible after import into a CAD tool. ISO 10303-221 is of main interest for the process industry since it contains details for the functional design of systems and engineering specifications for system components. Unlike the other parts of ISO 10303, AP 221 also relies on the reference data library described in ISO 15926-4, which is also noted therein [ISO 15926-4, 2007].

ISO 15926-2 (in competition to ISO 10303-221) details a data model for technical information of process plants, which does not rely on the EXPRESS architecture, but also uses the same reference data library (ISO 15926-4). However, no known commercial implementation exists thereof, which exchanges 3D data between CAD tools beyond the publication of the ADIIDS ISO-15926 3D model [Laud, 2008]. An ISO 15926 conforming 3D data exchange format with focus on exchange of graphical representation is suggested by Kim [Kim et al., 2016], but to the knowledge of the authors there is no commercial implementation available.

Outside of the process industry, the domain of building information modeling has generated the industry foundation classes (IFC) [DIN EN ISO 16739, 2017]. The use of IFC-compatible tools has already been required by several national governments for all public housing or road construction projects, e.g., in the UK [NBS, 2016]. IFC-SPF relies on ISO 10303-21 and IFC-*XML* on ISO 10303-28, hence working on the same EXPRESS modeling language.

Data Exchange Between Process Simulation Tools

The process simulation world differs from the aforementioned two in several regards. From a process simulation perspective, exchangeable data could be the results of a simulation, parameter and initial values, entire model equations, or executable code and solver settings (e.g. tolerances, numbers of iterations). Unlike in either P&ID or 3D CAD, a simulation model is inherently functional, i.e., results are generated based on nonlinear equation evaluations, etc. Hence, the standards available in the domain of process simulation are rather different.

The CAPE-OPEN Laboratories Network (CO-LaN) [CO-LaN, 2019] has issued a number of interface specifications. Based on these, it is either possible to exchange unit operation models in the form of precompiled executables (DLL) or to share property calculation packages between different software. In contrast to the other standards above, the actual model content is not open/visible data, only the interfaces are. In addition, the CAPE-OPEN specifications are currently limited to steadystate systems and there is no functionality in place to store and share results of simulations. Naturally, the CAPE-OPEN unit operation specification could be used to build entire flowsheets, but the specifications of the inlet streams to the process would only be stored in the flowsheet itself and, hence, would be lost on switching from one tool to another. Also, the topology of the flowsheet would need to be redone. Hence, the CAPE-OPEN specification – while being a very useful standard for process simulation in chemical engineering – is ill-suited for actual data exchange between process simulation software or with tools of other disciplines.

The Functional Mock-up Interface (FMI) [FMI, 2019] on the other hand is deeply rooted in the domain of dynamic process simulation and stems from the automotive industry. This standard is based on a combination of an *XML* description for a model referring to an *XML* schema defined by the FMI specification and associated precompiled C code containing the model, which are shared. Similar to CAPE-OPEN, the FMI specification is designed for co-simulation and model exchange.

The *XML* specification contains information on all exposed model variables of a unit operation, units of measurement and type definitions, additional static information, and describes the capabilities of the unit. Furthermore, it contains information on how to solve the model, i.e., solver settings and step sizes. The actual model equations can also be given in source (C code) or in binary form. The reference data for designing and using the *XML* schema of the FMI specification is contained within FMI and not related to any other standardization effort. At the moment, it is unclear whether this could, e.g., be aligned with ISO 15926-4.

Independent of the engineering discipline, all mathematical models can be described in an equation-oriented manner by the mathematical markup language (MathML) [W3C, 2019a]. Within MOSAICmodeling, MathML is combined with a generic set of *XML* schemas for model elements to supply all aspects of a dynamic or steady-state simulation model [Kuntsche, 2012]. This approach allows for maximum data transparency and accessibility of both functional models as well as initial and result values of simulation variables. While relying on standards for *XML* and $MathML$, this is not yet a formal standard and only implemented in MOSAICmodeling.

However, the set of *XML* files describing a model can be easily exchanged and transcribed into implemented model equations in any programming or mathematical modeling language. While the MathML parts of course only contain definitions of variables and equations, the more extensive set of *XML* files also includes information on simulation results, initial values, parameter values as well as solver settings for specific solution environments, e.g., solution parameters for MATLAB's fsolve.

Figure 2.2 depicts the relationships and dependencies of all the data formats and standards mentioned so far. This is not a complete overview, but it should already suffice to highlight the general complexity and issues of data exchange. While features such as the application of *XML* structures are recurring, model structure, reference data, and vocabulary do not always coincide or align.

At present, there is no general solution for a cross-disciplinary linking of plant planning tools in process engineering that allows intelligent data exchange between the various tools used. This paper presents a proposal for heterogeneous data exchange between commercial 2D and 3D CAD tools. Furthermore, the xml-based import of process simulation data from different simulation programs (commercial as well as in-house) for apparatus design is shown. The prototypical implementation is realized in *PlantDesign* MOSAICmodeling.

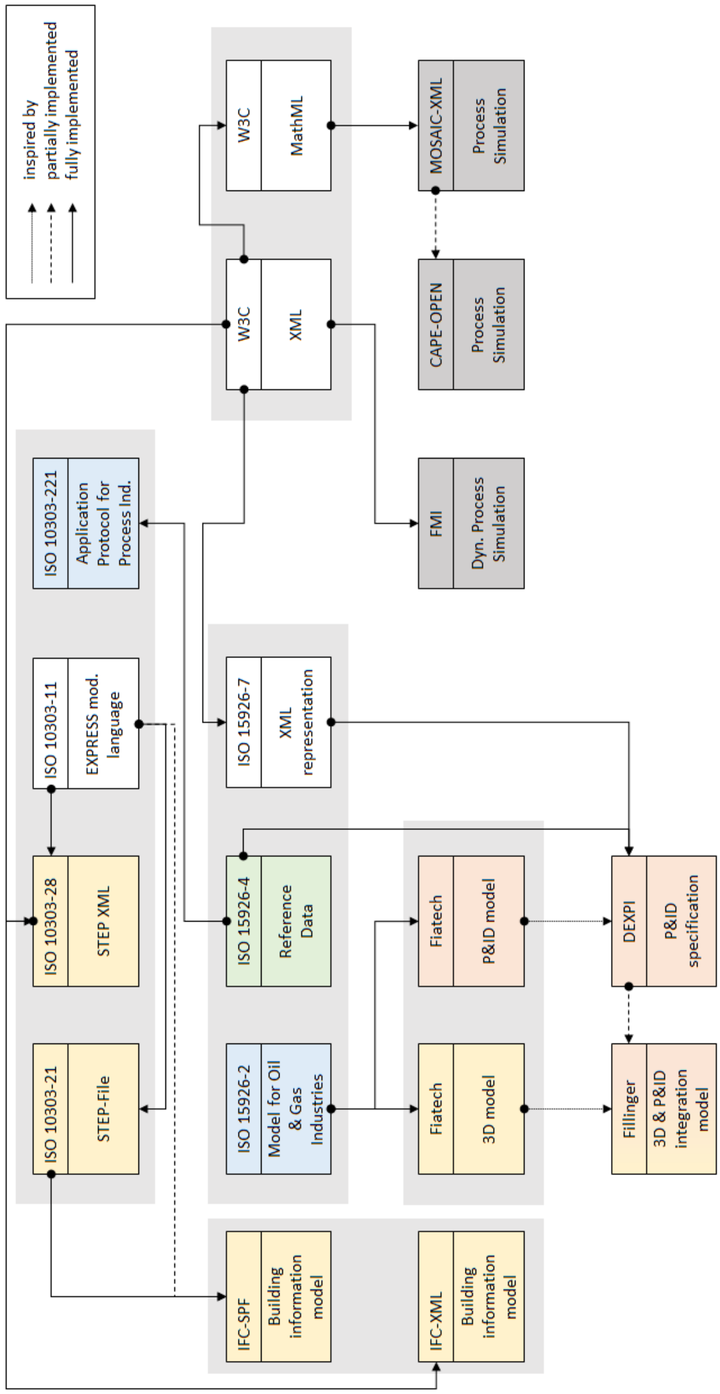


Figure 2.2: Sketch of relationships of international standards and formats mentioned above - *XML* is a recurring feature of the various data models used for P&ID, 3D CAD, and simulation, but beyond that the general overlap is rather limited [Fillinger, Esche, et al., 2019]

3 Integrated engineering solutions - prototypical implementation of *PlantDesign*

In contrast to industrial sectors like the automotive and manufacturing industries, design of unit operations for chemical and petro-chemical processes is highly specialized, tailor-made and requires a high level of experience and engineering know-how. One possibility to create a more efficient design procedure by reducing planning expenses and time to market is using a modular approach for the design of unit operations, especially to frequently used unit operations in industrial processes. This enables the reusability of best-practice engineering know-how.
The use of a modular approach enables a high degree of automation for the creation of plant models by defining a portfolio of implementation possibilities. In particular, the complex and time-consuming generation of 3D representations of process plants offers great potential for savings and improvement. Further enormously important potentials for the advancement of interdisciplinary, computer-aided planning processes lie in the enhancement of the consistency of data transfer as well as in the creation of transparency in the underlying decision processes.
The provision of data interfaces for data exchange between the applied highly specialized tools used in plant planning as well as the generic generation of import and export formats for a vendor-independent exchange of models are important prerequisites for integrated engineering solutions.

This chapter presents the underlying approaches and their prototypical implementation as integrated engineering tool in the *PlantDesign* environment of MOSAIC-modeling. In terms of content, these statements refer in parts to the following publications [Merchan et al., 2016], [Fillinger, Talaga, et al., 2017], [Fillinger, Tolksdorf, et al., 2017], [Fillinger, Bonart, et al., 2017], [Fillinger, Esche, et al., 2019] and [Fillinger, Seyfang, et al., 2020 (submitted)].

3.1 Concept of automated equipment design for adaptable modular process units

3.1.1 Adaptable Modular Process Units

Adaptable modular process units (MPUs) in this work are defined as 3D models of process units with a very high level of detail of the constructive design, created out of complex parametrizable templates. They include several constructive design options to guarantee a flexible adaptation to a wide range of process-specific conditions and constraints.
MPUs consist of equipment (apparatuses, machines), norm-compliant steel constructions like support beams, structural elements, ladders and platforms, foundations, close and internal piping (pipes and fittings), as well as control devices for the module-specific control loops. Further engineering working areas are not included yet, but an extension of this approach is feasible and desirable. An overview of the general hierarchical structure of MPUs is illustrated in Fig. 3.1. The MPU is structured into the «ProcessEquipment» level including constructive elements as well as structural elements, the «StationaryAccess» level including platforms (base as equipment, railing as structure) and ladders, the «ClosePiping» level for in- and outlet pipes, the «InternalPiping» for all internal pipework and finally the «PipeSupport» level. The applied module definition is related to [Lederhose, 2005] and [Hady, 2013, p. 43-50].

The design of the MPUs is individually adaptable to the process data, operating conditions, material selection and constructive design requirements. Besides the spatial information, also process and meta information like process variables, process conditions, constructive user specifications, heuristic information, and calculated design parameters are included in the 3D data model. Outcome of the tool is automatically generated source code of the process unit which can be imported into 3D CAD tools e.g. AVEVA E3D™/PDMS™ or Autodesk® Fusion 360.

The development for the prototypical implementation has been carried out mainly for distillation columns as well as for associated apparatuses (condenser, reboiler, pumps, reflux drums and storage vessels). Distillation processes are the most applied thermal separation process in chemical industry and have the required complexity regarding the costructive apparatus design to ensure the general applicability of the presented approach to the complex industrial problem statements.

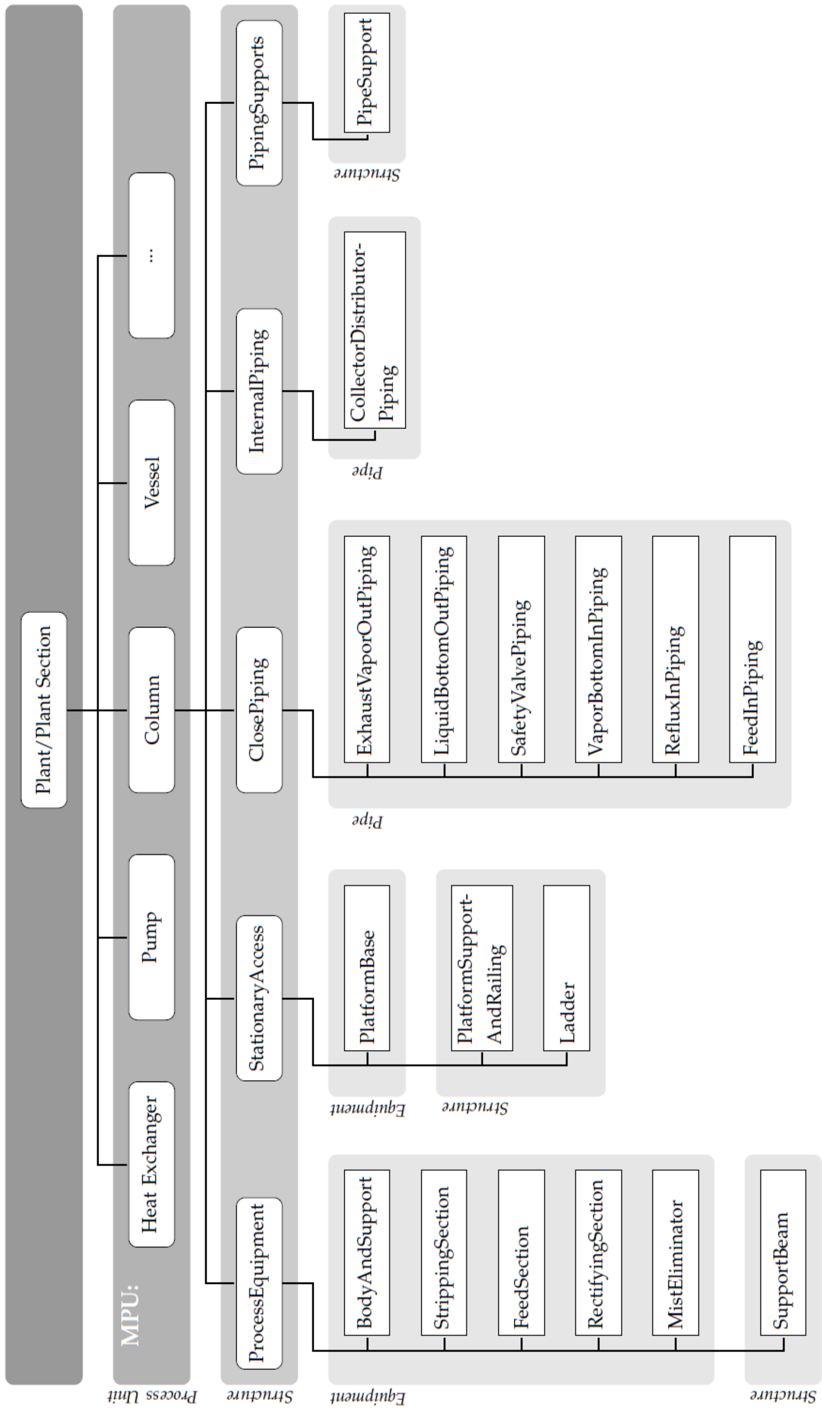


Figure 3.1: General structure of Modular Process Units, exemplary broken down for distillation columns

3.1.2 Constructive equipment design

The constructive design of process units is influenced by various determining factors. The fundamental dataset for the equipment design is determined during process simulation and/or optimization. This step delivers process variables such as material and energy flows and characteristic design variables like the number of theoretical separation stages of distillation columns, the heat transfer area of heat exchanger or the discharge head of pumps.
Process conditions such as operating pressure and temperature as well as the occurring media and chemical components affect the selection of appropriate materials and the spatial characteristics of structural elements, e.g. wall thickness of plant components.
In general operating pressure can be high pressure ($p > 10^5 Pa$), atmospheric ($p \approx 10^5 Pa$) or vacuum (low ($100 < p < 10^5 Pa$), medium ($0.1 < p < 10 Pa$) or high ($10^{-3} < p < 0.1 Pa$) [Sattler and Feindt, 1995, p. 102, Mersmann, Kind, and J. Stichlmair, 2011 p. 315]. Figure 3.2 illustrates the calculation routine as well as the general provision of required input data from different sources for the wall thickness (dimension variable). Detailed information for the calculation of the wall thickness is given in table A.3 in section A.2.1.
Direct user specifications, e.g. the input of the steel grade (marked in red), has to be provided via the graphical user interface. The import of simulation results makes the transfer procedure of data less error-prone and much faster. Required process variables like the temperature T, the pressure p as well as the calculated apparatus diameter D (marked in blue) are results taken from the process simulation, which is the design basis in the planning procedure. These values can be entered manually via the graphical user interface, but more comfortable imported automatically via data interfaces for simulation data, described more in detail in section 3.2.1. Of particular importance for an appropriate apparatus design are standard, heuristic and manufacturer data, which are stored in a database that has been developed especially for this purpose.

In this example the temperature-dependent yield strength of the steel grade $R_{e/t}$, the safety or welding factors S and ν and the nominal deviations of the wall thickness C_1 and C_2 (marked in green) can be queried automatically from the mentioned database. This calculation serves only as an example for the different types of input parameters used for the calculation basis of the constructive apparatus design. A more detailed description of important design calculations for the selected example of a distillation column is given in section 3.1.2.1.

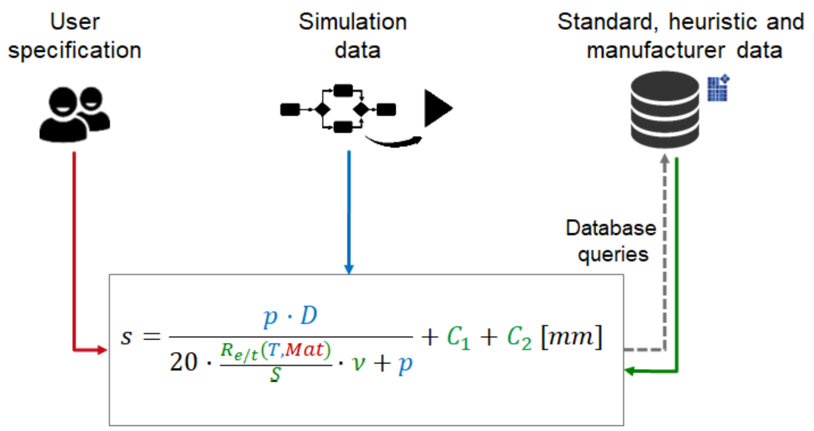


Figure 3.2: Input data sources and calculation routine for the internal calculation of dimensions, exemplary for the calculation of the wall thickness for high pressure apparatus based on the pressure equipment directive for pressure vessels [AD 2000-Merkblatt B1, 2000]

The approach allows various possibilities of equipment types and several detailed constructive design options, which can be chosen by process engineers. User options are for example types of columns and heat exchangers, selection of column internals like types of random or structured packing or tray types, supports, beams, and brackets for internals and piping, types of collectors and (re-)distributors in columns, internal piping options, the demand of demisters, standardized manholes diameters for maintenance, insulations - to mention only a few. Depending on the user selection regarding these options, the resulting 3D model is adapted respectively. A detailed description of the constructive design of distillation columns is given in section 3.1.2.1.

Flexible applicability for different processes is achieved by an adaptable module design that offers several constructive options for the plant components to the user. The sizing of the MPUs depends on the respective characteristic design variables, e.g. the heat transfer area and the length to diameter ratio for shell and tube heat exchangers. The sizing of more complex apparatuses such as rectification columns is affected by several process variables, e.g. the number of separation stages, gas and liquid loads, and type of column internals. Based on input information for the plant design, the sizing, arrangements, dimensioning, positioning and finally the resulting 3D representation of the MPU is processed automatically.

Finally, the storage of required information for the processing and creation of the detailed constructive design of MPUs is realized in a data model compliant to the [ISO 15926-2, 2003, ISO 15926-4, 2007] standard for data exchange in process industries. More detailed information to the development of the data model is given in section 4.2. Beside the import capabilities for process simulation data, a prototypical bi-directorial data interface for the import and export of 2D planning data from P&IDs has been successfully developed. The data is stored in *XML* format, in compliance with the standardized data exchange format (XMpLantPID-ProfileSchema [POSC Caesar Association, 2017]) developed by the DEXPI initiative. A more detailed description is given in section 4.3.1.
MPU designs has been prototypically developed for distillation, the most applied thermal separation technique in industrial processes [J. G. Stichlmair and Fair, 1998, p. 1ff.; Kister, 1992, p. 1ff.] as well as for associated apparatuses. Proceedings, engineering rules, heuristics and developed calculation algorithms related to the constructive design of these apparatuses are given in the following paragraphs. In doing so, the descriptions of the complex design of distillation columns are emphasized but the approach is similar for associated apparatuses.

3.1.2.1 Design of distillation columns

Continuous, countercurrent distillation or rectification is the most important and widely used separation technique with diverse applications in in chemical, petrochemical and pharmaceutical industries. This physical separation of mixtures is based on the different boiling behaviors of the components. Distillation requires large amounts of energy to apply the necessary evaporator and condenser duties during operation, which is associated with significant operational expenditures (OPEX). Referring to [Sattler and Feindt, 1995 p. 119], $60-80\%$ of energy in chemical industries are used for that purpose. In order to minimize the sum of capital expenditures (CAPEX) as well as OPEX costs, an appropriate process and constructive design is of great importance.
Process simulation delivers the basis for the design and sizing of columns as well as for associated apparatuses. Based on the type, quantity and state of the initial mixture (feed) and the desired product specifications, the required number of separating stages, the sizing of the column, the internal flow and hydraulic conditions and the cooling and heating utilities have to be determined. Hydraulics include the column pressure, internal-dependent pressure losses and the liquid hold up in the column. These variables represent important parameters to describe the mass transfer between the liquid and vapor phase, which are conducted in countercurrent principle within the column.

The separation efficiency correlates directly with mass and heat transfer between both phases. The transfer can be enhanced by internals which increase the interfacial surface area, the turbulence and contact time and therefore intensify the contact between liquid and vapor. The choice of the internals depend on various aspects like the separation performance (theoretical stages per column height), load capacities (vapor velocity or F-Factor, liquid load), pressure loss per theoretical separation stage (important for vacuum rectification), properties of the mixture (fouling tendency, corrosive or foaming systems), column capacity (quantity and purity of products) as well as the costs per theoretical separation stage (materials, processing, installation). [Christen, 2010, p. 437 ff]

This section deals with specific aspects of the constructive design of MPUs for distillation processes specifically for packed and tray columns. The given statements with respect to the column design are used to explain the general approach. Since the design of the process units is to be automated, different generic design options are considered in order to enable flexible adaptation to the respective process conditions and constraints.
Parts of the contents contained in this paragraph have been worked out as part of the supervised master's thesis by [Brodowska, 2017], [Gracjas, 2014], [Koczy, 2016] and [Jurga, 2015] as well as project works by [Molano, 2017] and [Klette, 2018].

Variable scheme for the generic design of columns

The algorithm for the generation of packed columns (as well as for tray columns) is divided into three constructive sections: (I.) stripping, (II.) feed and (III.) rectifying section, as depicted in figure 3.3.
The processing of the overall design as well as in the single sections is carried out from bottom to top. The description of the geometric properties (size, position and orientation in space) of all constructive items of the apparatus is realized using variables and formula expressions instead of fixed values. This is done in order to achieve the required full flexibility for the automated creation of 3-dimensional process models. Some of the dimensions and distances between internal components as well as orientation of nozzles are supplemented by the researched values and calculation formulas from technical literature. An overview of important design rules and heuristics taken into account for the constructive design of distillation columns are summarized in table A.7 in section A.2.2.

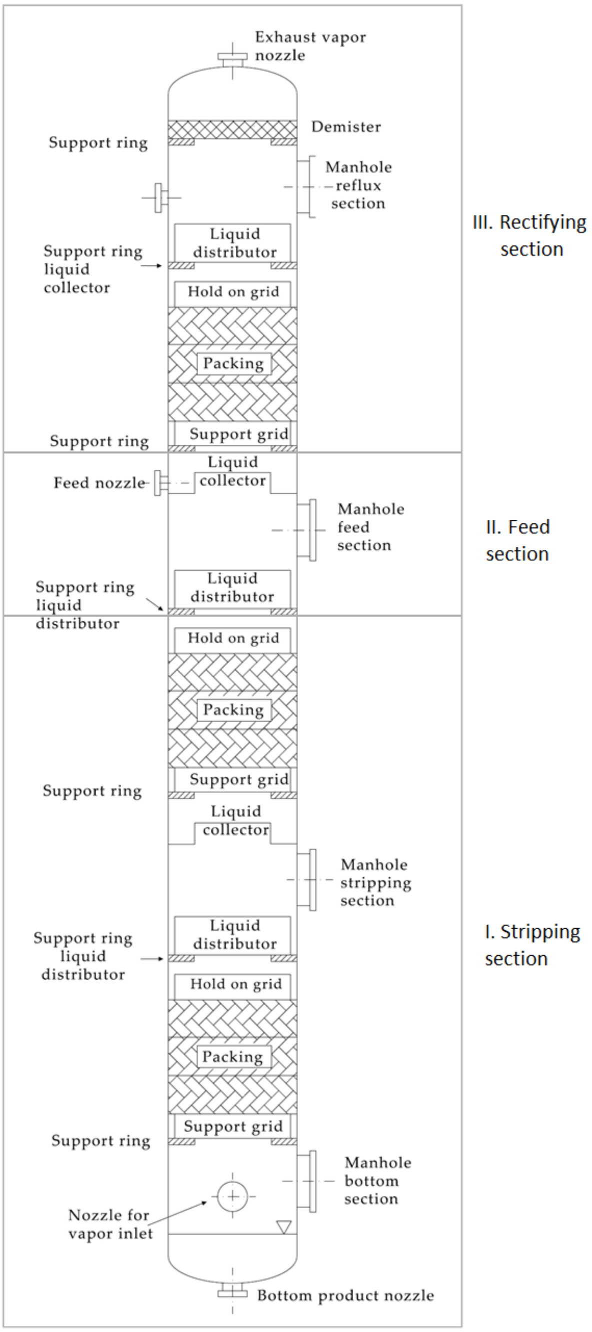


Figure 3.3: Constructive sections for the creation of packed columns during the programming algorithm

Liquid maldistribution, which has a negative influence on the separation performance by decreasing the heat- and mass transfer between the vapor and the liquid phases, can occur in packed columns. Particularly in random packings, phenomena like stream formations or the wall effect (displacement of down coming liquid closer to the wall due to the larger void fraction near the wall or stream formation) have to be considered. [Christen, 2010, p. 441]
In order to counteract these undesirable effects, the down coming liquid is regularly collected and redistributed over the column cross-section. The number and installation heights of the needed liquid-collector-distributor systems is depending on the total height of a specific packing in the rectifying and/or stripping section required to fulfill the desired separation task. A more detailed description of the distributor design is given in paragraph 3.1.2.1. Constructive solutions for a proper vapor distribution are currently not implemented but can easily be extended.

Calculation algorithm for the construction of packed columns

Figure 3.4 shows a schematic overview of relevant design variables applied for the design calculations of one design configuration of a packed column. This configuration includes a demister to avoid entrainment by the outgoing exhaust vapor stream, different shell diameters for the rectifying and stripping section, the positioning of the feed inlet as well as the manhole in the feed section are above the conus for the diameter change and the feeding of the inlet flow is carried out into the collector below the feed section.
Changing the column design settings partly leads to a deviation of the variables as well as of the calculation rules. Based on the selected user settings, the corresponding numbers of required collector-distributor sections, the resulting packing beds and the positioning of the feed section in between are determined at the beginning of the calculation algorithm for each column design. The results of these calculations are further applied by the usage of running indices. This is a required procedure to enable the calculation of the positions in space of all column items and finally the total column height.
A flowchart representing the overall algorithm for different constructive designs of packed columns is shown in figure A.1 and the creation of the stripping section is illustrated in figure A.2 of section A.2.2. Based on the user input, the total height of the packing in the stripping section is determined using the manufacturer's specification of the HEPT value (height equivalent to a theoretical plate) of the packing used and the calculated number of theoretical stages of this section. Using the maximum permissible height of a packing bed until the liquid has to be redistributed, the number of packing segments in the stripping section is determined.

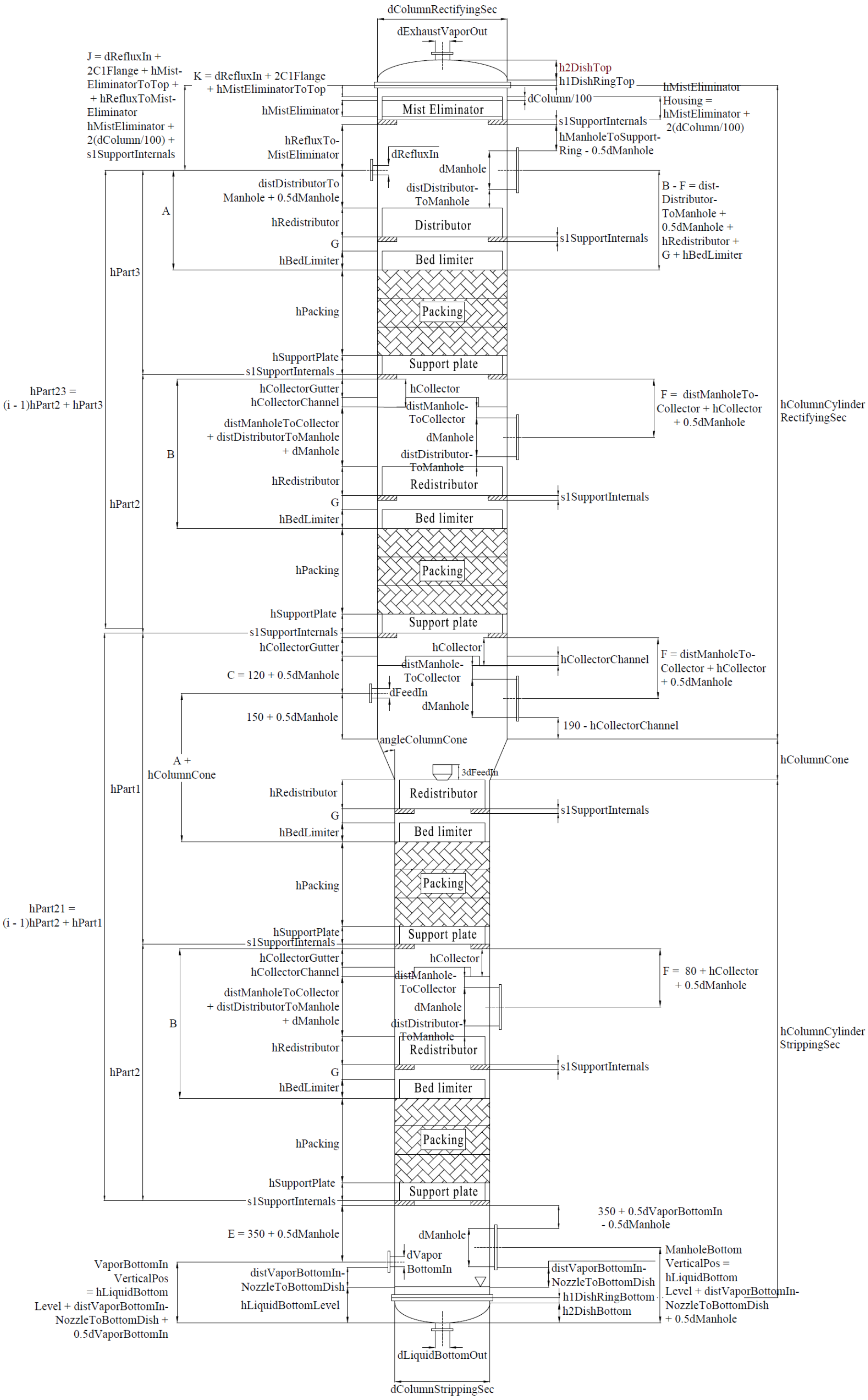


Figure 3.4: Overview of variables and distances for the calculation of vertical positions and total column height for packed columns including demister and feeding into the collector

In figure 3.5 the elements of a single packing segment, the distances between them and the dimensioning variables are shown. The structure of each segment is identical and contains a collector-redistributor system, a manhole for maintenance purposes and the packed bed with support elements - but the dimensioning can vary in the different column sections.

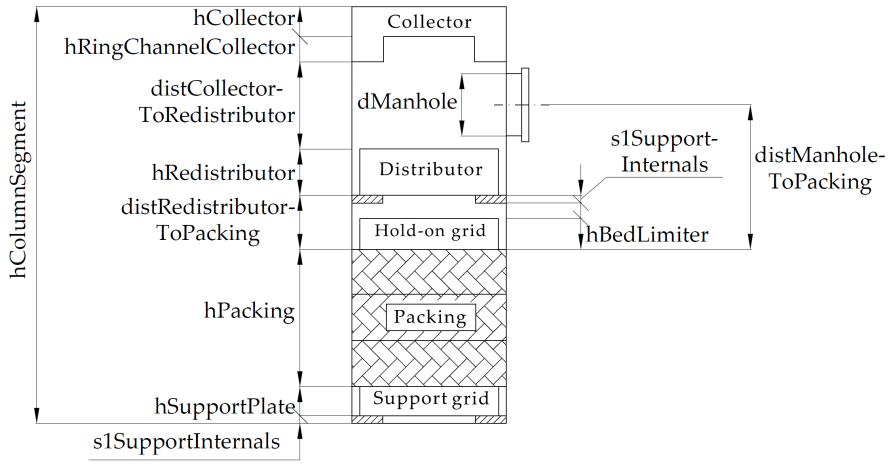


Figure 3.5: Elements and corresponding variables of a single packing segment within rectifying and stripping sections

The manufacturer's data on structured and random packing materials as well as required heuristic values for the constructive arrangement are stored in the *PlantDesign* database and are automatically queried from there during the design procedure. The dimensioning of the components, e.g. the supporting elements, are taken from standards. An overview of the standards used for the constructive design and the component geometries is given in Table A.4 in the appendix A.2.1. The dimensions are stored in the *PlantDesign* database just like the heuristics and are also automatically queried. A more detailed description is given in section 3.1.3. A similar procedure is used for the design of the rectification part.

The required user-specific input variables for the general apparatus design, the column internals as well as manholes and nozzles are listed in tables A.5 and A.6 in section A.2.2. These variables are the minimum input data for the processing of the calculation routines and can be specified via the graphical user interface or at least in parts by data import interfaces.

To ensure a proper operation of distillation columns the design and the arrangements of the internals have a major influence. Referring to [Kister, 2006], poor liquid or vapor distribution, the tower base level and the vapor return in the bottom section are among the most common malfunctions in packed columns. Other typical malfunctions, that are not directly linked to the constructive column design, such as a failure of the evaporator or reboiler, misleading measurements, leakages, foaming, coking, undesired reactions in towers, water-inducted pressure surges, problems during start-ups, shutdown, commissioning and abnormal operations as well as control problems are only mentioned for the sake of completeness.

In order to avoid malfunctions, which can be traced back to the constructive design, common heuristics are applied and integrated in the presented approach in the best possible automated way. The recommended design rules are usually linked to specific process or apparatus conditions, which are automatically checked to use the selection of the correct heuristic recommendations for column design. An overview of important heuristics rules is compiled in table A.7 in section A.2.2.

The determination of the position of the vapor inlet nozzle in the bottom area of the column, which is set via the position variable *!verticalPosVaporBottomInNozzle*, is presented as an example. Figure 3.6 illustrates the used position variables.

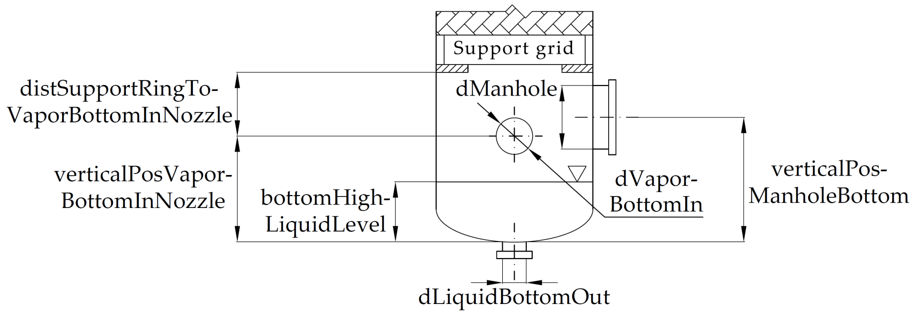


Figure 3.6: Variables for the calculation of the positioning of the bottom part of packed columns

The vapor inlet nozzle has to be positioned in such a way that it does not get into the liquid. According to [Kister, 1990, p. 83-87] and [Branan, 2005, p.97] this is ensured by positioning the lowest point of the vapor inlet nozzle at minimum $300mm$ above the highest bottom liquid level (*!bottomHighLiquidLevel*). If this recommendation is not met, turbulence on the liquid surface, fluctuating level control and entrainment of liquid into the rising vapor may occur [Kister, 1990, p. 83-97].
Slightly different guidelines are proposed by the Saint-Gobain NorPro company [Saint-Gobain NorPro, 2001, p. 50], where the center position is calculated as 2 times the diameter of the vapor inlet nozzle or at least $500mm$ in the case of large and $450mm + 0.5 \cdot !dVaporBottomIn$ in case of small columns.

Furthermore, the vapor inlet nozzle has to be placed above the torospherical head to enable a proper installation in terms of distance between weldings. Equation 3.1 represents the applied calculation of the vapor inlet nozzle position referring to Kister, 1990 and Branan, 2005 and with consideration of the distances for welding. The variables *!h1BottomDishRing* describe the height of the cylindrical border h_1 (see figure A.19 in section A.2.2) and *!h2BottomDish* the height h_2 of the curved part of a dished bottom.

$$\begin{aligned} &!verticalPosVaporBottomInNozzle = \\ &\quad \mathrm{MAX}[(!bottomHighLiquidLevel + 300mm + 0.5 \cdot !dVaporBottomIn), \\ &\qquad (!h1BottomDishRing + !h2BottomDish + 2 \cdot !spaceForWeld))] \end{aligned} \tag{3.1}$$

Changing the heuristic values used can be useful for specific applications. For such cases the user has the possibility to influence the design by setting optional variable values (e.g. for the variables *!verticalPosVaporBottomInNozzle* or *!spaceForWeld* in the example above).

The general procedure of defining the calculation routines for variables required for the constructive design of the process units has been performed in a similar way. Norm values, manufacturer specifications as well as heuristic rules are used as basic data set for dimensioning and the positioning of elements and possible restrictions with regard to the installation are also taken into account in the calculation methods.

Design of tray columns

In figure 3.7 an overview of variables and formula expressions for the determination of geometric properties for tray columns is given. In tray columns, the arrangement and design of the trays ensure the return liquid flows across the horizontal tray during contact with the ascending vapor penetrating it vertically through perforations. Vapor and liquid are thus passed through the column in cross counterflow. [J. Stichlmair, 2005, p. 72]

The design and geometries of the trays are regular, but may vary according to internal flow rates in different sections. In this approach only single-pass trays are considered - further possibilities like multi-pass (two-, three- or four-pass), radial flow, stepped or reverse flow trays [Sattler and Feindt, 1995, p.213] are currently not implemented, but these design options can easily be extended.

Specific malfunctions referring to the constructive design in tray columns are for example the feed entry arrangement, vapor maldistributions, draw-off malfunctions, tower liquid base levels and the reboiler return arrangement [Kister, 2006]. In order to achieve good mass transfer between the two phases and to avoid capacity and separation bottlenecks, special attention must be paid to the design of the tray geometries, weir and down comer area. The overall algorithm of the creation of internals in tray columns for different configurations is illustrated in figure A.3 in section A.2.2.

Furthermore, the manhole arrangement within tray columns is of importance for achieving good conditions for maintenance tasks and during the turnaround. The column internals (trays, support rings) have to be created depending on the number and the positions of additional manholes. The programming algorithm is shown in the figures A.4 and A.5 in section A.2.2. The construction of the tray column is created from bottom to top. A closer description to the determination of the manhole arrangement is given in paragraph 3.1.2.1.

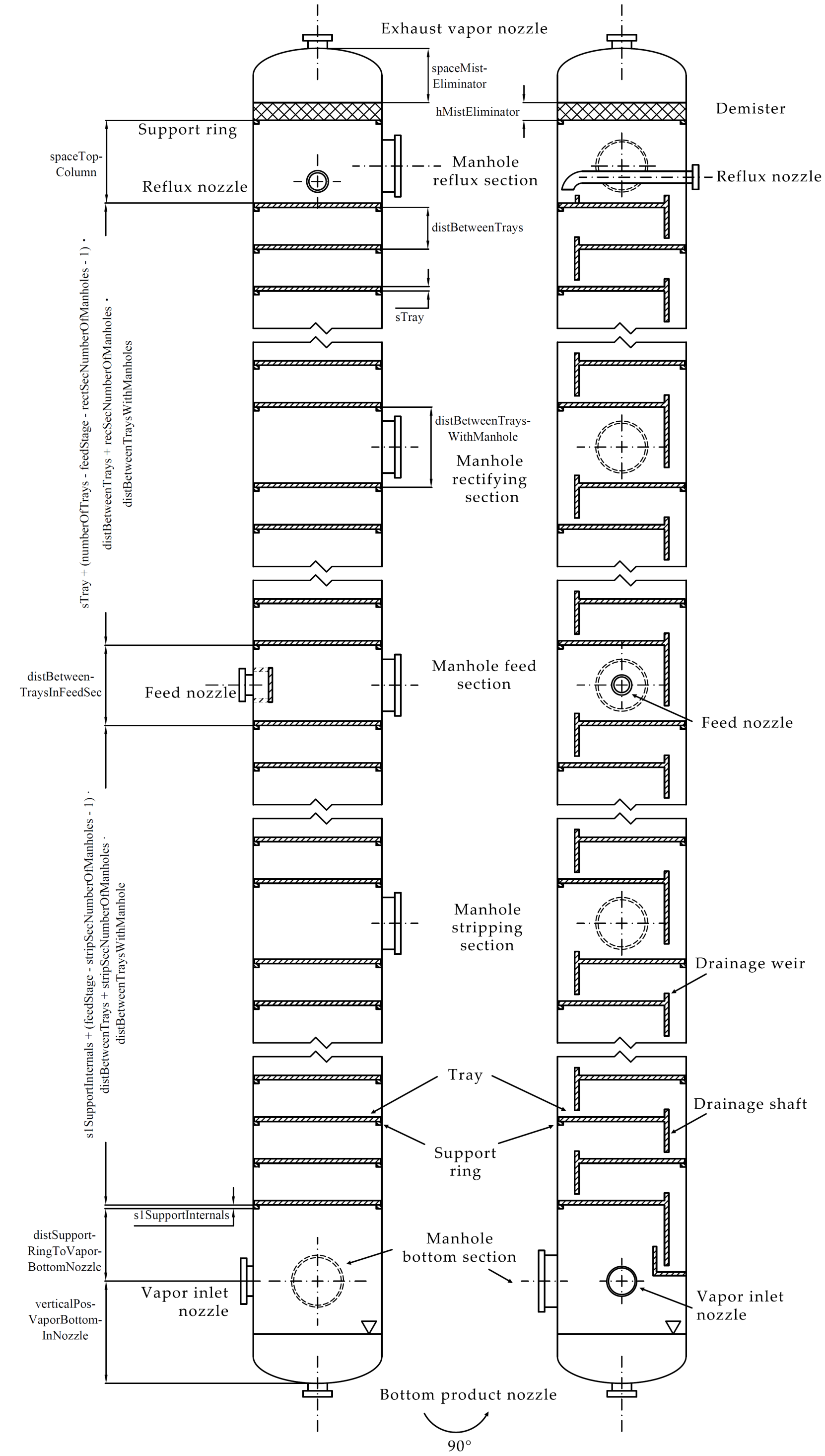


Figure 3.7: Variable overview for the calculation of vertical positions and total column height for tray columns (including demister)

Process and design variants for distillation columns

Depending on the separation tasks and the thermal state of the feed, columns can have different configurations. Figure 3.8 depicts a continuous, countercurrent distillation column including stripping and rectifying section, a stripping or exhausting column and a rectifying or enrichment column as typical column configurations in process industries. A stripping column has no rectifying section and a good bottom purity can be achieved with a small throughput and small amounts of overhead product. Rectifying columns have no stripping sections and instead of a reboiler a vapor bottom feed (saturated or wet vapor with a small fraction of the liquid phase) is used. The overhead product can be achieved with high purities with a small throughput. [Sattler and Feindt, 1995 p. 102 ff., p. 119 ff.]
The general design of a column and consequently the programming sequences for the generation of a design are highly influenced by these characteristics.

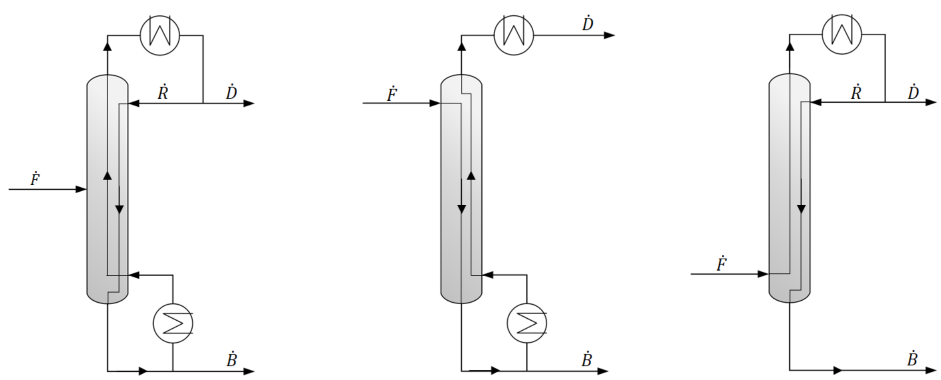


Figure 3.8: Schematic overview of typical column configurations depending on position and thermal state of feed: standard column including stripping and rectifying section (left), stripping column (middle) and rectifying column (right) [based on Sattler and Feindt, 1995]

Design of column feed sections

The thermal state of the feed q is characterized by equation 3.2. The thermodynamic state (saturated liquid or vapor, two-phase, subcooled liquid or superheated vapor) affects the internal vapor and liquid loads, as illustrated in figure 3.9, as well as the (optimal) feed position in the column.

Different internal flows lead to different column diameters for rectifying and stripping section assuming the F-Factor, representing the gas load of the column, is approximately constant.

$$q = \frac{\dot{L}^{str} - \dot{L}^{rec}}{\dot{F}^{f}} = \frac{\dot{L}_j - \dot{L}_{j-1}}{\dot{F}_j^{f}} \tag{3.2}$$

The q-line locates the intersection of rectifying and stripping component balance or operating lines in the McCabe-Thiele diagram. The McCabe-Thiele diagram provides a simple way to graphically construct the total number of theoretical stages for a distillative separation as well as to capture of feed location, which divides the rectifying and the stripping section as illustrated in figure 3.10.
The validity of the McCabe-Thiele diagram is given only for binary mixtures at constant pressure and under certain assumptions (e.g. equal molar evaporation enthalpies of both components, constant molar overflow instead of consideration of energy balance) [Sattler and Feindt, 1995, p. 82-83; Kister, 1992, p. 29-32]. Nevertheless, this design method offers a good possibility of graphical representation of relevant correlations. The q-lines as function of different thermal states of the feed represent the influence on the optimal feed position.

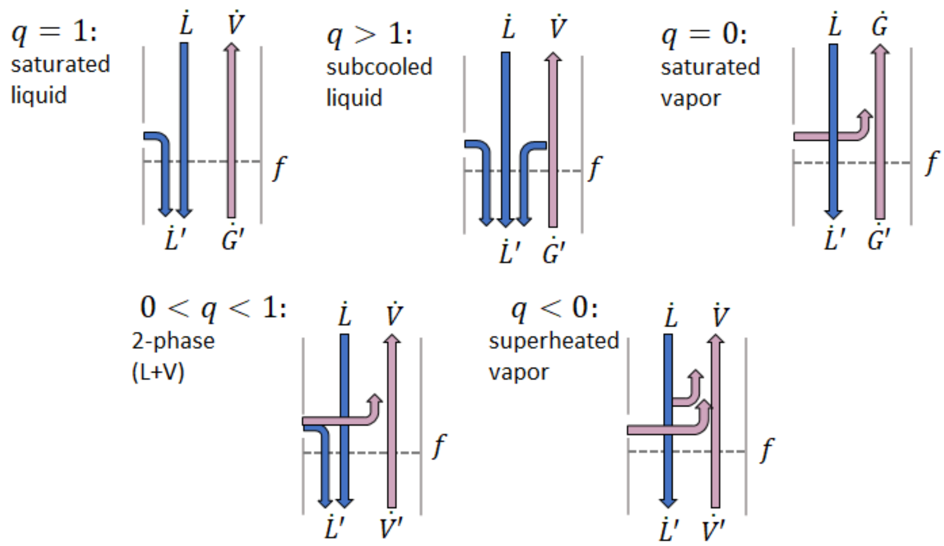


Figure 3.9: Schematic overview of the influence of the thermal feed state on the internal liquid and vapor flows of a distillation column

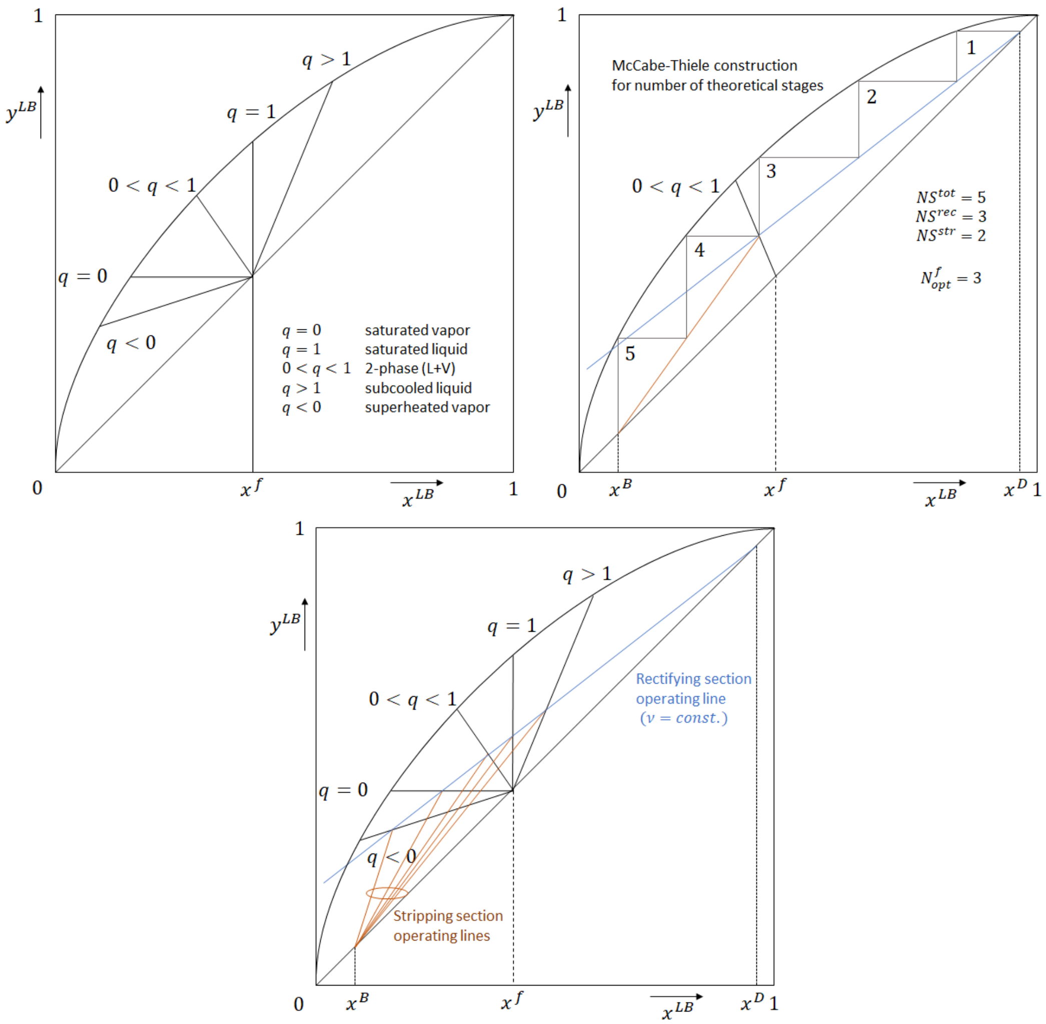


Figure 3.10: q-line as function of the thermal feed state (a), examplary construction of number of theoretical stages (b) and effect on the operating lines of the stripping and rectifying section at constant reflux ratio (c) [related to Kister, 1992, p.38 ff]

In figure 3.11 possible constructive configurations of the feed section for packed and tray columns are shown. The differences refer to the position of feed nozzle and manhole above, below or within the conus for the change of the external column diameter within the stripping and rectifying sections.

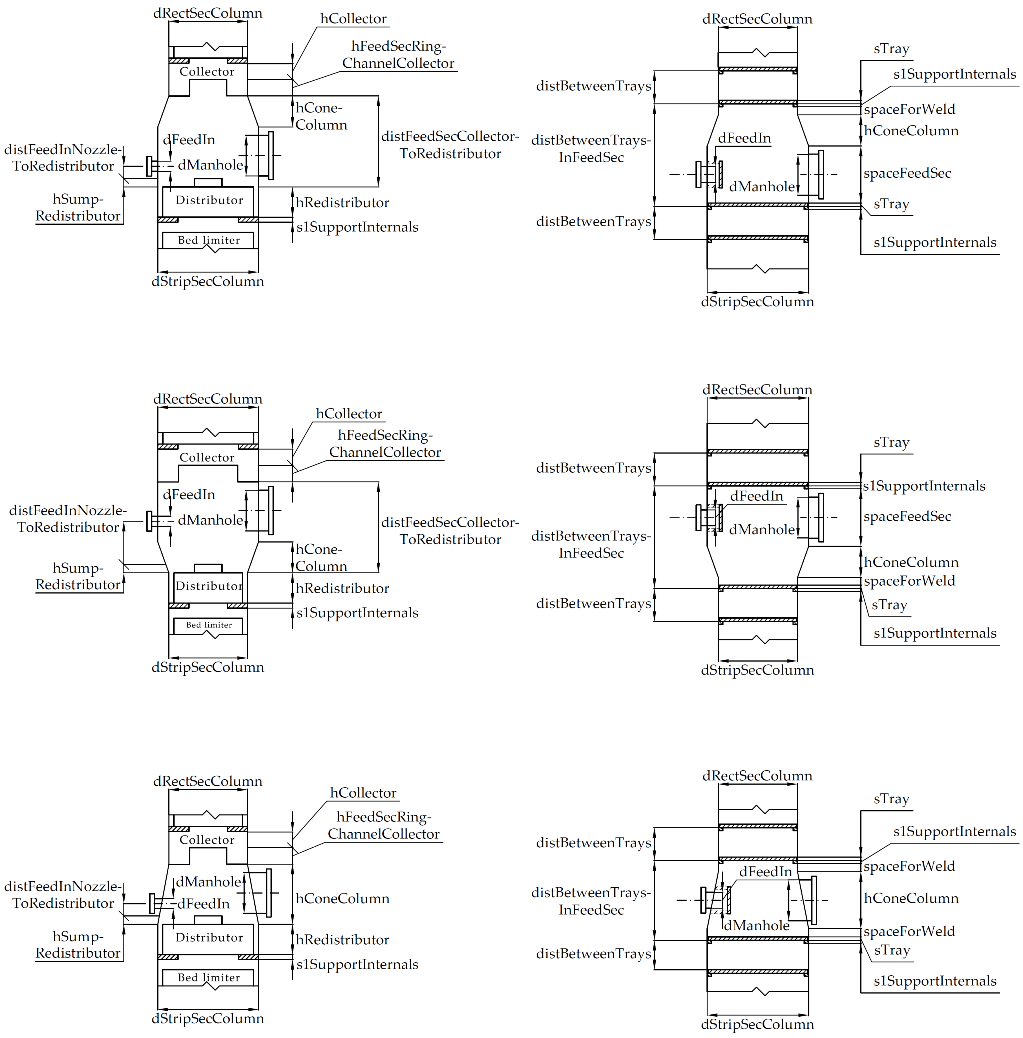


Figure 3.11: Possible configurations of feed sections for packed (left) and tray columns (right) with different diameters in the stripping and rectifying sections: $D_{rec} < D_{str}$ and nozzles in stripping section (top); $D_{rec} > D_{str}$ and nozzles in rectying section (middle); $D_{rec} < D_{str}$ and nozzles in conus (bottom)

Figure 3.12 illustrates the configurations of the internal feed arrangement within packed columns with constant column diameter. The possibilities for the input of the feed are within the ring channel of the collector (left) or outside of the collector (right).

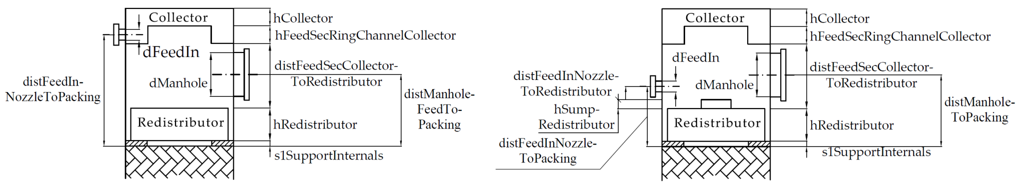


Figure 3.12: Possible configurations of internal feed arrangements in packed columns: feed inlet inside ring channel of collector (left) and outside of the collector (right)

Mist eliminators

Figure 3.13 depicts the rectifying section of packed and tray columns with and without mist eliminator. The mist eliminator/demister has the task of separating liquid droplets from the leaving exhaust vapor. This can reduce the loss and improve the quality of the distillate product, prevent corrosion in the downstream systems due to corrosive liquid droplets, protect compressors and vacuum pumps against liquid drops and reduce emissions by droplet ejection [Nitsche, 2014, p. 376].
In vertical separators like columns, the fall velocity w_{fall} of the droplets must be greater than the upward vapor flow velocity w_V. Referring to Nitsche, 2014, for the design $50-75\%$ of the drop velocity is used ($w_G \leq 0.5 \dots 0.75 \cdot w_{fall,drops}$). Referring to [Nitsche, 2014, p. 376 ff.] wired meshes with wire diameters of $0.1-0.28mm$ and a package depth of $100-300mm$ are most widely used. The steam flows around the wires, but the drops cannot do this because of their inertia. This causes droplet coalescence, whereby the droplets that hit the wires flow together and fall down as large droplets. The knitted wire mesh separator is particularly suitable for separating small droplets in the range from $5 \dots 10\mu m$. Lamella separators are advantageous for larger liquid loads and at the risk of contamination. Droplet separation is achieved by inertia, because the droplets do not follow the gas flow when flowing through the zigzag corrugated laminae and collide with the sheets and run down in countercurrent to the gas.

Liquid collector-distributor systems for packed columns

As mentioned above, liquid (re-)distribution ensures an appropriate distribution of the liquid phase which is the prerequisite for an appropriate packing efficiency - according to [Kister, 1990, p. 35] it may decrease by factor 2...3 due to maldistribution.

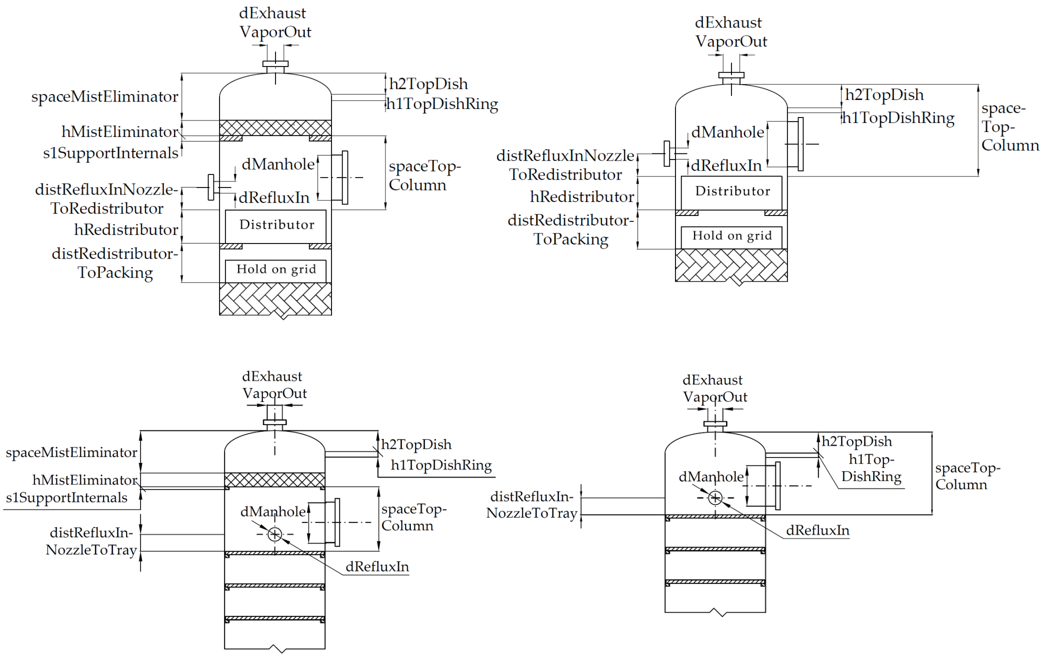


Figure 3.13: Rectifying section of packed column (top) and tray column (bottom) including mist eliminator (left) and without mist eliminator (right)

Figure 3.14 shows qualitatively the variation of HEPT (height equivalent to a theoretical plate) as function of vapor or liquid rate at constant vapor-to-liquid ratio. The two upper curves represent the progress of a lower quality of liquid distribution in comparison to the standard or high-performance distribution curves below. The packing turndown with maldistribution is largely reduced. [Kister, 1990, p. 37 ff]
Distributors are required at each position where a liquid stream is fed into the column [Branan, 2005, p.88]. Since the relative void fraction of the packing close to the wall is larger than in the center, the downflowing liquid tends to preferentially trickle down the wall with increasing distance from the liquid distributor. To restrict this specific effect of maldistribution, liquid redistributors are used to interrupt the packing [Sattler and Feindt, 1995, p. 198].
To provide distributor designs for different scopes of application, frequently used distributors for varying operating windows (liquid load, column diameter, turndown ratio) with different operating principles and robustness in terms of risk of contamination are investigated and implemented.

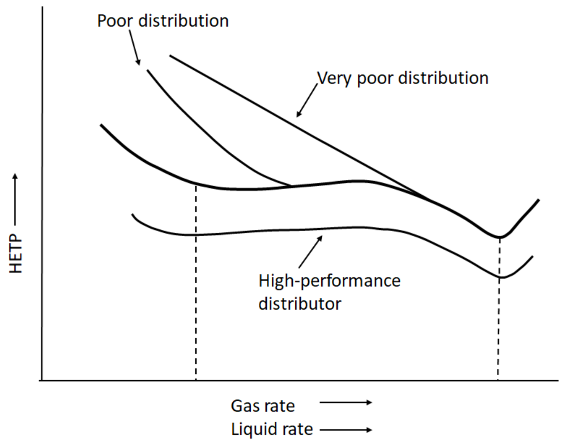
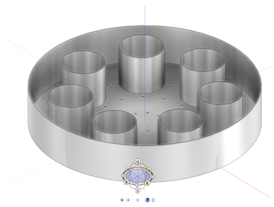
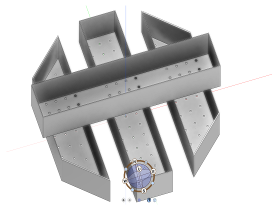
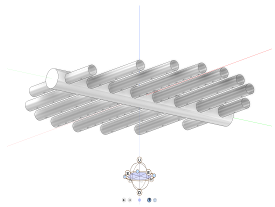


Figure 3.14: Effect of liquid distribution on HEPT (on constant liquid-to-vapor ratio) [according to Kister, 1990, p.37, figure 3.7]

The current *PlantDesign* model library includes orifice pan (pan with discharge holes for the liquid and gas risers for the rising gas, gravity-driven), channel type (through distributor with outlet holes at the distributor base, gravity-driven) and perforated pipe distributors (closed pipe distributor with central inlet). An overview of the main characteristics is given in the upper part of table 3.1. Detailed design information for column internals e.g. distributors are typically manufacturer-depended and not completely published. However, in literature there are operating ranges and the corresponding typical design parameters for internals that are commonly used in industries. In the case of liquid distributors, the automated design is realized using specifically developed computation algorithms, which determine automatically geometries and arrangements of the components with respect to the information and restrictions given from manufacturers as well as typical values and ranges from literature [referring to Molano, 2017]. These values are queried from the *PlantDesign* database. Calculated and iterated values are for example the number, diameters and arrangements of holes, risers and pipes, the dimensions and arrangements of main and sub channels or the height of the channel depending on the column diameter, the turndown ratio and the fluid load representing the hydraulic conditions.
In table 3.1 the specifications using manufacturer and heuristic data and the iterated variables for the construction based on the user input are summarized for the different distributors. Exemplary, an overview of the design procedure to create orifice pan distributors is illustrated in figures A.6 and A.7 in section A.2.2.

Table 3.1: Liquid distributors - types, characteristics and calculation variables

Orifice pan distributor	**Channel type distributor**	**Perforated pipe distributor**
		
Distributor models are drawn and visualized in AVEVA E3D™ 2.1		
Small to medium-sized columns	Medium-sized to large columns	Small to large columns
$d_{col} = 300 - 1200mm$	$d_{col} = 800 - 3000mm$	$d_{col} = 500 - 3600mm$
Flowrate: $> 5\frac{m^3}{m^2 \cdot h}$	Flowrate: $5 - 80\frac{m^3}{m^2 \cdot h}$	Flowrate: $60 - 100\frac{m^3}{m^2 \cdot h}$
Turndown ratio: 2 : 1 up to 4 : 1	Turndown ratio: 2/10 : 1	Turndown ratio: 3 : 1
Raschig GmbH, 2017, p. 44-46	Raschig GmbH, 2017, p.41-43	Raschig GmbH, 2017, p. 50-52
User specifications:		
Column diameter Liquid volumetric flow Free area for gas flow	Column diameter Liquid volumetric flow Free area for gas flow	Column diameter Liquid volumetric flow
Manufacturer and heuristic values:		
	Number of channels	Number of pipes Diameter of main pipe
Iterated variables:		
Number of holes Hole diameter Positions of holes Height of distributor Number of gas risers Diameter of gas risers Position of gas risers	Number of holes Hole diameter Positions of holes Number and positioning of holes in main channel Height of main and sub-channels Width of main channel	Number of holes Hole diameter Positions of holes Diameter of lower pipes

Based on the user-specifications the number, sizing and positioning of liquid orifices and gas risers are determined for an equal distribution. In figure A.8 relevant geometric variables for the positioning of orifices are illustrated. Starting with an initialization using typical default values for the constructive variables, the algorithm iterates the final values fulfilling constraints and conditions for a proper distributor design. Important heuristic rules and manufacturer information applied within the algorithm has been found in [Perry and Green, 2008, p. 14-73 - 14-80], [Kister, 1990, p. 35-82], [Branan, 2005, p. 88-97], [Lehner, 2006, p. 55-58], [Nitsche, 2014, p. 339-343], [Raschig GmbH, 2017, p.35-75], [Koch-Glitsch, 2010a, p. 3-17], [Koch-Glitsch, 2010c, p. 15-16], [Montz, 2019, p. 30-39], [AMACS, 2012, p. 11-13], [GEA, 2014, p. 10-25], [Schultes, 2000, p. 1381-1389], [Robert J. Cordingley, 1986, p. 2-4]. Thus a very detailed dimensioning and positioning of the distributor as well as a very exact overall model of the column (e.g. determination of the exact overall height) is already available without a concrete design of the internals by the specialized manufacturers. The iterated design is adapted to all relevant process parameters, e.g. the liquid load but also physical properties (e.g. mixture densities of the phases, viscosity of the liquid) and offers a good reference for the design for comparison of the design by the manufacturer of the internals.

Algorithm for the design of sieve trays

Tray design is - for most column internals - manufacturer specific and there are typically no publications regarding the geometries and the distribution of the boreholes or constructive details for advantageous effect on separation performance. Similar to the design of liquid distributors, an algorithm designing sieve trays automatically has been successfully developed based on heuristics found in literature [J. Stichlmair, 1978, p. 281-284], [J. G. Stichlmair and Fair, 1998 p. 176-187], [Mersmann, 1963, p. 103-107], [Ruff, Pilhofer, and Mersmann, 1976, p. 759-764], [Kister, 1990, p. 146-151], [Sattler and Feindt, 1995, p. 167-187]. Parts of the implementations are done within the project work of [Klette, 2018].

In figure 3.15 a sieve tray and the corresponding variables for construction used in the calculation algorithm are illustrated. The unknown target variables for the sieve tray design are the bore diameter d_h, the distance between them (pitch) p and the number of holes n. The algorithm for the determination of the dimensioning and positioning of sieve trays using available heuristic information from literature has been developed as illustrated in figure A.9 in section A.2.2.

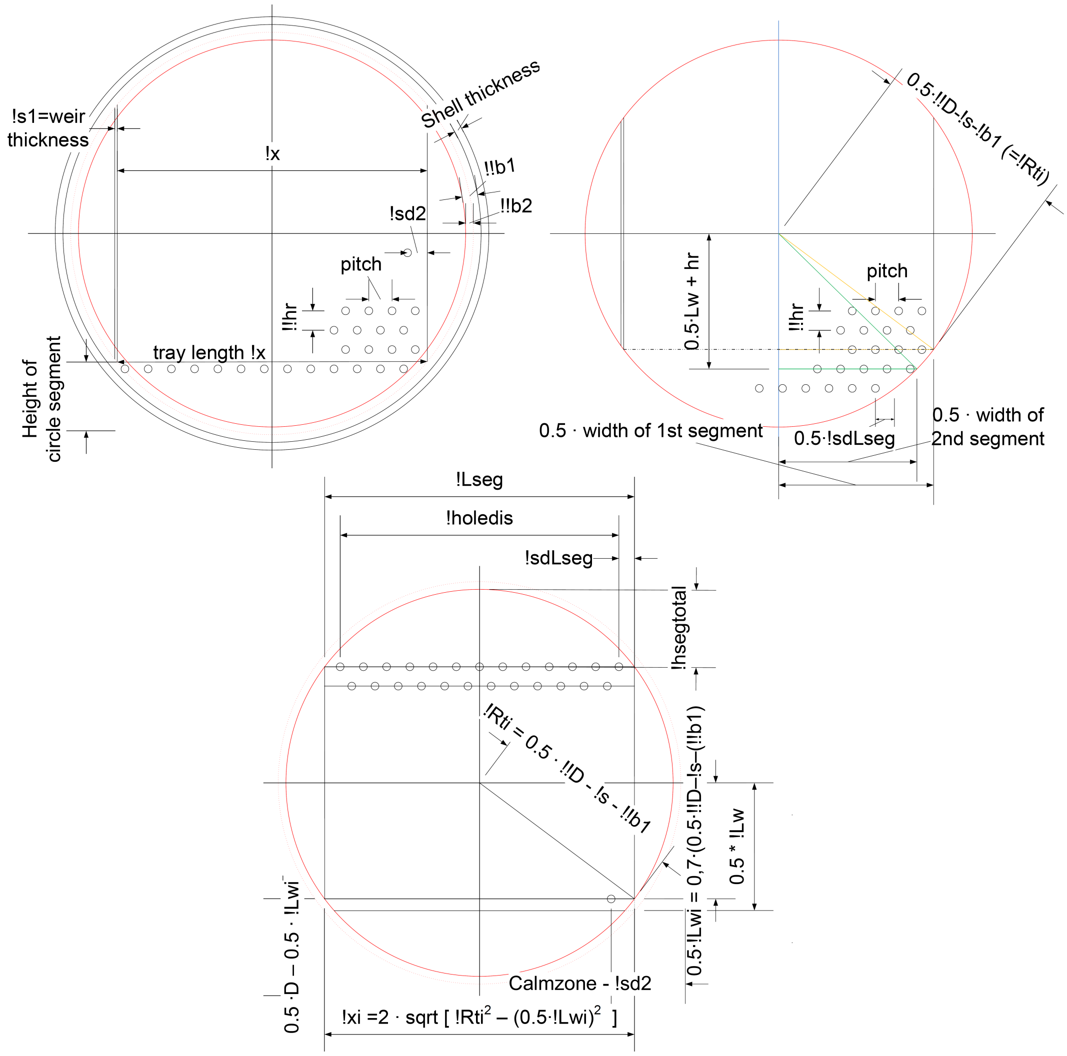


Figure 3.15: Constructive variables for sieve trays

Starting point is the determination of reasonable starting values for the distance between holes p (determination based on Kister, 1990, p. 149) and the hole diameter d_h by providing better known starting values for the hole diameter $d_{h,start}$, the relative fractional hole area Φ_{start} as well as a tolerance value ϵ for Φ.

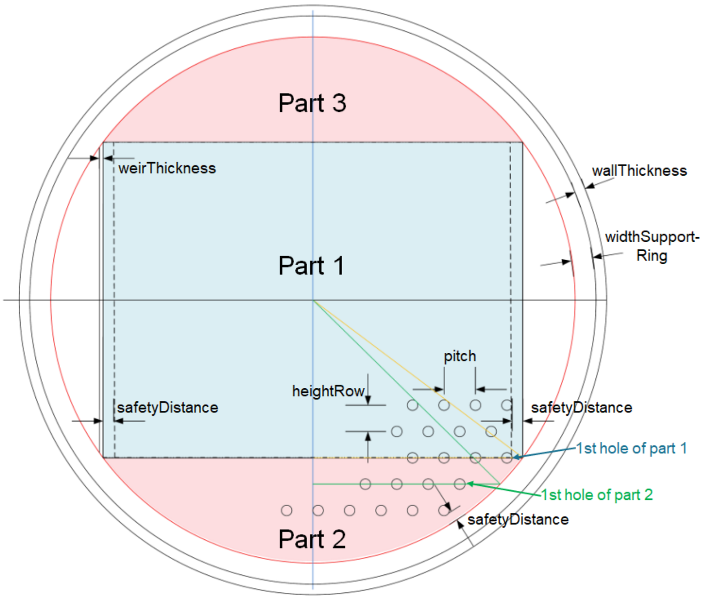


Figure 3.16: Procedure of constructive design of sieve trays

All intermediate and final results are checked against typical values from literature. Heuristic values for the design of sieve trays as well as recommendations for valve and bubble cap trays are listed in table A.8 in paragraph A.2.2. Based on simulation variables (e.g. internal vapor flowrates, liquid and vapor mixture density, liquid surface tension) the required active area is calculated referring to the approach [J. Stichlmair, 1978, p. 281-284]. This makes it possible to subsequently calculate the number and diameter of the holes as well as their distance from each other (pitch). Afterwards the algorithm for positioning and drawing the holes, which is subdivided into three parts as shown in figure 3.16, is started using these results. *Part 1* is a square area of the active tray area, *Part 2* and *Part 3* are mirrored circle segments above and below the square area. The holes are distributed equally with a triangular pitch in all parts, taking into account to leave a free safety distance on the edge for installation purposes.

The approach of the sieve tray design can be easily adapted for valve and bubble cap trays. Depending on the specific design variables, the distribution of these elements can be calculated in a similar way, only the bores in the tray have to be replaces by valves or respectively bubble caps. The extension of these designs can be realized in future work.

Maintenance tasks - manhole arrangements

Manholes and handholes (for columns $d_{col} < 700 \ldots 900mm$) are entries into the shell of the column, typically positioned where internal piping's are arranged or internals e.g. distributors should be accessible [Kern, 1977a, p. 156; Kister, 1990, p. 137]. In contrast to the manhole distribution in packed columns, tray columns have additional access possibilities beside in the reflux, feed and bottom sections. Further manholes are provided for maintenance tasks within the stripping and rectifying sections to reduce installation and maintenance times, especially for high columns.
It is recommended to install manholes at each $10 \ldots 20$ trays. If the service is clean and non-corrosive up to 30 trays can be served by one manhole. If a frequently cleaning is required, or the trays are very large and removing internals through the hole is slow, the distance between two manholes should be reduced [Kister, 1990, p. 137]. The number of additional manholes within the stripping or rectifying section is defined by the variable *!minNumberOfTraysBetweenManholes*, which can be chosen by the user. To ensure an equal distribution of the manholes in both sections, an algorithm has been developed to check and adapt the setting if necessary to ensure a regular arrangement. The overall algorithm is shown in figure A.11, the determination for the optional manholes in the stripping section in figure A.12 in section A.2.2. The procedure is analog for the rectifying section.

The variable *!distBetweenTraysWithManhole* stores the distance between two trays in the stripping and rectifying section, between which a manhole is located. Their value is determined by the manhole diameter (*!dManhole*) and the space for the welds (*!spaceForWeld*), which default value is set to $200mm$ for this calculation, but can be adjusted by the user (but a minimum value of $50mm$ must not be exceeded). According to [Kister, 1990, p. 138, referring to Bolles, 1956] the tray clearance must be at least $900mm$ to ensure sufficient working space. If the calculated tray clearance with handholes is smaller than without, the larger distance is selected. In addition, it must be mentioned that the down comers of the trays with additional manholes are extended automatically according to the higher distance between the trays.

The variable *!headroomPlatform* describes the clear height, which provides enough free space for working below a stage (see figure 3.17). This ensures that the platforms can be placed one below the other and the access to a manhole is not obstructed or impeded. A reference value of $!headroomPlatform = 6.75ft = 2060mm$ is taken from [Kern, 1977b, p. 123-129].

For a proper constructive design, the required number of trays to ensure enough headroom from the platforms is determined as illustrated in figure A.10 in section A.2.2. If it is necessary, the variable value is increased incrementally. In this case, a warning message is given to the user and too low user-specific values of the variable *!minNumberOfTraysBetweenManholes* can be detected easily.

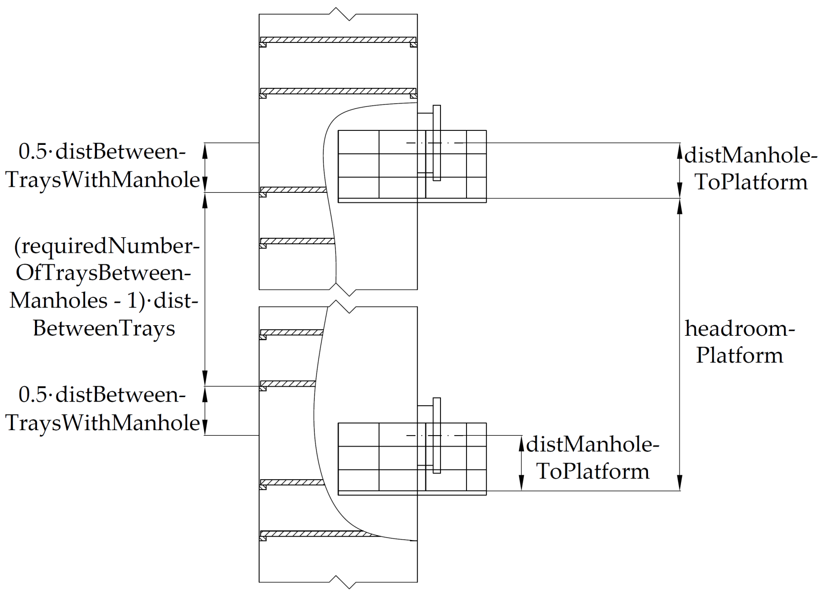


Figure 3.17: Accessibility to manholes in tray columns - positioning of platforms and manholes

Within pure stripping or rectifying columns, but also if the number of trays in the stripping or rectifying section is too low, it can happen that no manholes will be installed in the bottom, feed or reflux area. The corresponding checks in the program sequences are shown in figures A.13 and A.14 in section A.2.2. The possible scenarios for the manhole arrangements are listed in table 3.2.

According to [Kister, 1990, p. 138], the accessibility of manholes through platforms should be ensured at heights greater than $12ft \approx 3700mm$ and all manholes should be oriented in the same direction, whenever possible. These guidelines are taken into account for the automated constructive design of the modular distillation columns.

Table 3.2: Possible scenarios for bottom, feed and reflux manhole arrangements in tray columns

Type of tray column	Installed manholes*
Stripping column	MF, MB
↦ too few trays	MF
Rectifying column	MR, MF
↦ too few trays	MR
Column including stripping and rectifying section	R, MF, MB
↦ too few trays in rectifying section	MR, MB
↦ too few trays in stripping section	MR, MF
↦ too few trays in both section	MR

**MR: Manhole reflux, MF: Manhole feed, MB: Manhole bottom*

Accessibility - platforms & ladders

Accessibility to columns for assembly and dismantling tasks as well as for inspections and maintenance work are stationary entrances on the outer shell in the form of platforms and ladders, as shown in figure 3.18. Figure 3.19 illustrates the schematic layout and variables used for the design. The constructive design is realized based on [DIN 28017-1, 2014] for stages, [DIN 28017-2, 2012] for railings, [DIN 28017-3, 2012] for ladders and [DIN 28017-4, 2012] for fall protections. Access is provided for the existing manholes in the reflux, feed and bottom sections. Additional manholes are used in the stripping and rectifying sections in tray columns (after 10-20 trays), in areas of re-distribution systems in packed columns as well as for the bottom manhole. As already mentioned in paragraph 3.1.2.1, the presence of manholes for feed, reflux and bottom manholes must be verified in each case.
Permanent means of access are positioned at each manhole places at minimum $3700mm$ above the bottom plate [Kern, 1977b p. 153-160; Kister, 1990, p. 138], at minimum each $(!maxDistBetweenPlatforms = 10m)$ and for column diameters $d_{col} > 1000mm$. According to [DIN 28017-3, 2012], ladders can be inclined at a maximum of 10° to the vertical and a back protection must be installed. The inclination is relevant for columns with different column diameters in the rectifying and stripping section.

If the column is insulated, the platforms are placed at a distance of $100mm$ plus the insulation thickness (*!insulationThickness*) referring to [DIN 28017-1, 2014]. The positioning is based on the cylinder axis of the apparatus.
The flowcharts representing the general algorithms for the creation of means of access are illustrated in figures A.15 to A.18.

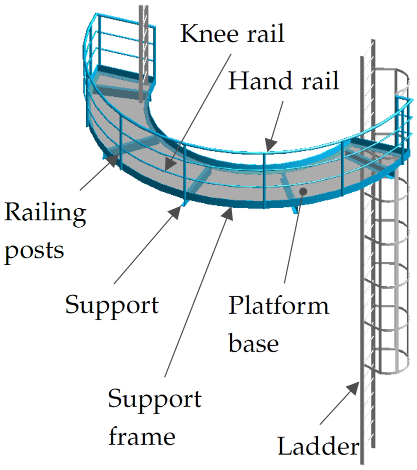


Figure 3.18: Components of permanent means of access

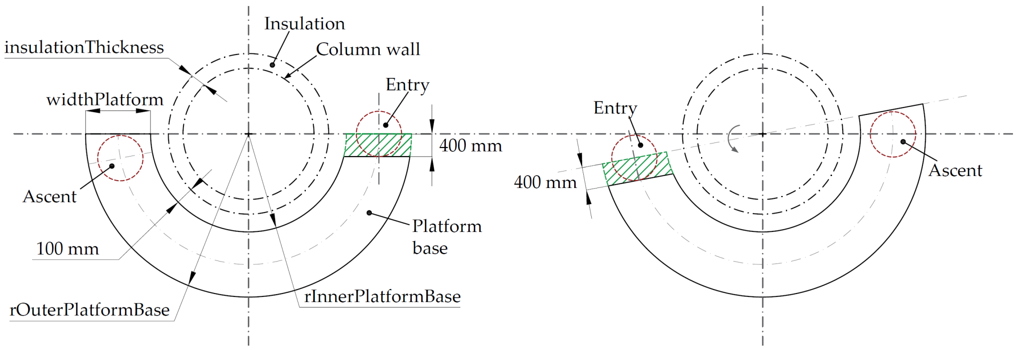


Figure 3.19: Schematic layout and constructive variables of permanent means of access

Control schemes for distillation processes

The aim of the process control system is to achieve and receive the desired operating state with regard to the production level, safety and economic efficiency despite any disturbances that occur in the process. Typical disturbances are for example changes in the feed quantity, composition and state (temperature, pressure), inlet conditions of utilities like cooling water and heating steam, as well as fouling in the heat exchangers, corrosion, formation of deposits in the column, etc. Column control can be divided into two categories - the basic control to regulate material accumulation in the column and setting stable conditions for operation (top pressure, level control in the bottom part and the reflux drum in case of distillation columns) as well as the control of the product specifications [Kister, 1990, p. 487; Goedecke, 2006, p. 728ff]. Typical manipulated variables for distillation column control are depicted in figure 3.20.

The assignment of manipulated and controlled variables to level control can be carried out using simple rules. For level control, it makes sense to use the largest flow as the manipulated variable, since a greater effect on the change of the level can be achieved. With small reflux flow ratios and thus also low reflux flow quantities, the level in the reflux drum should be controlled with the distillate flow as manipulated variable (as shown in schemes *a* and *b* in figure 3.21).

For high evaporation rates, it is recommended to select the heating medium quantity as the manipulated variable for the bottom level, for low evaporation rates, the bottom product flow (as illustrated in scheme *c* in figure 3.21). For the respective flow a quantity control should be provided. The setpoint for this is either fixed or results from a ratio control such as reflux ratio $\frac{\dot{R}}{\dot{D}}$ or $\frac{\dot{V}_{hm}}{\dot{B}}$ (see figure 3.20).
The column pressure is one of the most important control variables since it affects condensation, vaporization, temperatures, compositions, relative volatilities and almost all processes in a distillation column [Kister, 1990, p. 490]. The control is usually carried out by adjusting the coolant flow for total condensation, normal or positive pressure columns. However, it should be noted that low speeds and high outlet temperatures when using cooling water can cause fouling in the condenser. The control function is best guaranteed if the condenser is located above the reflux drum. This arrangement allows the condensate to flow by gravity. In case of vacuum rectifications with non-condensable components the discharge flow to the vacuum pump is usually chosen as manipulated variable [Goedecke, 2006, p. 783]. If a vaporous distillate product is present, it is recommended in [Kister, 1990, p. 490; Sloley, 2001, p. 39-48] to control the pressure directly by adjusting the product itself as illustrated in figure 3.21 schema *d*.

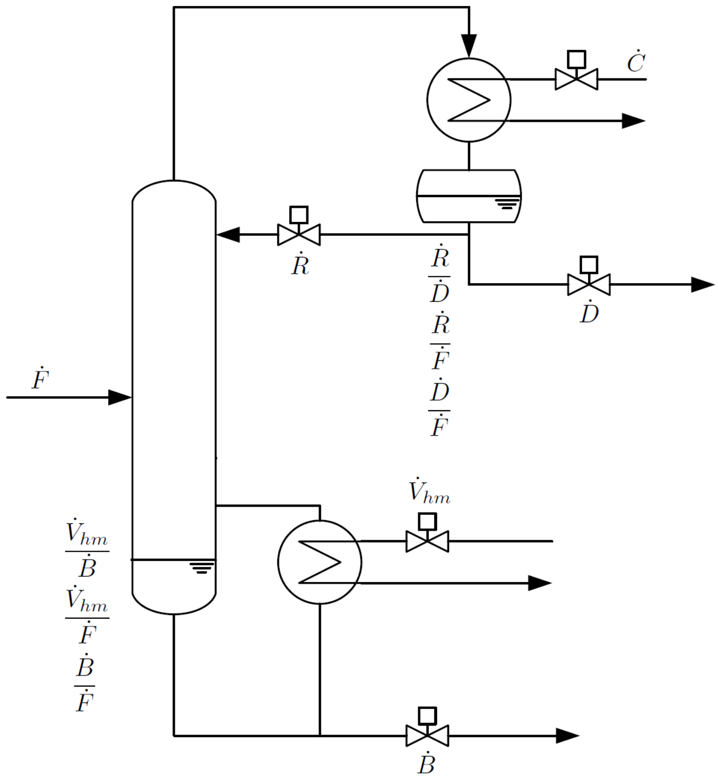


Figure 3.20: Typical manipulated variables for distillation column control loops [adapted from Goedecke, 2006, p. 782]

The composition control is of particular importance for distillation columns, since it is only possible to operate the columns as intended by achieving the product specifications. The product compositions are rarely measured directly (e.g. via online gas chromatographs), as this is too expensive and does not provide continuous measured values. [Deshpande, 1985, p. 293-294] For this reason, the temperature is often used as a substitute control variable using the dependencies of the boiling temperature of a mixture with the composition at constant pressure. Other representative physical properties like density, vapor pressure, refractive index or freezing points can also be used as substitute for composition [Kister, 1990, p. 488]. Referring to [Kister, 1990], temperature control is advantageous because it is cheaper, easier to maintain and faster than direct composition control, whereby it does not react sensitive to changes in product composition in high-purity product streams [Goedecke, 2006, p. 728ff]. By analyzing the temperature profile of the column, a suitable temperature sensor position shows a high sensitivity as well as symmetric temperature changes for positive and negative deviations of the manipulated variable.

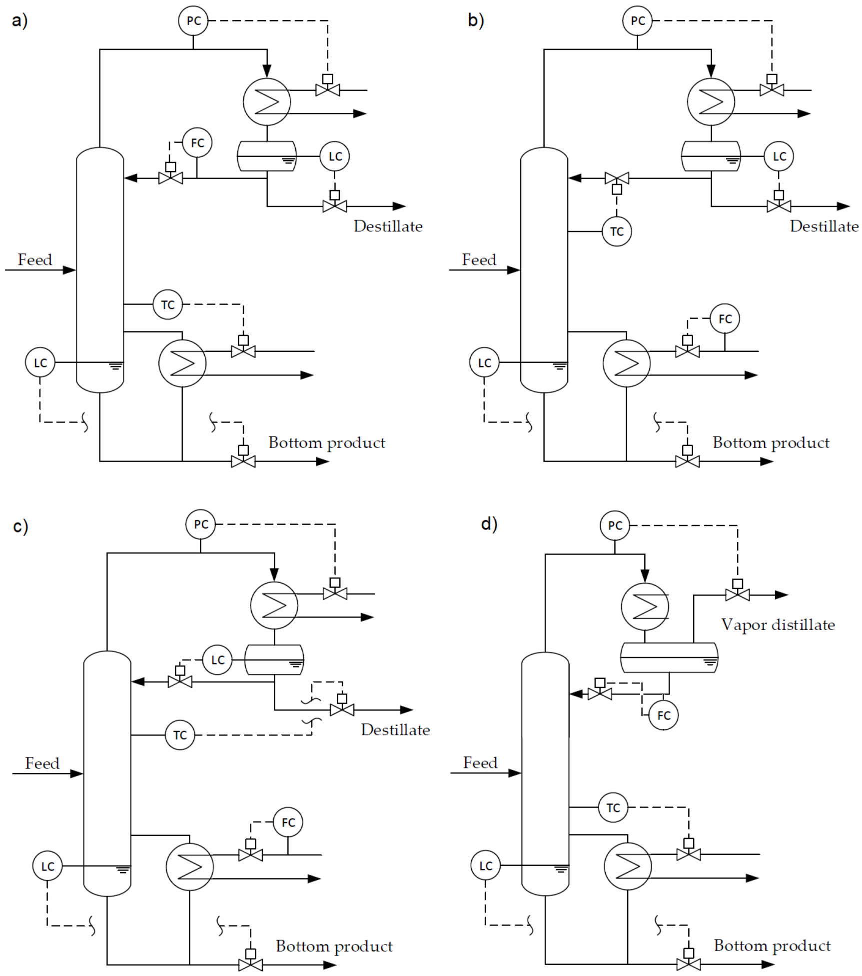


Figure 3.21: Single composition control structures for distillation columns [related to Kister, 1990, p. 498 and Sloley, 2001, p. 39-48]: (a) Indirect control, compositions regulates boilup; (b) indirect control, composition regulates reflux; (c) direct control, composition regulates distillate flow; (d) pressure control with vapor distillate product flow

In this work, the three most common control concepts from [Kister, 1990, p. 485 ff; Deshpande, 1985, p. 286 ff] are modeled (see figure 3.21 a, b, c). Beside them, further control concepts are listed in table A.9, but these are not often applied in practice. Application cases for the different control schemes are listed in table A.10 in section A.2.2.
The first two variants (figure 3.21 a, b) represents indirect mass balance control schemes, which means that the quality/temperature control is not directly controlled by the product take-off flows, i.e. the mass balance, but for example via reflux flow or heating steam quantity. Within direct mass balance control like in scheme (figure 3.21 c), a product stream, in this case the distillate flow, is the manipulated variable to control the quality/temperature.

The graphical representation of the control structure is realized within two-dimensional PFDs and P&IDs, whereas in 3D models not all control elements are represented. Sensors used for control (TC, PC, FC, QC, LC) or for indication (TI, PI, FI, QI, LI) are typically not drawn in 3D models, but actors like control valves are included within the piping. Information lines between sensors and actors of the control loops as in 2D diagrams are not illustrated. Within the close piping included in MPUs for distillation columns no control valves are positioned, but in the MPUs of associated apparatus (e.g. condenser, reboiler and pumping groups) control elements are present. The accessibility of these actors and corresponding piping elements (like shutoff valves in front and after the control valve) has to be guaranteed. They are typically placed close to the associated apparatus within the equipment rack or in the ground level depending on their position. The flexible implementation of the control structure in 3D models for distillation processes therefore does not depend on the MPUs of the columns but rather on those of the associated apparatus modules, especially to the condensers and reboilers. The presented control schemes in figure 3.21 (a-c) can be put into practice if the flowrates of the heating steam inlet pipe of the reboiler and the cooling medium inlet pipe of the condenser can be controlled using a control valve. The required control valves are included in the close piping of the condensers and reboilers implemented in *PlantDesign*. The other sensors for implementing the control concepts (in particular level and temperature sensors for level and purity control) are not necessarily represented in the 3D model. This allows a flexible adaptation of the control scheme to the respective process conditions if the various MPUs contained in *PlantDesign* are interconnected.

3.1.2.2 Design of associated apparatus

In this section the automated design of associated apparatus of distillation columns is briefly discussed. As mentioned above, the development of the automated MPU design is in general identical as for columns. For this reason only a short overview of the design of heat exchanger und pump assemblies is given.

Shell and tube heat exchanger

Shell and tube heat exchangers as widely applied type of heat exchangers in process industries (approximately 65% of the market share, [Thulukkanam, 2013 p. 293]) are implemented in *PlantDesign*. The design of the implemented floating head heat exchanger is related to several norms, listed in, table A.4, and heuristics found in literature [Thulukkanam, 2013, p. 237-236], [Verein Deutscher Ingenieure, 2006, p. Ob1-Oc36], [Pope, 1997, p. 33-42], [Shah, Mueller, and Sekulic, 2015a, p. 29-38], [Shah, Mueller, and Sekulic, 2015b, p. 48-52], [Shah, Mueller, and Sekulic, 2015c, p. 1-17], [Shah, Mueller, and Sekulic, 2015d, p. 1-9], [TEMA, 2019], [Edwards, 2008, p. 1-30], [Scholl, 2010, p. 2179-2187].
The number of input parameters required for the design of the heat exchangers is comparatively low. Beside the type of heat exchanger (condenser, reboiler), design parameter from the process simulation as the heat transfer area ($0.79m^2 \leq A \leq 363m^2$ assuming a maximum length $l_{max} = 5000mm$), operating temperature and pressure of the shell and tube side and volumetric flows as well as constructive parameters e.g. the length-to-diameter ratio ($150mm \leq d_{nominal} \leq 1200mm$ according to [DIN 28191, 2009]) have to be specified. Furthermore, the orientation of the close piping (horizontally or vertically) and the baffle spacing as optional parameter can be adapted. In figure 3.22 an automatically generated reboiler designed as floating head shell and tube heat exchanger is shown. The pipe to the right in front of the reboiler is the heating steam supply with the control valve and a bypass system for maintenance work. The rear, lower pipe is for the discharge of the heating steam condensate and contains a steam trap.
Figure A.20 of section A.3 depicts the schematic overview referring to [Pope, 1997, p. 34] of the floating head design. The implemented shell-side tube layout is triangular according to [DIN 28184-1, 2010], which is the most applied pipe setup and provides the tightest arrangement of holes at a constant pitch. Further arrangements e.g. orthogonal (used if cleaning service for outer pipes is required) or concentric (rarest applied setup, most compact build heat exchanger) pipe positions are not implemented yet, but can be extended in future works.

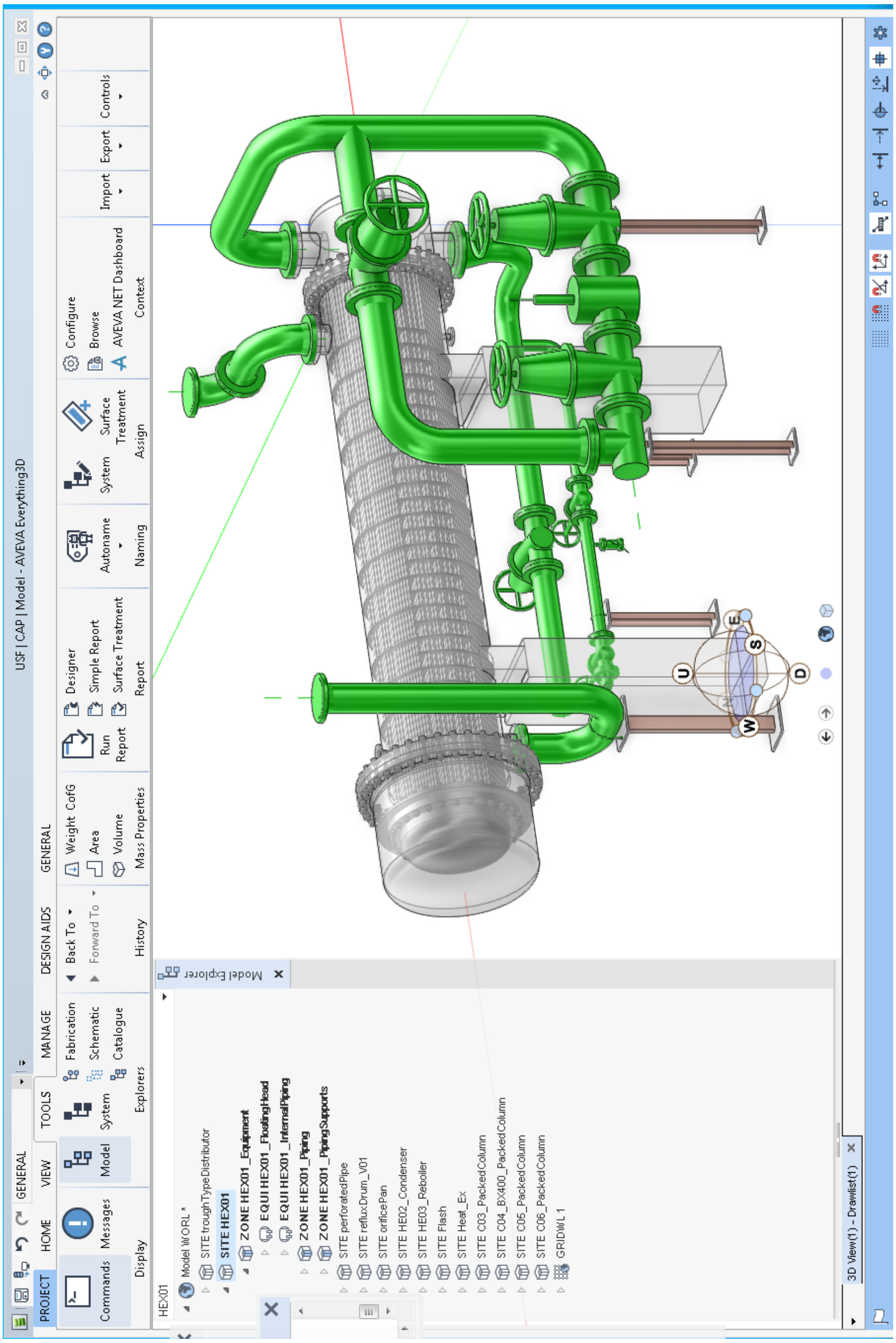


Figure 3.22: Reboiler, designed as floating head shell and tube heat exchanger, automatically created with MOSAICmodeling *PlantDesign*, visualized with AVEVA E3D™ 2.1

Pump assemblies

Redundant pump assemblies are used for the forced circulation of the distillate and the bottom product. The standby pump is identical in construction and is piped in the bypass with the main pump. In the event of a failure or during maintenance work, it can be taken directly into operation so that the entire process can continue. This configuration is often found in the process industry in areas where downtime due to maintenance-intensive technical units has to be avoided.

In this approach, centrifugal pumps (sub-class of dynamic axisymmetric work-absorbing turbomachines) are used due to their robustness (low maintenance effort in comparison to displacement pumps) and their suitability for large volume or large volume-to-pressure ratio applications. Horizontal centrifugal pumps are widely applied in process industries. [Pope, 1997, p. 94-96] Very detailed graphical representation pump models are mostly provided by the manufacturer, only the piping has to be applied within the detailed engineering. Based on the best-practice suggestions for a general piping design made by [Hady, 2013, p.73-79, p. 133-139, p. 173-200], different close piping arrangements for the suction and discharge pipes (H-H horizontal-horizontal, H-V horizontal-vertical, V-V vertical-vertical) are implemented within *PlantDesign*, as shown in figure 3.25 for the H-H and H-V arrangements. Hereby, the pumps are built as a kind of simplified placeholder, including steelwork, supports and base socket.

The size is automatically adapting to the input parameter referring to standardized sizing of centrifugal pumps for $PN10$ [DIN EN 733, 1995], $PN16$ [DIN EN 2858, 2011] and the dimensioning for the base sockets [DIN 24259, 1979].
The input parameters for the parametrization of the pump assemblies are the speed of rotation, classified in $n \leq 14501/min$ and $n \leq 29001/min$, the nominal capacity $6.3m^3/h \leq \dot{Q} \leq 315m^3/h$, nominal head $5m \leq H \leq 80m$ (depending on $\dot{Q}$) and the orientation for the close piping. The classification is done according to [DIN EN 733, 1995] and [DIN EN 2858, 2011]. An illustration of the pump sizing based on [DIN EN 2858, 2011] is given in figure A.21 in section A.3.

3.1.3 Database-based appliance of norm, heuristic and manufacturer data

As mentioned above, the processing of detailed constructive design for MPUs requires norm, heuristic and manufacturer data beside the process variables determined in process simulation. In practice, this information are typically not stored centrally, but are introduced by internal, company-specific engineering guidelines and in particular by the expertise of experienced engineers during planning. The systematic storage of these kind of information enables a much more efficient planning procedure and a long-term transparency for the plant life cycle. In this approach, the data storage is realized in a MySQL database [MySQL, 2019] which can be accessed automatically at run time of *PlantDesign*. The diverse information coming from different sources have a significant influence on the structure of the database.

In figure 3.23 the structure of the relational *PlantDesign* database is shown. The boxes represent the single tables or *relations* of the database including the *attributes* (table columns) and their formats. The dotted lines represent 1:1, 1:n or n:m relations between entities of different tables, which are called *foreign keys*. In case of 1:1 relation, for every data set or *tupel* of one table exactly one dataset in a second table exists. A 1:n relation is characterized by the fact that any number of $0 \ldots n$ data sets exist for a single data set in the other table. In case of n:m relation, each data set in table one is assigned $0 \ldots m$ data sets in table two and on the other hand, $0 \ldots n$ data sets are assigned to each data set from table two in table one. The tables represent one *entity type*, the rows represent *instances* of that type of entity and the columns are representing values attributed to that instance. Each row in a table has a unique key consisting of one or a combination of several attributes, which is called *primary key* and marked with a yellow key in front of the primary key attributes in figure 3.23, whereas the non-key attributes are marked with a trapezoid symbols. [Unterstein and Matthiessen, 2012, p. 19-20, Studer, 2016, p. 9-15]

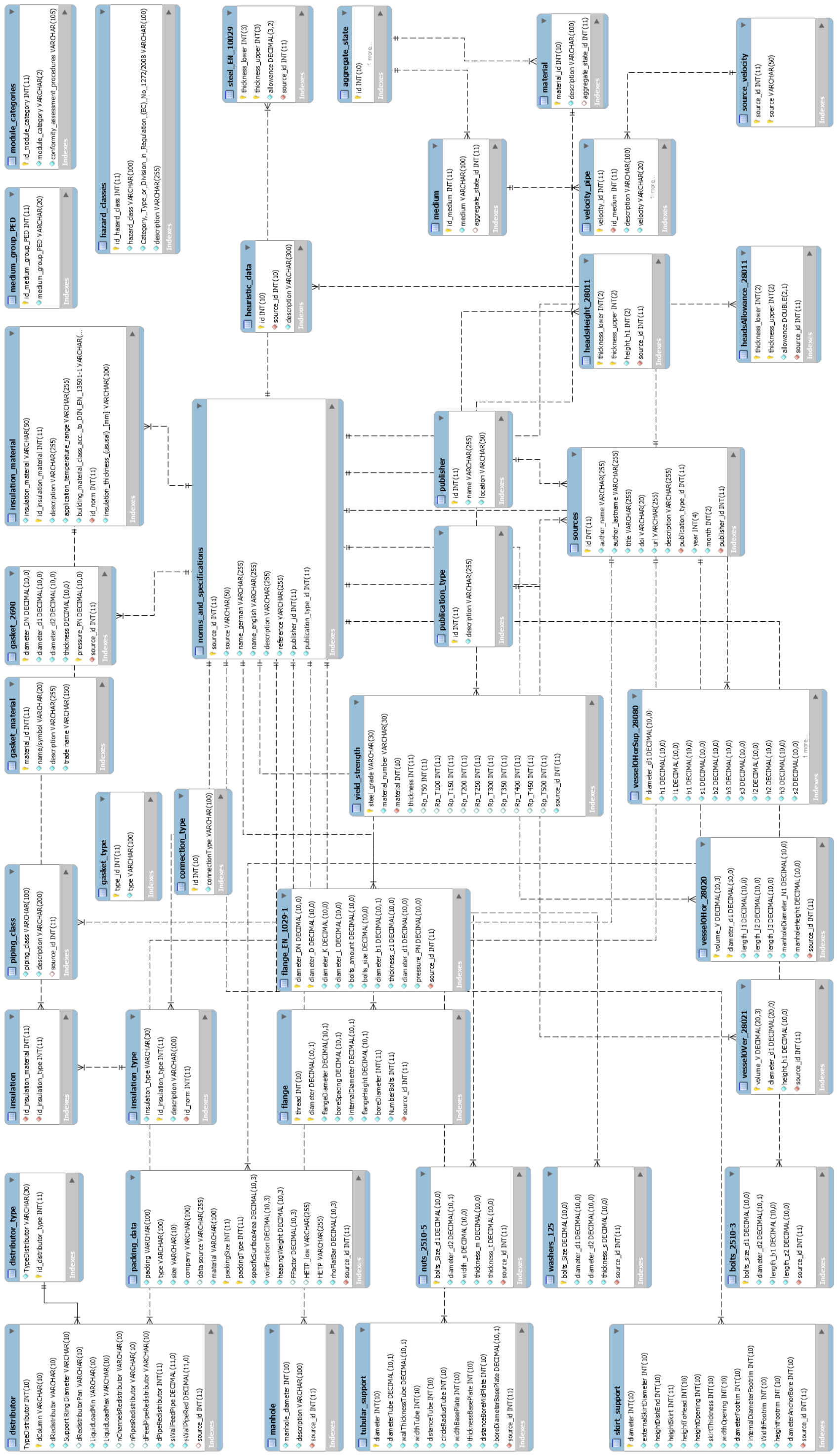


Figure 3.23: EER (enhanced entity-relationship) diagram representing the structure of the relational *PlantDesign* database [**A3 version in appendix**]

In order to reduce data redundancies and to improve the data integrity relational databases should be structured in so-called normal forms (first ($1NF$), second ($2NF$), third ($3NF$), Boyce-Codd ($BGNF$), fourth ($4NF$) and fifth ($5NF$)). Redundancies are duplicate information in a database or database table and therefore a sign of bad database design. A redundancy-free database is achieved if all duplicate information can be removed without any loss of information - this can be realized using normalization techniques. Normalization of a database schema can be achieved by splitting of attributes into several relations. The normalization avoids inconsistencies due to update, insertion or deletion anomalies [Codd, 1990, p. 317-321].
If all data elements of the real world are summarized and listed in one table, this table is in the zeroth normal form, i.e. unnormalized. Meeting the conditions of $1NF$ means that each attribute of a relation has to be atomar (the value range of the attribute cannot be splitted in further subranges) and the relation must be free of repeating groups (attributes containing the same or similar information must be moved to another relation), which facilitates or even enables queries of the database. The $2NF$ requirements are fulfilled if the $1NF$ is met and no non-primary attribute (attribute that is not part of primary key) functionally depends on a real subset of a key candidate (non-key attributes really depend completely on **all** keys). This reduces redundancies and the associated risk of inconsistencies because each relation models only one fact.
The third normal $3NF$ form is reached when the relation scheme is in the $2NF$ and no non-key attribute depends transitively on a key candidate. An attribute A_2 is transitively dependent on the key candidate P_1 if there is an attribute set A_1 so that $(P_1 \rightarrow A_1)$ and $(A_1 \rightarrow A_2)$. A non-key attribute must not be dependent on a set of non-key attributes, but only directly on a primary key (or a key candidate).

The more advanced standard forms are only mentioned for the sake of completeness, since these forms have not proved to be suitable for practical use. The Boyce Code Normal Form $BCNF$ is a further development of the $3NF$. In the third normal form it can happen that a part of a key candidate is functionally dependent on a part of another key candidate. The $BCNF$ prevents this functional dependency. A key candidate is an attribute or an attribute combination that uniquely identifies a data set, i.e. forms a primary key. The $BCNF$ only needs to be used if several key candidates exist and overlap each other partially. If there is only one candidate key in the relation or if there is no overlap between several candidate keys, the relation is automatically in the BCNF.
The fourth normal form follows the $BCNF$ and its normalized data modeling, but has the additional condition that dependencies on multi-value attribute sets are trivial and an attribute set is the key candidate of the relation must be fulfilled. This means that no redundancies can exist in functionally dependent attributes.

The fifth normal form $5NF$, like the $4NF$, deals with multi-value dependencies. The prerequisite of the $5NF$ is a relation in the $4NF$, in addition, all key candidates of the relation must also be keys of the subsets of the relation, which means that the separated attributes must be keys of the new relations. In the fifth normal form, it is no longer possible to divide the relation types further into relation types of a lesser degree, so that the original state can be restored at any time without loss of information. $5NF$, unlike the other normal forms, serves to discover new information, because new correlations emerge in the data. It is only used if one wants to express possible connections from three relations and does not represent concrete connections between three tables.

Too much normalization of the data has negative consequences, since it requires additional tables that generate administrative effort (e.g. storage space, authorization, referential integrity). In addition, it slows query speed because the tables must first be linked using joins. Therefore, especially in data analysis and reporting, normalization is removed to speed up results through redundancy. In the creation of relational data models, the $3NF$ has proven to be practical to ensure the perfect balance of redundancy, performance, and flexibility for a database. It also eliminates most anomalies in a database, but not all.
The *PlantDesign* database schema is set up in the third normal form.

Norm data mainly refers to geometric information of standardized process units, for instance, heat exchangers and vessels or plant components like flanges, platforms and ladders, nozzles, supports, heads and manholes. Furthermore, material information such as physical and mechanical properties, e.g. density or the temperature depended yield strength for different kind of steels are provided in norms (see figure 3.2).

Manufacturer data, for example performance characteristics, recommended application areas and constraints as well as constructive and material information about packed and tray types, collector and redistributor systems, are provided for the design of process units, too. Furthermore, heuristic data is applied to achieve appropriate engineering solutions for process units. Heuristics have an influence on the general design of the equipment, especially for dimensioning, e.g. standardized nozzle diameters or height to diameter ratios for apparatuses. The specification of arrangements of components are set following heuristic recommendations, for instance, reboiler arrangements, distances between components, liquid levels and nozzles, access area below platforms or height of and spacing to mist eliminators. An overview of important heuristic values is listed in A.7 in section A.2.2. To achieve more flexibility, experienced engineers can optionally replace the default values for these specifications with user-specific values.

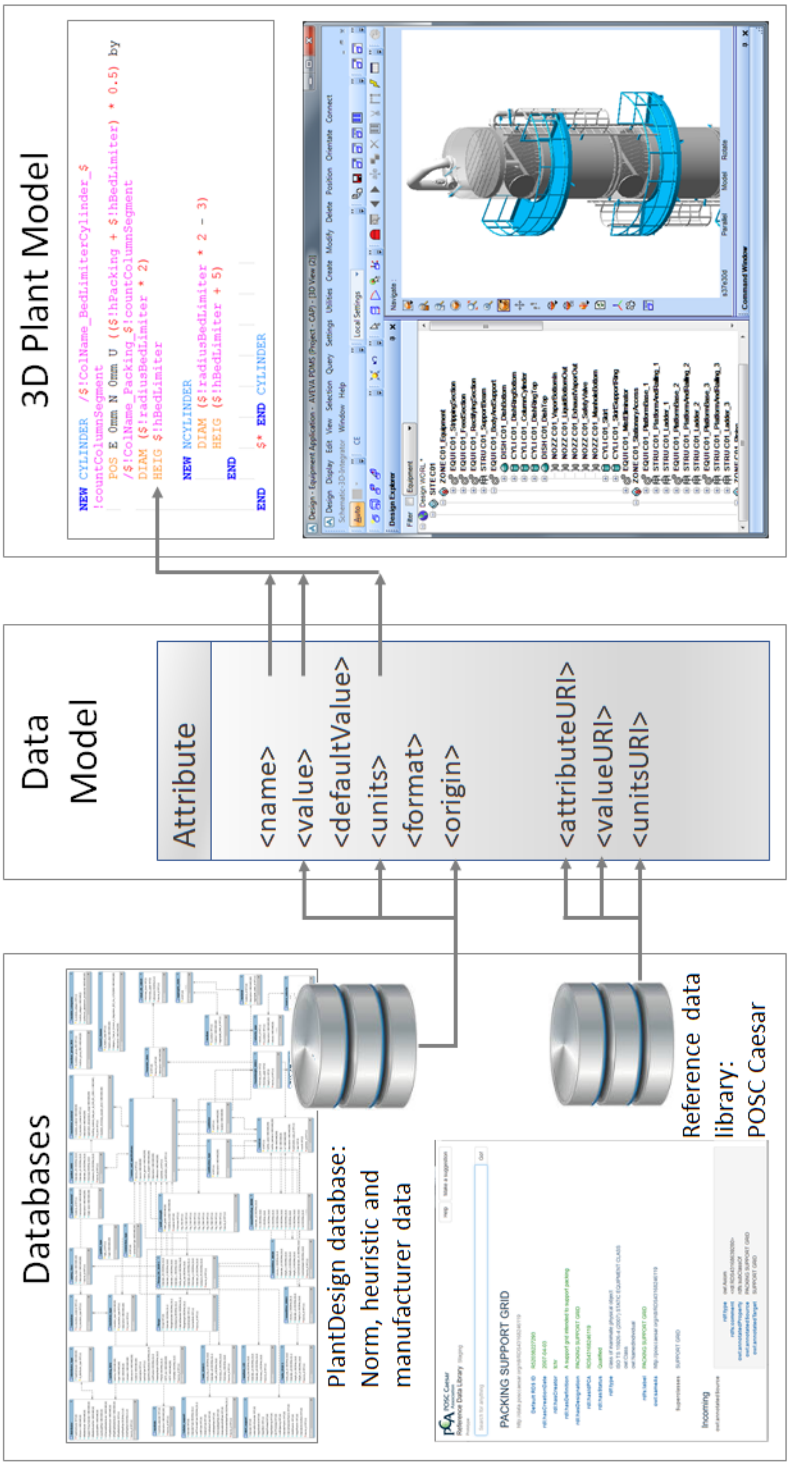


Figure 3.24: Usage of database-based norm, heuristic and manufacturer data for design specification

The required database queries are performed automatically during runtime. The queries depend on the user input and on the intermediate results of the constructive calculations, which are the transfer parameters to the queries. The results, e.g. component geometries from norm or manufacturer tables or mounting distances from heuristic tables, are directly used for the generation of the 3D model. 3D model information is stored in form of attributes with the help of a data model. Each attribute consists of *name*, *value*, *default value*, *unit*, *format* of value and the *origin* of the information. Furthermore, Uniform Resource Identifier (URI) for the specifications (*attributeURI*), value (*valueURI*) and unit (*unitsURI*) of each attribute are given with respect to publicly available Reference Data Libraries e.g. from the POSC Caesar Association), where standardized descriptions of the attributes are referenced.
Figure 3.24 illustrates the interrelations between the databases (*PlantDesign* database, POSC Caesar reference data library), the data model storing the information in form of attributes and the usage of this information for code generation of the 3D plant model. The information within the generated source code is partially transferred to the CAD environment (in this example AVEVA PDMS™, right bottom part of figure 3.24), where it can be accessed via the attributes of the 3D model elements in the explorer. Prerequisite for the transfer to the CAD environment is that the information can be internally processed and assigned to the eco system of the tool.

3.2 Prototypical implementation in MOSAICmodeling *PlantDesign*

A prototype of the automated creation of 3D models for MPUs applied in chemical plants is successfully implemented within the *PlantDesign* feature of the modeling environment MOSAICmodeling [Merchan et al., 2016]. MOSAICmodeling is a free, web-based modeling, simulation and optimization environment developed at the Process Dynamics and Operations Group at TU Berlin [MOSAICmodeling, 2019], [Kraus et al., 2014]. It enables the source code generation of simulation and optimization problems for a wide range of programming languages and simulation tools based on mathematical models written in LaTeX [Kuntsche, 2012]. The generated source code can be executed directly in the environment of choice, e.g. Matlab [Mathworks Matlab, 2019], Aspen Custom Modeler [Aspentech Aspen Plus, 2019], gPROMS [Process System Enterprise gPROMS, 2019] and others. The portfolio of functionalities contain various features, e.g. Model Transformation and Analysis, automatic reformulation of equation systems, the export of CAPE OPEN unit operations [Tolksdorf et al., 2016] and the newly developed *PlantDesign*.

PlantDesign is an engineering assistant system for the detailed constructive design of process units based on simulation/optimization results, user specifications along with norm, heuristic, and manufacturer data. The schematic workflow is shown in figure 3.26. The engineer has to set different kind of information as input data for the constructive design. Process data and conditions as well as characteristic values for the apparatus design typically are determined within process simulation/optimization. Further settings regarding the choice of supports, internals, materials, insulation and piping have to be specified too via a graphical user interface.
The input data are further processed and the dimensioning and positioning of all elements is performed within different calculation algorithms as previously described in section 3.1.2. For this procedure different constructive calculations are performed and required norm, heuristic and manufacturer data are queried in the background. The generated outcome of this procedure is source code for the automated creation of 3D models, which can be imported into specific CAD software. Exemplary 3D MPU models imported into AVEVA PDMS™ are shown in figure 3.25.
Besides spatial information for the graphical representation also process and constructive information are transferred into the 3D CAD tool. Exemplarily, material types of apparatus, pipework, insulation, operation conditions, piping class information, types of internals, and site-specific information of the plant are included as attributes in the model. After importing the MPU model into a 3D CAD environment, all this information is available for further usage within the tool.

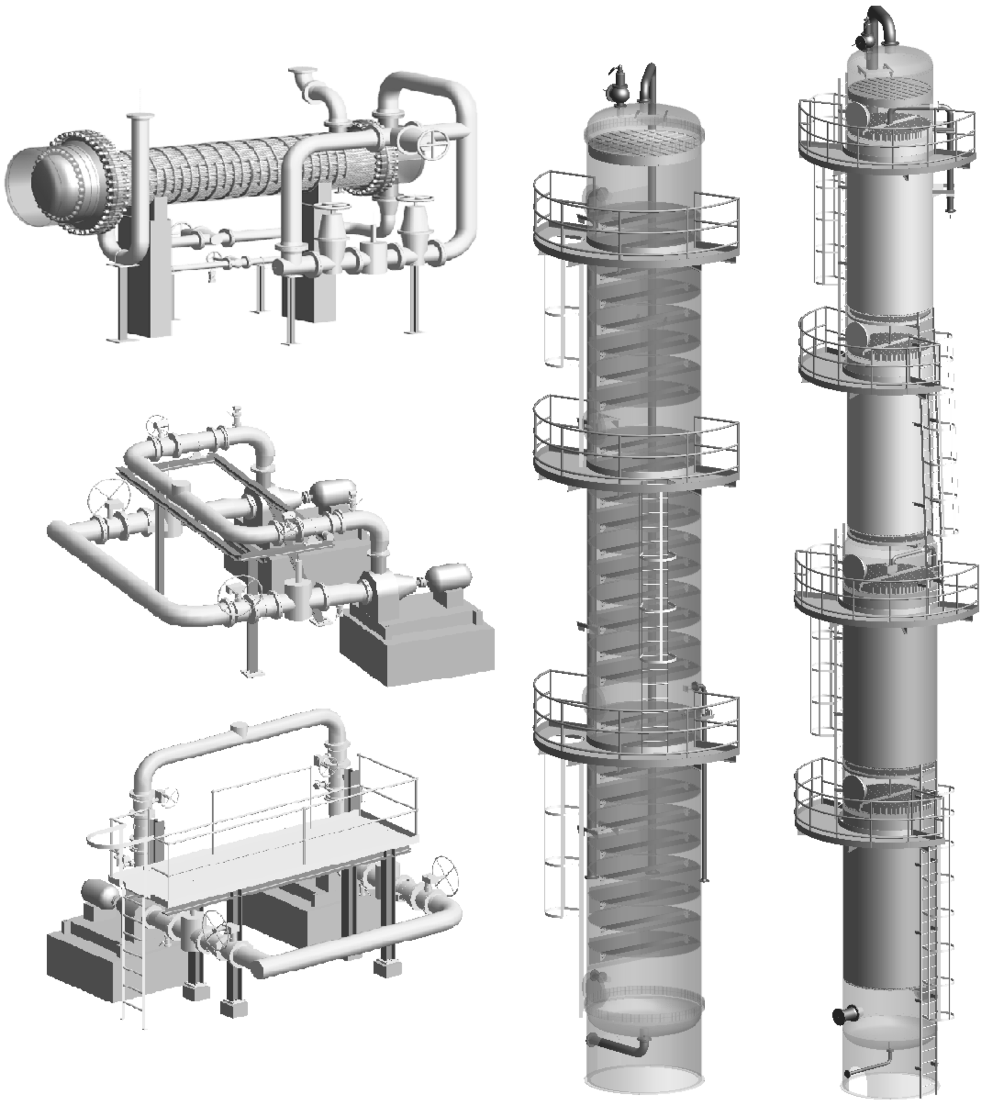


Figure 3.25: Examples of automatically generated 3D models of Modular Process Units (MPUs) for a shell and tube heat exchanger, pump assemblies, tray and packed columns in the *PlantDesign* feature of MOSAICmodeling, imported and visualized in AVEVA PDMS™ 12.1 SP4

Therefore, this approach allows the automated generation of intelligent 3D models already including relevant information from the previous planning procedure. In contrast, the classical plant design workflow is more time-consuming, error-prone, and needs a lot more manual work to specify planning data into 3D plant design.

The prototypical *PlantDesign* library includes rectification columns and associated apparatuses (pump assembly, condenser, reboiler, reflux drum). A compilation of the individual tabs of the graphical user interface of the *PlantDesign* tool is shown in figures A.22 to A.31 in section A.4 of the appendix.

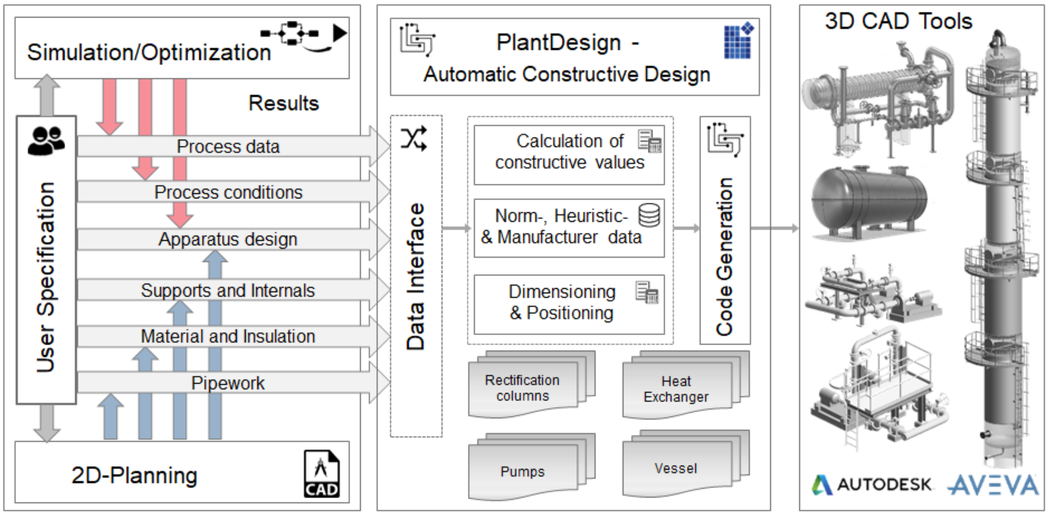


Figure 3.26: Schematic overview of the *PlantDesign* feature in MOSAICmodeling - input and processing of data; outcome is a source code of a 3D model which can be imported into different 3D CAD tools

3.2.1 Linkage of *PlantDesign* to other CAE environments

Nowadays, the variety of different specialized software environments applied in chemical engineering necessitates a seamless data handover to avoid undesired manual data transfer. Unfortunately, the absence of standardized data interfaces respectively the limited acceptance and support of existing standards from software vendors requires proprietary data interfaces to connect different software tools in many cases.
The basic data set for the design of equipment is obtained through process simulation and optimization during the basic engineering. The dimensioning of apparatuses typically bases on steady state simulation results for the desired operating point of the process unit within the whole process. Additionally, optimization results with respect to thermodynamic and economic considerations can be applied to the constructive design.

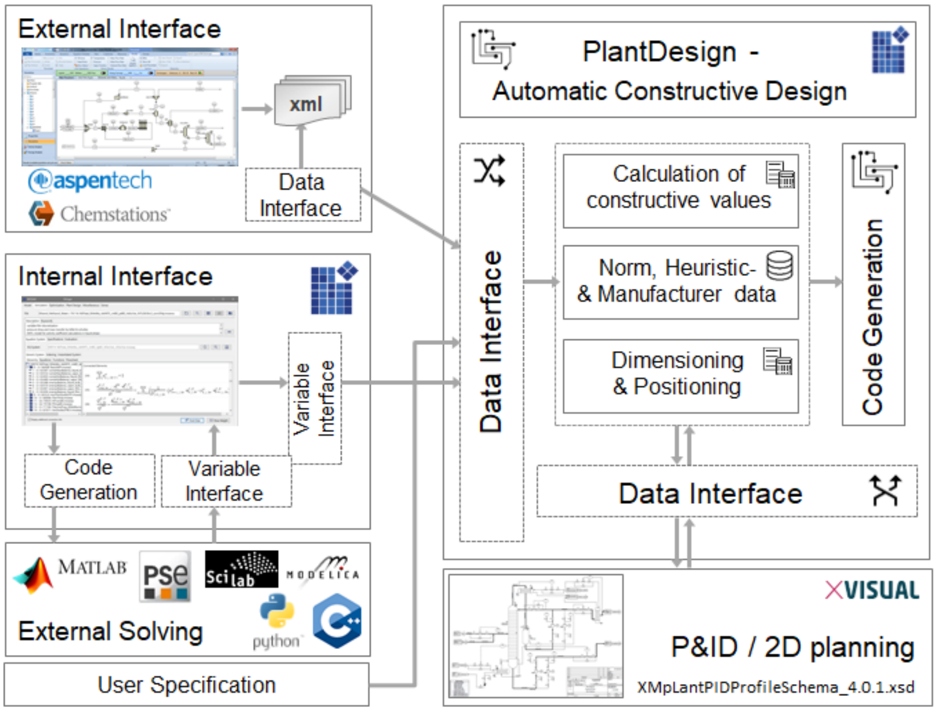


Figure 3.27: Realized connections of MOSAICmodeling *PlantDesign* to other CAE tools

Provision of the required input values for the constructive equipment design can be realized in different ways. One possibility is a manual data handover via a graphical or command user interface, which has no requirements to data interfaces. However, this procedure is time consuming and error prone. A second option is the usage of an internal variable interface to the MOSAICmodeling simulation functionality [Fillinger, Tolksdorf, et al., 2017] to import simulation results into *PlantDesign*, as illustrated in the middle left box in figure 3.27. After modeling of a process in MOSAICmodeling the user can generate executable source code for different simulation environments. Generating source code for libraries like BzzMath [Guido Buzzi-Ferraris, 2012, p. 1312-1316, Buzzi-Ferraris, 2011, p. 1215-1225] or the Gnu Scientific Library [Gnu Scientific Library, 2019] can be internally executed on the MOSAICmodeling server. This enables the direct linkage of the simulation results to the *PlantDesign* feature using a variable interface. For this a variable mapping between the result list from simulation and the internal variables applied in *PlantDesign* is required as shown in figure 3.28. On the left-hand side, the tab for the setup of process data is shown.

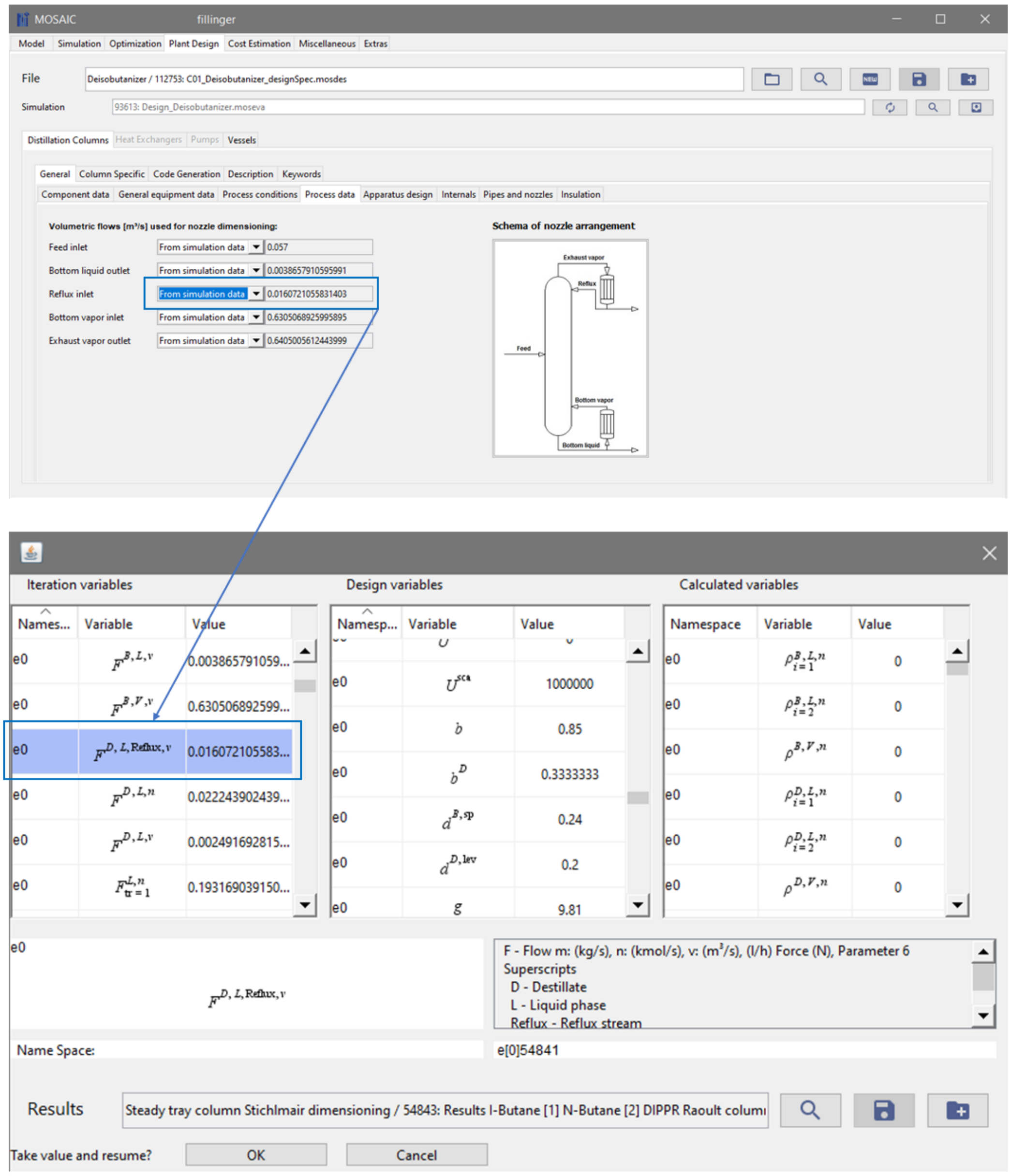


Figure 3.28: Internal variable interface between MOSAICmodeling simulation functionality and *PlantDesign*

When choosing the option «*From simulation data*» as data source (after loading a MOSAICmodeling evaluation), the result table as shown in the right-hand side opens and the mapping between the simulation result variable and the internal *PlantDesign* variable can be set. In this case the mapping has to be done manually since the setup of process models in MOSAICmodeling is equation-oriented, using a flexible, user-specific variable naming.

Beside the internal simulation options, also an external execution of source code generated by MOSAICmodeling can be performed. After problem solving, the simulation results can be imported from tools like PSE gPROMS Model-Builder or MathWorks MATLAB, to MOSAICmodeling and via the same variable interface to *PlantDesign*, as illustrated in in the bottom left box of figure 3.27.

Furthermore, prototypical external data interfaces are developed for several process unit models within ASPEN Plus [Aspentech Aspen Plus, 2019] and Chemcad [Chemstations, 2019] simulation tools as representatives of commercial flow sheeting environments, as illustrated in the upper left box of figure 3.27. Both tools provide an *XML* export for simulation data, in case of Chemcad and depending on the process unit models, there are further exports for physical properties and for tray and packed sizing data for the sizing of columns.
In table 3.3 there is an overview of import variables for different models for distillation columns. Shortcut and rigorous models for the process units vary in the level of detail in the mathematical descriptions and offer different result sets for the import. The variable naming of each model is fixed in the commercial flow sheeting environment, so that the mapping to the *PlantDesign* variables is automatically done during the import.

This advantage is in contrast to the disadvantage that the process variables within the models in the libraries are limited and an extension by further variables (as with equation-oriented approaches) is usually not possible.

Table 3.3: Overview of import variables for different distillation column models from Chemcad and Aspen Plus

	Chemcad		Aspen Plus
Variables/Models	**SCDS**	**ShortCut**	**RadFrac**
Components	I.	I.	I.
FeedAggregateState	I.	I.	I.
FeedRate	I.	I.	I.
RefluxRate	I.	I.	I.
BottomVaporRate	II.		I.
ExhaustVaporRate	II.		I.
BottomLiquidRate	II.		I.
NumberOfStages	I.	I.	I.
FeedStage	I.	I.	I.
MaxPressure	I.	I.	I.
MinPressure	I.	I.	I.
MaxTemperature	I.	I.	I.
MinTemperature	I.	I.	I.
F-Factor	IV.		
ColDiameterRecSec	III.		
ColDiameterStripSec	III.		

I. Simulation (*XML*)
II. Tray Properties (Excel-*XML*)
III. Tray/Packed Sizing (Excel-*XML*)
VI. Calculated Variable

As shown in table 3.3 the proprietary export files are storing different information. Due to this, the import interface has to take into account the specific, internal attribution of each program to manage the mapping to *PlantDesign*. The *XML* export files from AspenPlus as well as from Chemcad are for example storing only the component names (in a string/character format), but no CAS numbers. The nomenclature of chemical substances can vary a lot between different environments. This can lead to problems with the automatic mapping with the components of the physical property database of MOSAICmodeling. Unfortunately, the tools are not supporting neither a unique nor a standardized naming policy and a string comparison is difficult in between different eco systems. This simple example is very representative for the effort of providing and maintaining proprietary data interfaces to different tools and shows the enormous potential for improvement that standardized definition of the interfaces could offer.

All presented options for importing simulation data requires further user specifications, as already shown in figure 3.26.
Beside import of simulation data, a prototypical import/export interface to P&IDs has been developed and successfully implemented. A closer description is given in section 4.3.1. For the generation of 3D models for different CAD environments, a prototypical source code converter framework has been developed, which is described more in detail in the following section.

The *PlantDesign* feature is part of the functionalities provided in the MOSAICmodeling tool suite. The structure of the MOSAICmodeling programming code is modular and features like *PlantDesign* can easily be added to the core of the implementation. In future work it would be also possible to connect or integrate the functionality of *PlantDesign* into other CAE tools. It can for example be integrated as a program library (e.g. dynamic link library (DLL)), which can be linked during the compilation or by runtime of the other software. The required data input for processing the design of MPUs can be managed by providing a suitable data interface. For this purpose, the knowledge of the input set of information (mandatory and optional) for each process unit of the *PlantDesign* library including the format and engineering unit specification is necessary. The input data can be applied via a user interface (command or graphical) or with the help of a data transfer file.

3.3 Generative programming for generation of 3D plant models

3.3.1 Concepts for generic creation of 3D plant models

The 3D equipment models are created based on the constructive solid geometry method (CSG), which constructs 3D objects from simple parametrizable primitives like cylinders, cuboids or spheres transformed and combined by Boolean operations (union, intersection, and difference) [Foley, Dam, and Feiner, 2013, p. 450]. The geometry of 3D objects based on CSG is exact/valid and guarantees a closed topology of the surface and the data files are concise [Kamrani and Nasr, 2010, p. 217] The high quality of the geometry ensures that the requirements for further planning procedures are met without further pre-processing of the model. For example, the basic models for static analysis using finite element methods or the analysis of flow conditions using CFD methods can be established. The definition of primitives is realized by characteristic variables, which are represented by parameters, equations or constraints. The creation of each primitive is made depending on a set of arguments to describe the volumetric body (by variables like diameter, height, length, angle) as well as the position of an origin vector in space. The set of primitives and the corresponding transfer parameter lists used in this work is shown in figures 3.29 and 3.30.

3.3.2 Command-oriented creation of 3D plant models

The graphical representation of the plant models is formulated in a command-oriented programming language that can be imported into and interpreted by the CAD environment. In addition to the spatial information, process and meta information, e.g. process conditions, hierarchical location-based information of the site, material specification, and piping class information are also transferred to the CAD environment. Prerequisite and restriction for the exchangeability of data sets is the availability of similar planning functionalities within the tools. This ensures that an internal interpretation and processing of the data is possible. Exemplary, some CAD environments applied in the mechanical engineering are not supporting the creation of pipework and related functionalities like piping consistency checks.

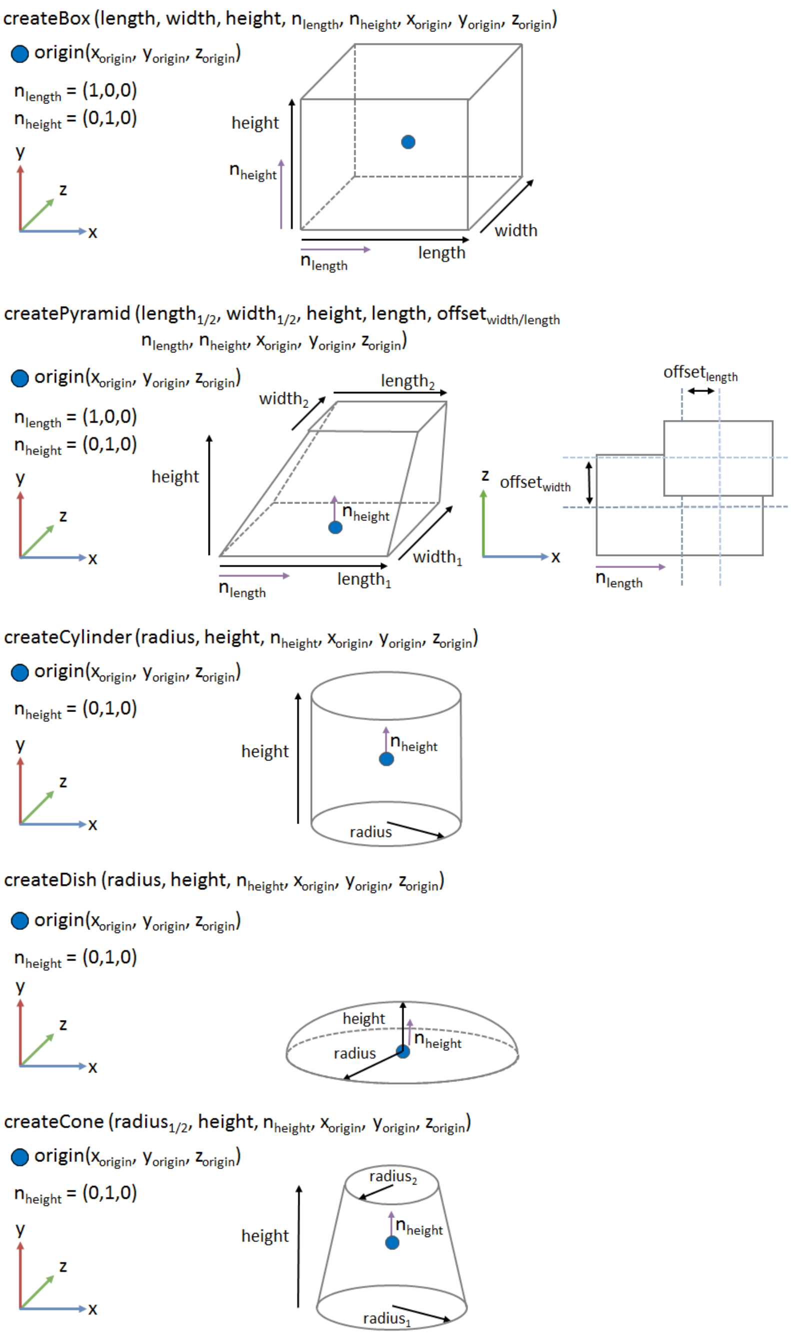


Figure 3.29: Parametrizable geometric primitives and the corresponding transfer parameter lists as basis for the creation of 3D plant models in *PlantDesign* - part 1

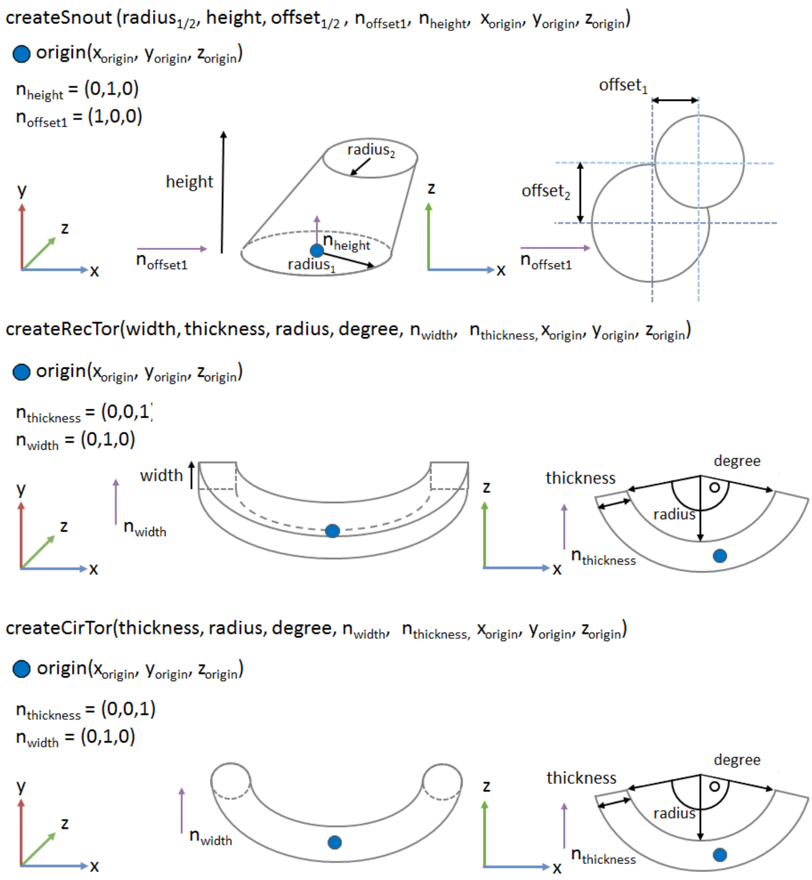


Figure 3.30: Parametrizable geometric primitives and the corresponding transfer parameter lists as basis for the creation of 3D plant models in *PlantDesign* - part 2

As introduced in section 2.3.2, there are different methods to create volumetric primitives, as illustrated in figure 3.31. One creation method is the usage of parametrizable primitives, as used for example in AVEVA 3D CAD tools (E3D™, PDMS™). In case of creating a cylinder, the parameter which have to be defined are height and diameter as well as the spatial information of the origin vector to set the position in space. A second method of creating volumetric primitives is the extrusion of 2D planes, as used for example in Autodesk 3D CAD tools (Autodesk® Fusion 360). Here, the basis is a circle around a centerpoint on a plane (bottom left picture of figure 3.31), which is extruded afterwards to create the volumetric body (bottom right picture of figure 3.31).

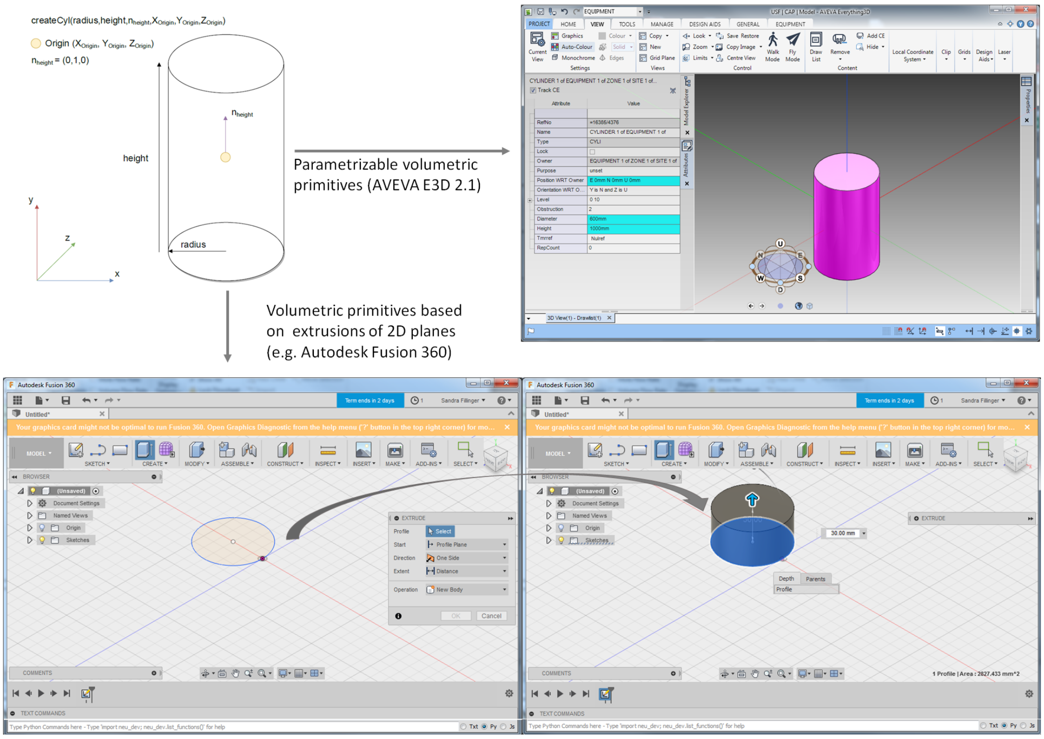


Figure 3.31: Methods for creation of volumetric primitives, exemplary for cylinders in form of parametrizable volumetric primitives (e.g. in AVEVA E3D™ 2.1, top right) and volumetric primitives based on extrusion of 2D plane (e.g. Autodesk® Fusion 360, bottom left and right)

The primitives for both methods can be created via the graphical user interface of the CAD environments or in a command-oriented manner, as shown in figure 3.32. The graphical representation for both methods has to be identical, not only with respect to dimensions like height and diameter but especially in terms of positioning in space. This can be realized by using the same basis vectors for the primitives. In doing so, the transfer parameters for both methods are identical. This is the prerequisite for the development of the source code converter framework, which is introduced in the following section.

```
NEW CYLINDER  /$!ColName_BedLimiterCylinder_$
!countColumnSegment
    POS E 0mm N 0mm U (($!hPacking + $!hBedLimiter) * 0.5) by
    /$!ColName_Packing_$!countColumnSegment
    DIAM ($!radiusBedLimiter * 2)
    HEIG $!hBedLimiter

    NEW NCYLINDER
        DIAM ($!radiusBedLimiter * 2 - 3)
        HEIG ($!hBedLimiter + 5)
    END

END      $* END CYLINDER
```

[AVEVA PML Code]

```
product = app.activeProduct
rootComp = product.rootComponent

# Creation of construction Point and Vector for Plane
Point= adsk.core.Point3D.create(0,5,0)
normal = adsk.core.Vector3D.create(0,1,0)
plane = adsk.core.Plane.create(Point,normal)
cons_planes = rootComp.constructionPlanes

# Determine as construction plane
cons_planeInput = cons_planes.createInput()
cons_planeInput.setByPlane(plane)
cons_plane = cons_planes.add(cons_planeInput)

 # Create sketch in plane
sketches = rootComp.sketches;
sketch = sketches.add(cons_plane)

# Create sketch circle
sketchCircles = sketch.sketchCurves.sketchCircles
centerPoint = adsk.core.Point3D.create(0, 0, 0)
sketchCircles.addByCenterRadius(centerPoint, 5.0)

# Get the profile
prof = sketch.profiles.item(0)

# Create an extrusion input
extrudes = rootComp.features.extrudeFeatures
extInput = extrudes.createInput(prof, adsk.fusion.FeatureOperations.
NewBodyFeatureOperation)

# Define that the extent is a negative distance extent
distance = adsk.fusion.DistanceExtentDefinition.create(adsk.core.
ValueInput.createByString("100 mm"))
extInput.setOneSideExtent(distance, adsk.fusion.ExtentDirections.
NegativeExtentDirection)

# Create the extrusion
ext = extrudes.add(extInput)

# Get the body created by the extrusion
body = ext.bodies.item(0)
```

[Autodesk® Python Code]

Figure 3.32: Command-oriented creation of volumetric primitives, exemplary for cylinder - top: *PML* (AVEVA E3D™ 2.1) and bottom: python (Autodesk® Fusion 360)

3.3.3 Source code converter framework

The initial development of adaptable MPU models was performed in programmable macro language (*PML*). *PML* is a domain specific programming language, which can be interpreted in AVEVA PDMS™/E3D™. It contains commands to create the graphical representation as well as the transfer and setting of plant information within the CAD environment. Furthermore, the code includes different programming constructs (e.g. nested conditional branches) to build up the different design options that *PlantDesign* offer. The usage of a 3D CAD environment for the development is mandatory to be able to test and debug the MPU models by checking the calculation results, the correct graphical representation of the constructive design and the transfer of the planning and process data of the plant into the CAD tool. Parts of work introduced in this section has been implemented within the project work [Skarabis, 2017].

To enable the source code generation of the 3D models of MPUs in different domain-specific programming languages, a new source code converter framework has been developed. The source code converter enables the automatic generation of a code generator written in a higher programming language, in that case *JAVA*, based on a domain-specific source code for the MPU model, in that case written in *PML*. A schematic overview of the source code converter framework is shown in Figure 3.33.

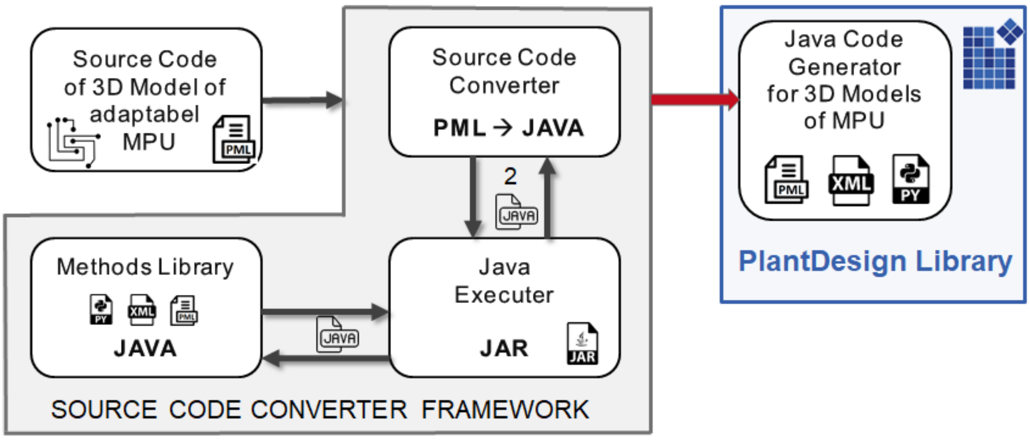


Figure 3.33: Schematic procedure of generation of a source code generator using the newly developed Source Code Converter Framework

Input for the converter is the *PML* code of an adaptable MPU model including the complete set of constructive options, as illustrated in the left top box of figure 3.33. For example, there are two constructive options available for the column support - pillar or skirt support. Both options are included in the *PML* code, but only one of them is executed within a conditional branch depending on the user selection. All further constructive options for the MPU are included within nested conditional branches, loops etc., too. This leads to a very extensive code of single MPUs, which is strongly branched and not so easily comprehensible and extensible.
During the source code conversion, general programming constructs for calculations and the setup for specific constructive options are directly converted into executable *JAVA* code. Within these constructs, function calls including the corresponding arguments for the creation of code representatives in the specific target language are inserted. This is illustrated in the middle top box «*Source Code Converter*» of the gray highlighted «SOURCE CODE CONVERTER FRAMEWORK» of figure 3.33. The aim is to translate the program logic of the *PML* source code into a higher programming language (*JAVA*) which can then generate *PML* source code again, as illustrated in the top right box of 3.33. Important is, that the preprocessing should take place within the higher programming language and the generated source code should only receive the constructive options which the user has selected. For this reason, the generated *PML* code is much leaner and tailored for the specific purpose afterwards.

In a first step, the source code is analyzed line wise by searching for specific key syntaxes of *PML*. All nested programming constructs like loops and conditional branches as well as the functions for the creation of plant hierarchy and information elements and the parametrizable primitives shown in figures 3.29 and 3.30 are detected during this procedure. *PML* is not very restrictive during execution, which means that certain programming structures can be implemented in different ways, but produce the same results after compilation.
PML is for example not case sensitive and programming structures do not necessarily have to be closed. In order to simplify and conserve resources in the development of code-analyzing and converting programs, the syntax in *PML* is restricted to such an extent that not all possible cases of syntax have to be intercepted. Comments can be introduced in the PML code in two ways, either by setting two hyphens («–») or by combining dollar signs and *p* («$*p*»). These comments always occupy whole lines and are not attached to a functional program line, therefore, the partial commenting of lines with «$*p$» should not be used. All keywords should be capitalized in their entirety and to interpret the hierarchy level of the commands in the right way, it is required to close all commands in a correct way, e.g. by using the «*END*» command.

To guarantee the exact interpretation of the code a pre-analysis is made, and incorrect or unknown commands are reported line wise. If new or missing commands are detected, they have to be added to the source converter to be able to interpret them afterwards automatically.

The creation of language-specific code fragments for primitives or the setup of plant-specific hierarchy elements is stored within a method library, as illustrated in the left bottom box of figure 3.33. The method library includes domain-specific command-oriented methods to set geometric information of volumetric primitives, plant and process information as well as general CAD-specific commands, as illustrated in figure 3.34. This structure allows an easy extension of new target languages for different 3D CAD environments like Intergraph, Siemens, Bentley or others. It is required to store a code representative for each function and programming construct and their arguments that can occur in the *PML* code.

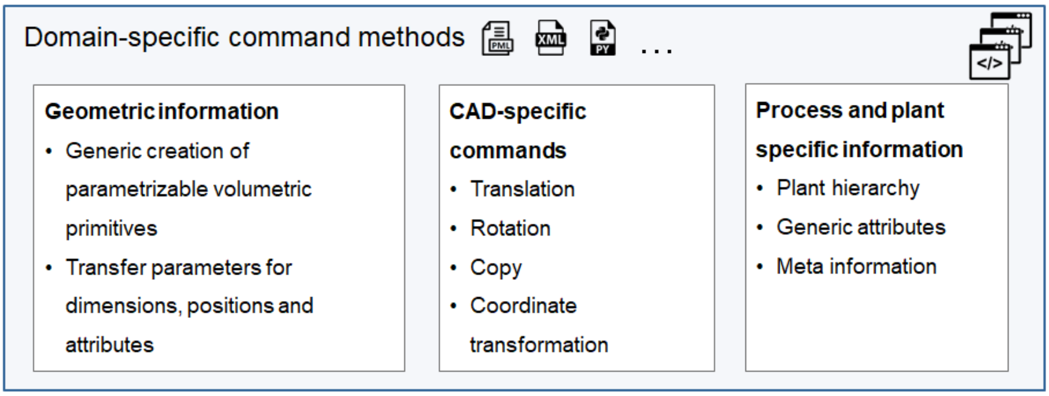


Figure 3.34: Schematic overview of content of the methods library in the SOURCE CODE CONVERTER FRAMEWORK

After execution of the source code converter with a special *PML* input for an MPU, a code generator for an MPU is available in the PlantDesign library and the code generation for all programming languages in the methods library is possible. The code generation is done depending on the user specifications, database queries and internal calculations and the user get, in contrast to the *PML* input file for the converter framework, a code including only the chosen constructive options – this makes the generated code much leaner and more efficient.

For development purposes, the required standard or heuristic information for the flexible constructive design of MPUs have been included in the original *PML* code in form of library files, which are called during the execution of the *PML* code within the CAD environment.
For each call, the return value is set for a constructive variable used in the MPU code. During the code conversion procedure, these library files are replaced by database queries to the *PlantDesign* database (introduced in section 3.1.3, figure 3.23, which are executed directly executed from the *JAVA* code to get the standard and heuristic data and written in the variables within *JAVA*. This procedure is done manually and is not processed within the source code converter framework.

In figure 3.35 the MPU of a horizontal vessel is shown exemplary as a result of the Source code converter framework. The development of the vessel design was performed in AVEVA PDMS™, the logic was transferred using the source code converter including a method library for python, which can be interpreted in Autodesk® Fusion 360.

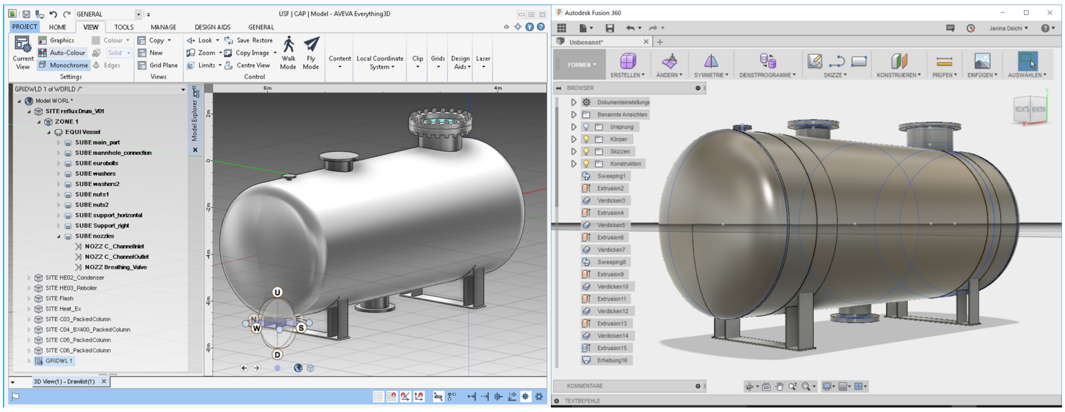


Figure 3.35: Generated MPU of horizontal vessel in AVEVA E3D™ (left) and Autodesk Fusion® 360 (right) created using the Source code converter framework

In principle, an analogous development of the source code converter is also possible for other input languages. For this purpose, it is necessary to define all possible programming control structures (e.g. loops, if-else-statements) in the desired source language and to create a link to the corresponding programming control structures in the target language.
Especially desirable is the creation of methods referring to standardized formats, e.g. the Onthology Web Standard (OWL, W3C, 2019b, applied in Kim et al., 2016), which is listed in figure 3.34.

The *PlantDesign* approach allows the direct creation of 3D models in a command-oriented way for different CAD environments. The use of an exchange format for the transfer into another CAD environment is not necessary, so that no loss of information is associated with the generation of the graphical representation. A much more important advantage using the presented approach is that a further processing of the 3D model is possible after importing the plant model into the CAD environment. By this, the disadvantage resulting from the use of non-intelligent 3D data exchange formats such as STEP can be completely avoided.

3.4 *PlantDesign* workflow - application of automated generation of 3D plant models

3.4.1 Integration of *PlantDesign* into classical engineering workflow

The classical engineering workflow of plant design in process industries, as illustrated in figure 2.1, starts with feasibility studies, followed by conceptual design, basic and detailed engineering. These planning phases are followed by procurement, mechanical completion and commissioning, which are not directly considered in this work. The typical planning documents and files, e.g. simulation studies, PFDs, P&IDs, piping isometries and 3D plant models are created using specialized software.
To improve the data handover between these tools during the planning, data exchange interfaces of *PlantDesign* enable the integration of different planning information. On the one hand, the calculation basis of connected process units achieved by simulation can be imported from different environments, e.g. MOSAICmodeling, Aspen Plus or Chemcad. On the other hand, planning data can be imported and exported via an interface to the P&ID tool PlantEngineer, using the standardized data exchange format [POSC Caesar Association, 2017] developed by the DEXPI initiative. The planning data has to be complemented by additional user inputs, e.g. the piping class, sealing surface or design options. The set of input information is processed within *PlantDesign* and the 3D construction of the MPU is provided in the form of code for the creation of the 3D plant model within a CAD environment.

PlantDesign can be integrated easily into the classical workflow of plant design in process industries. The design of process unit modules (MPUs) can be combined with the design of units, that are created manually during the classical planning procedure. The manual design is very complex and the time savings using *PlantDesign* are enormous - despite the much more detailed design that is achieved.

A schematic overview *PlantDesign* workflow is illustrated in figure 3.36. The upper part shows the workflow with *PlantDesign* and the lower part the classical workflow in plant planning. A distillation column, highlighted by a blue box, is illustrated as example for the integration. Process simulation data (bottom left box) as well as planning data from PDF or P&ID diagrams (2nd and 3rd bottom box) can be transferred via data interfaces automatically into the *PlantDesign* tool (top left boxes). After processing of the column design, the code export can be used for the creation of the graphical representation in a 3D CAD environment (3rd top box) and the MPU can be integrated into the overall model in the classical workflow (4th bottom box), which is the starting point for the pipework.

The spatial planning is basis for the generation of isometries (top right box) and finally for the installation of the plant (bottom right box). The comparison clearly documents the support functions provided by the new approach and highlights how the design of individual MPUs can be integrated into the overall design of a plant using the data interfaces to other planning tools, which are described more in detail in chapter 4.
In the following sections, two case studies for the application of *PlantDesign* are introduced. First, the utilization of MOSAICmodeling *PlantDesign* within an academic course for teaching computeraided plant design is presented. Hereby, the focus is on the evaluation of the classical workflow in comparison to the *PlantDesign* workflow for the constructive design of process units. The view of unexperienced engineers is shown.
The second case study shows the application of the *PlantDesign* workflow for designing an plant in cooperation with an industrial company. Here, the focus lies on the evaluation of the applicability of the *PlantDesign* workflow from an expert point of view.

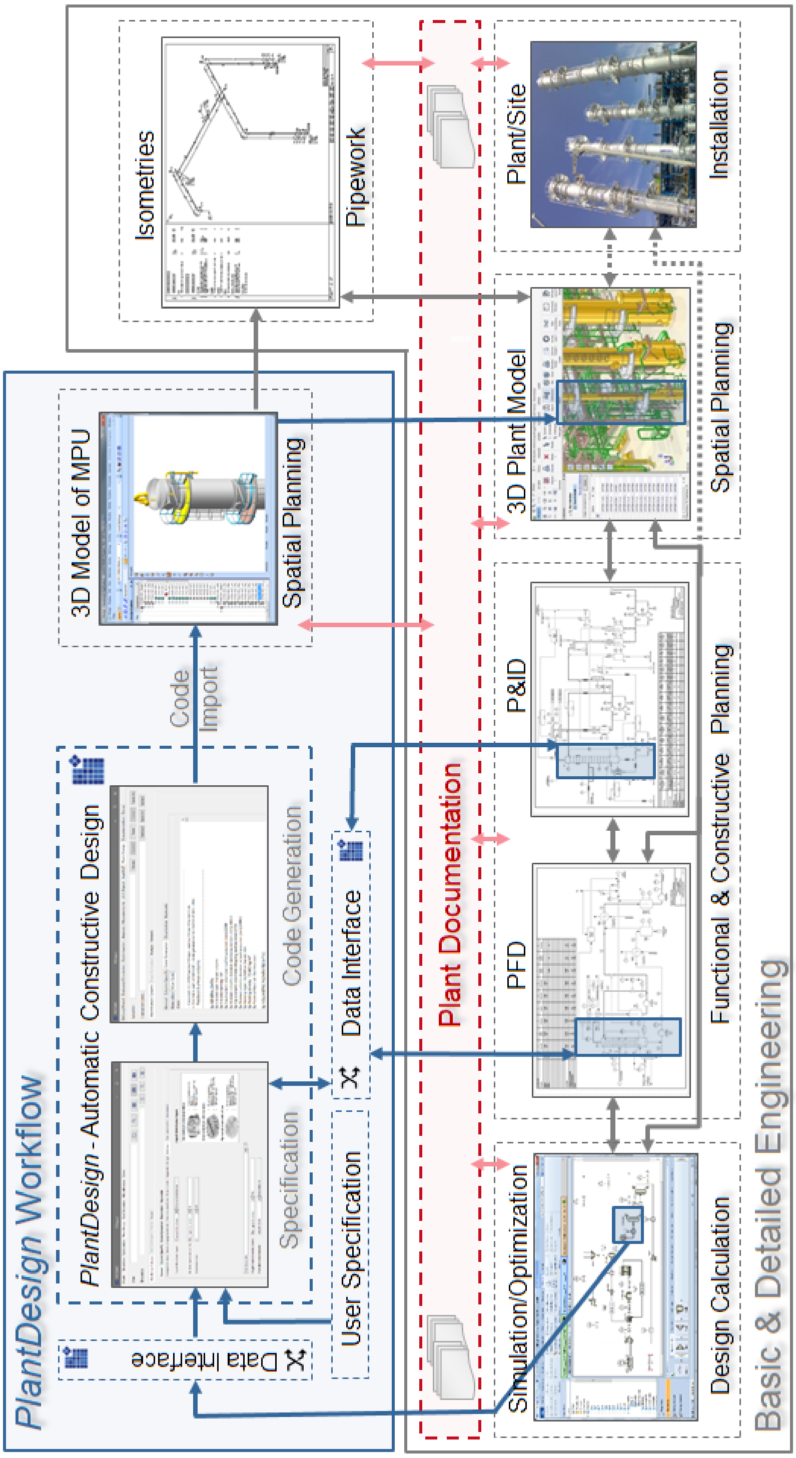


Figure 3.36: Integration of *PlantDesign* into the basic and detailed engineering of (petro-)chemical plants exemplary for distillation columns

3.4.2 Teaching application of *PlantDesign*

The *PlantDesign* feature has been successfully applied in a lecture called Computer-aided Plant Design at Technical University Berlin since summer semester 2016. The objective of the course is to carry out the sub-steps of the plant planning. The goal is to design an isobutane process applying specialized CAE software. The tasks are carried out in groups of two to a maximum of three students. The planning process includes the following aspects:

- Simulation of the whole process in a commercial flowsheet simulator
- Thermodynamic and economic optimization of the process with a focus on one distillation column and the associated apparatusses
- Preparation of a piping and instrumentation flow diagram (P&ID) including control structures for the distillation column and the associated apparatuses
- Constructive equipment design for the distillation column, the heat exchangers and the reflux drum
- Cost estimation of CAPEX and OPEX for the distillation column and associated apparatuses using a commercial flowsheet simulator
- Preparation of 2D site planning documents (equipment plot plan, equipment elevation plan) using a commercial 2D piping and instrumentation diagram tool
- Manual equipment design and 3D drawing (classical plant design workflow) of the distillation column (deisobutanizer, configured as tray column) and associated apparatuses using a commercial 3D CAD environment
- Automatic equipment design of distillation column using the MOSAICmodeling *PlantDesign* workflow (stabilizer, designed as packed column) to compare the approaches
- Pipeline planning for the entire planning process (with specification of the equipment models for the reactor, the pump groups, the equipment rack and the pipe rack) using a commercial 3D CAD environment

In figure 3.37 the result of the final 3D planning after finishing all tasks is shown.

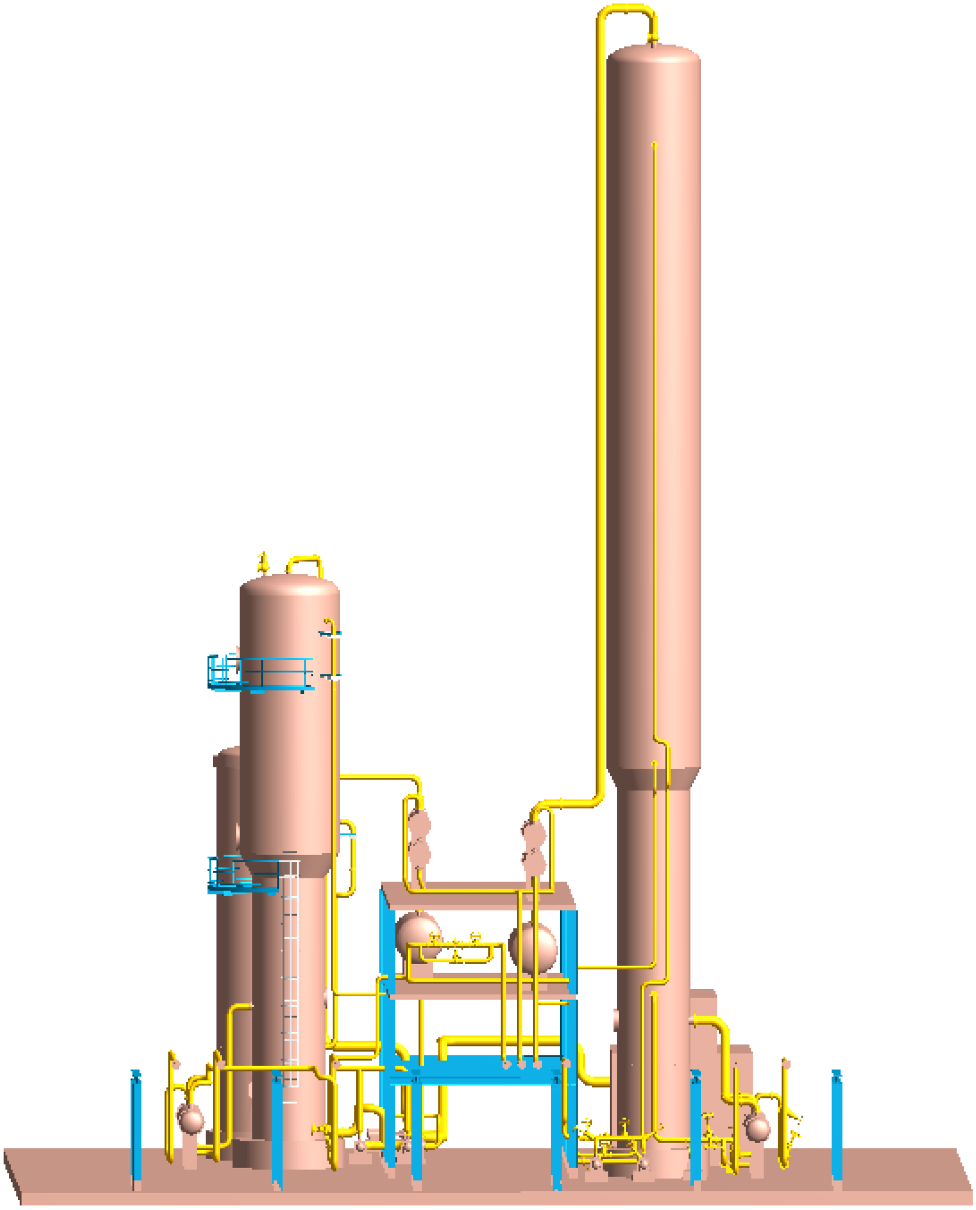


Figure 3.37: Exemplary resulting 3D planning of the isobutane process planned within the CAP course

On the right-hand side of the picture the deisobutanizer column for the separation of iso- and n-butane is placed. This column is designed manually by the students as a tray column. On the left-hand side, the stabilizer column for removal of light components, which are formed as side products during the reaction, is shown. This column including all internals, platforms and ladders and the close piping is created automatically using *PlantDesign*. In the background associated apparatuses, the ofen (right-hand side) and the reactor (left-hand side) are also depicted, but they are given and not designed during the course. The students are combining both planning approaches together to create the overall model for the pipework. Both columns are designed with different external column diameters in the stripping and rectifying sections.

Comparison between classical and *PlantDesign* workflow

During the exercises a comparison between the classical, manual constructive design of a distillation column and the automated design with the help of the assistant system *PlantDesign* is made regarding the evaluation of the following points:

- Time effort for the creation of the 3D model of the distillation column in a 3D CAD environment
- Assessment of the workflow, in particular regarding the degree of difficulty creating the detailed constructive design of the distillation column
- Comparison of the level of detail of 3D models created with both procedures
- Advantages, disadvantages, constraints and limitations of the different approaches of apparatus design

Starting point of the comparison of both approaches is the completed process simulation as well as the dimensioning (column diameter and tray spacing) with the Stichlmair method for the deisobutanizer column. The manual equipment design includes creation of a technical sketch (hand-drawn or using a 2D CAD tool) of a tray column, which includes the detailed design of all internals and distances between elements as well as the dimensioning and positioning of inlet and outlet nozzles, the internal piping and manholes. An examplary hand-sketch is shown in figure A.32 in section A.4. This is a particular challenge for the students, as they usually have a very limited experience with the constructive design and the installation requirements.

The sketch is the basis for the creation of a 3D equipment model, which is created in a 3D CAD environment as starting point for the pipework of the overall process.

Evaluation results

Up to now, 18 groups consisting of 41 students in total finished the course and evaluated the *PlantDesign* workflow against the classical one. All students have had neither experience with the 3D CAD tools of AVEVA nor with the *PlantDesign* environment. The evaluation was carried out in form of reports, the main outcomes with regard to the experience made by the student groups are summarized in table 3.4.

For the evaluation it has to be mentioned that the discussion scope of the individual groups is quite different. A quantification of the time savings using *PlantDesign* has not been carried out in all groups. Furthermore, the evaluations of the workflows have been conducted partly very extensively, partly very scarcely. Common to all groups was the mention of the enormous time savings in *PlantDesign* workflow compared to the classic approach. The more exact details to the time savings (partly related to the considered work steps, e.g. the creation of the 3D CAD graphic or the creation of the hand sketch) are also listed in table 3.5. The comparison is made very different within the groups, especially regarding the scope of the tasks considered (e.g. including hand sketch or only the 3D CAD drawing) - for this reason a summarizing statement is hardly possible.

Furthermore, in almost all groups the comparatively high level of detail of the constructive design of the column (platforms, ladders, local piping, internals) compared to the manually created column and the clear, very intuitive and user-friendly workflow of *PlantDesign* were positively emphasized.
More than half of the groups also pointed out the advantages of a quick comparison of different designs (e.g. varying design for different internals) as well as the automated dimensioning and positioning of nozzles and components, which represent a particularly high effort in manual design. As limitation of the *PlantDesign* approach more than 60% of the groups mentioned the restriction of the design options, but most of these groups also figured out that the a subsequent adaptation of the constructive design of the column (e.g. adaption of nozzle positions or change of direction for exhaust vapor pipe) is easy to implement.

Other positive aspects mentioned for the *PlantDesign* workflow are the avoidance of human errors in the design of the apparatus due to the high level of automation, the consideration of accessibility for maintenance tasks (steel construction), which was neglected in the manual design, the combination of various work steps of the basic and detailed engineering in one tool, the help functions and descriptions in the graphical user interface and the advantages resulting from the storage of heuristics for the design.

Disadvantages of using the *PlantDesign* approach are, for example, that the internal, computational design is hidden for the user and therefore a verification of the results is time-consuming. Not all results and intermediate calculations are made available to the user - here an automated documentation would be suitable, which however has not yet been implemented but can easily be extended. Furthermore, the provision of definitions and assistance should be expanded so that confusion and ambiguities of terms are avoided.

Some reports also pointed to the learning curve during the manual apparatus design - which is of course a major concern of the course. However, it was also frequently noted that the enormous time savings in the use of *PlantDesign* in an industrial environment seems to be promising from an economic point of view.

In one of the last courses, the extension of the interfaces to the Chemcad process simulator was also introduced and met with a very positive response. The avoidance of data transfer errors and the time saving through the automated transfer of simulation results and process information has further simplified the workflow and the extension of such interfaces is desirable as an extension according to the students.

In summary, the *PlantDesign* tool has been used very successfully in the CAP course and has been evaluated by the students as a valuable support for their plant design project.

Table 3.4: Overview of evaluation of the *PlantDesign* in comparison to the classical workflow within CAP course at TU Berlin from summer semester 2016 up to now (black: advantages, red: limitations)

Group	**Saving of time**	**Higher level of detail**	**User-friendly workflow**	**Less research effort**	**Automated dimensioning & positioning**	**Fast comparison of designs**	**Limited flexibility of design**	**Proof of design**
1	x	x	x					
2	x	x	x	x		x	x	x
3	x	x	x	x	x	x	x	
4	x	x	x	x	x		x	
5	x	x	x	x	x		x	
6	x						x	
7	x	x	x			x		
8	x	x	x		x	x	x	x
9	x	x						
10	x	x	x				x	
11	x	x	x		x	x	x	
12	x	x						
13	x	x				x		
14	x	x	x		x			
15	x	x	x	x	x	x		
16	x	x	x	x	x	x	x	
17	x	x	x	x	x	x	x	
18	x	x	x		x	x	x	x
$\sum$	100%	94.4%	77.7%	38.8%	55.5%	55.5%	61.1%	16.6%

Table 3.5: Comparison of time savings (for the creation of a distillation column) between *PlantDesign* and classical workflow within CAP course at TU Berlin from summer semester 2016 up to now

Group	***PlantDesign* workflow**	**Classical workflow**
1	$20min$	Very time-consuming
2	$7hr$ time savings	n.s.
3	$5-6hr$ time savings (without re-work due to changes and errors in the classical workflow)	n.s.
4	$45min$	much more time effort, especially for 2D hand sketch of column
5	Several minutes	Minimum factor 10 longer
6	Significantly faster	n.s.
7	$1hr$, significantly faster	n.s.
8	$< 30min$	Several hours (only 3D CAD drawing, no hand-sketch)
9	n.s	n.s.
10	$3hr$	$12hr$ (including hand sketch and 3D CAD drawing)
11	$10min$, significantly faster	$3h$ (only 3D CAD drawing, no hand-sketch)
12	Significantly faster	n.s.
13	Faster	n.s.
14	Approximately $1hr$	$> 8hr$ (only 3D CAD drawing, no hand-sketch), estimation of $40hr$ for drawing internals
15	Significant time savings	n.s.
16	Significant time savings	n.s.
17	$1hr$ (mostly for calculation of required input data)	$15hr$, much longer for creation of internals, platforms & ladders
18	$15min$	$12hr$

n.s.: not specified

3.4.3 Case study for industrial example process

A theoretical case study for an industrial application has been performed in cooperation with the Lonza AG, one of the world's leading suppliers to the Pharma&Biotech and Specialty Ingredient markets [Lonza AG, 2019]. The content of this section refers in large parts to [Fillinger, Seyfang, et al., 2020 (submitted)].
Starting point of the investigation is a steady state process simulation at an early phase of the engineering, comparable with the basic engineering stage, after establishing the process concept for the desired production. The process is designed for a multipurpose plant to produce an agricultural intermediate with several thousands of tons per year. The two-stage chemical process has a broad by-product spectrum with a variety of solvents, so that the downstream purification process is complex and expensive. A Basic Flow Diagram of the process is shown in Figure 3.38. The steady state process simulation has been performed in Chemcad 7.

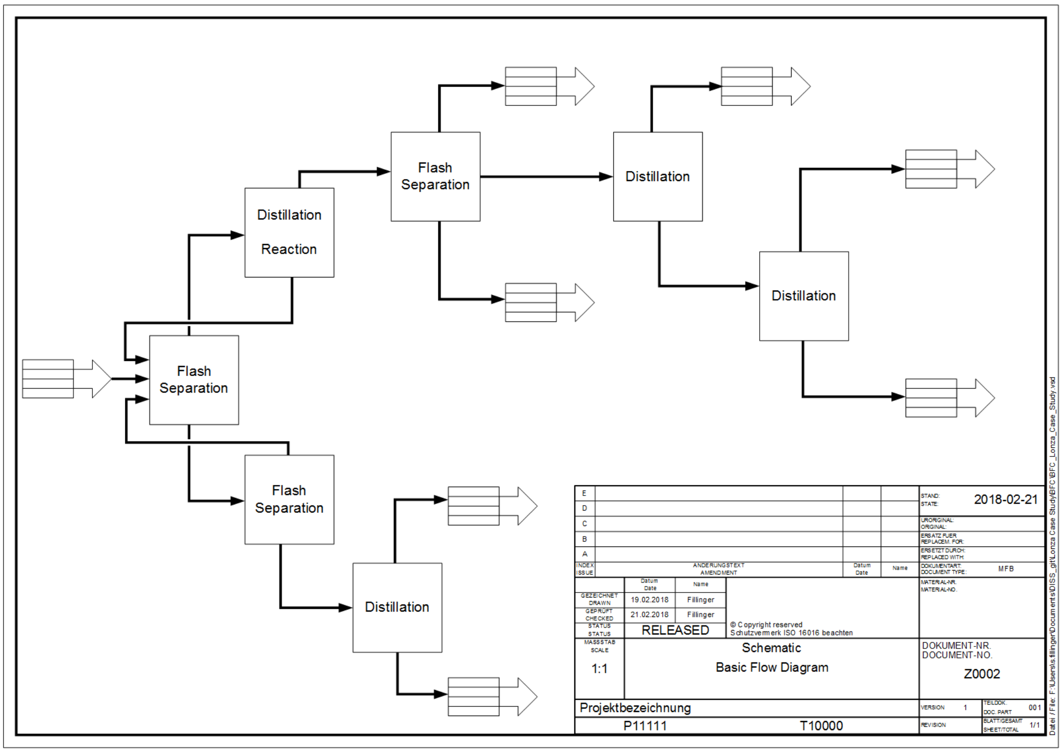


Figure 3.38: Basic Flow Diagram of the process

3.4.3.1 Setup

The process units considered for the automated constructive design are packed columns for the distillative separation [modeled with the rigorous SCDS column model], shell and tube heat exchangers as condensers and reboilers, pressure vessels as flash units and redundant pump assemblies. Only associated apparatus for distillation columns, no pumps to control the pressure-driven flows between process units, are taken into account.
The sizing and design calculations for flash units bases on [Branan, 2005], the constructive design of internals is not considered i.e. only the outer shell of the apparatus is created automatically. The simulation settings and results are exported as Chemcad *XML* files storing data from simulation as well as physical properties and packed sizing information in case of distillation columns. The set of simulation values used for the constructive design are imported via the *PlantDesign XML* interface – these values are the fundamentals of the engineering base. During the import of the flowsheet information, an automated detection of the type of process unit (e.g. rigorous or short cut model) and the data handover of the corresponding process variables that are available is performed. Information about the simulation file is stored as an attribute in the *origin* tags of the imported values and transferred to the exported 3D data file. This is an efficient way to document the decision-making process and to improve the transparency within the planning procedure, but the sustainability of the information is limited for locally stored simulation files. A more comfortable option is the storage of database references to the process simulation, but this is of course depending on the storage strategy of the simulation tool.
An overview of the import variables is given in table 3.6. The required conversion of engineering units is performed automatically during the import of data using the *XML* interface.

Table 3.6: Engineering base automatically imported from Chemcad simulation for the case study

MPU	**Variables & settings**
Packed column	Tag name Calculated column diameter (rectifying and stripping section) $[mm]$ Component list $[-]$ Molar composition of feed, distillate, bottom product $[mol \cdot mol^{-1}]$ Volumetric flowrates $[m^3 \cdot s^{-1}]$ Operating temperature [°C]

Continuation table 3.6 of previous page

MPU	Variables & settings
	Operating pressure [bar] Feed stage [$-$] Total number of separation stages [$-$] Feed aggregate state [$-$]
Heat exchanger	Tag name [$-$] Heat exchange area [m^2] Volumetric flowrates [$m^3 \cdot s^{-1}$] Operating temperature medium [°C] Operating pressure medium (shell side condenser/ tube side reboiler) [bar]
Pump assembly	Tag name [$-$] Capacity [m^3/h] Inlet/outlet pressure [bar]
Pressure vessel (Distillate drum, Flash)	Tag name [$-$] Volume [m^3] Operating temperature [°C] Operating pressure [bar] Volumetric flowrates [$m^3 \cdot s^{-1}$]

3.4.3.2 Linking of process units

Following the generation of the MPU models using *PlantDesign*, the unit models have to be positioned manually into the global 3D plant model. For this example, a greenfield site planning with existing equipment and pipe racks is assumed and the units are arranged spaciously to have a better graphical view. If necessary, adaptions of the MPU, e.g. the orientation of close piping or manholes for maintenance tasks, can be performed to prepare the global piping of the process. In doing so, general guidelines should be taken into account for the overall piping of installations, which may be influenced by various factors, such as the media as well as the condition or phase transitions of fluids in the pipelines, the accessibility and mounting capability, etc. The arrangement of units should be realized in a way, that the connecting elements like nozzles are situated in the same plane to simplify the pipework by avoiding offsets.

Additional user specifications for the constructive design of the process units are listed in table 3.7. This engineering information is typically not available in process simulation, often refers to company- and country specific guidelines and directives for the plant design and requires a high engineering expertise. For the sake of clarity, further optional settings, e.g. the welding distance or the safety factor for the calculation of the wall thickness, are not considered in this list. For these variables default values from literature are assumed. Additional data is entered manually via the GUI. The decision-making process for the user selection is supported by providing heuristic and manufacturer information for the constructive design. This is of particularly beneficial to less experienced engineers enabling them to develop practicable and working engineering solutions.

Table 3.7: Additional specifications for the constructive design of the case study

MPU	**Variables & settings**
General settings (all process units)	Equipment material (steel grade) $[-]$ Min./max. temperature [°C] Min./max. pressure $[bar]$ Piping class (pressure rating) $[-]$ Piping material $[-]$ Nozzle connection type $[-]$ Nozzle length $[mm]$
Packed column	Type of internals (Packing type, packing size) $[-]$ Equipment insulation (type $[-]$, material $[-]$, thickness $[mm]$) Piping insulation (type $[-]$, material $[-]$, thickness $[mm]$) F-Factor (calculated from simulation data) $[\sqrt{Pa}]$ Liquid bottom level $[mm]$ Column end shape (torispherical head, ellipsoidal head) $[-]$ Feed inlet design option $[-]$ Column support type option (Skirt support, tubular support) $[-]$ Mist eliminator (installation option $[-]$, material $[-]$, height $[mm]$) Manhole diameter option $[mm]$ Close piping option $[-]$ Flow velocities (in-/outlets) $[m \cdot s^{-1}]$ Type of liquid distributor $[-]$ Process unit description $[-]$
Heat exchanger	Close piping orientation (vertically, horizontally) $[-]$ Length/diameter $[mm]$

Continuation table 3.7 of previous page

MPU	**Variables & settings**
	Baffle spacing (optional) [m]
Pump assembly	Rounds per minute [min^{-1}] Delivery head [mm] Orientation close piping (suction and pressure line: horizontal, vertical) [$-$]
Pressure vessel	Length/diameter [mm] Orientation (vertical, horizontal) [$-$]

3.4.3.3 Results and workflow

The resulting 3D models of the single process units are illustrated in figure 3.39. The generated source code of each MPU created with *PlantDesign* is imported and visualized in AVEVA E3D^{TM}. The placing of the MPUs into the 3D model of the entire plant is done manually using one global coordinate system by moving the whole MPU model. Afterwards, the modular design of the units can be adapted and modified for the specific purposes of the entire plant. For example, the pipe outlet orientation of the exhaust vapor pipe or nozzle positions in the shell side of a heat exchanger are possible changing points. The adaptions that has been performed for this case study are marked in figure 3.39 - orange arrows show the adaption of close piping, green ones the change of positions of the whole MPUs. Figure 3.40 shows the MPUs after the adaptions of piping orientations and the placing of each MPU as preparation for the global piping.
Major modifications, e.g. changing the apparatus diameter, can be adapted only with a very high effort within the 3D CAD environment afterwards due to the strong dependencies of this design variable to further variables of the entire equipment. The faster way of realizing a change is to adapt the specifications directly in *PlantDesign*. This enables an easy comparison between designs related to different operating points of a plant or changes regarding the separation performance of columns and the resulting effects on the associated apparatuses. Also, the effects of the constructive design and the sizing based on the selection of different internals (for a similar separation task) can be realized very efficiently. By this, the fitting of the apparatus into brownfield sites can be simplified massively.

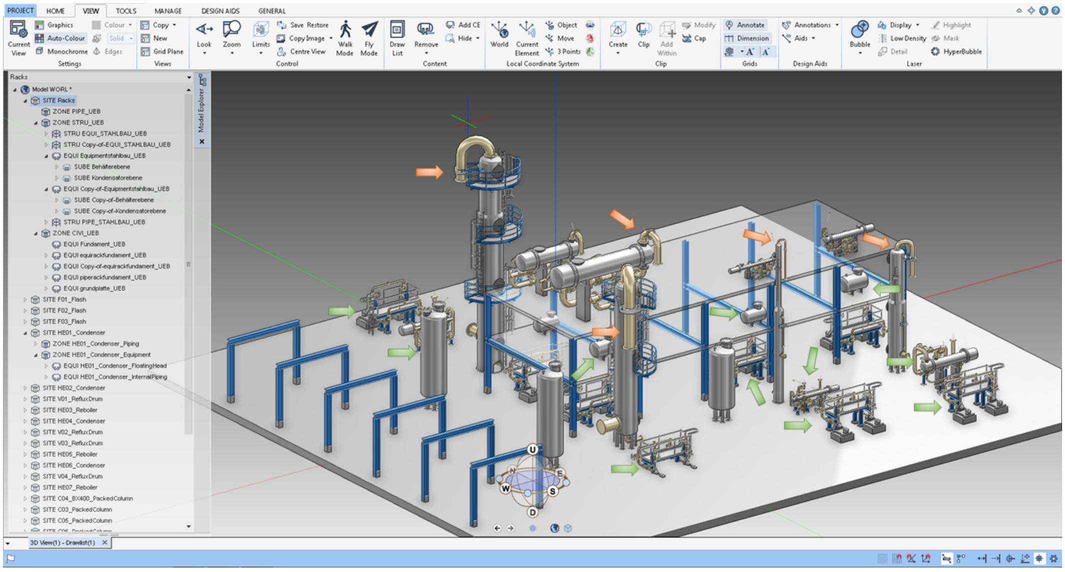


Figure 3.39: Generated 3D models of MPUs, orange arrows illustrate the required adaptions to the close piping, green arrows signal the replacement of whole MPUs as preparation for the global piping, visualized in E3D™ 2.1

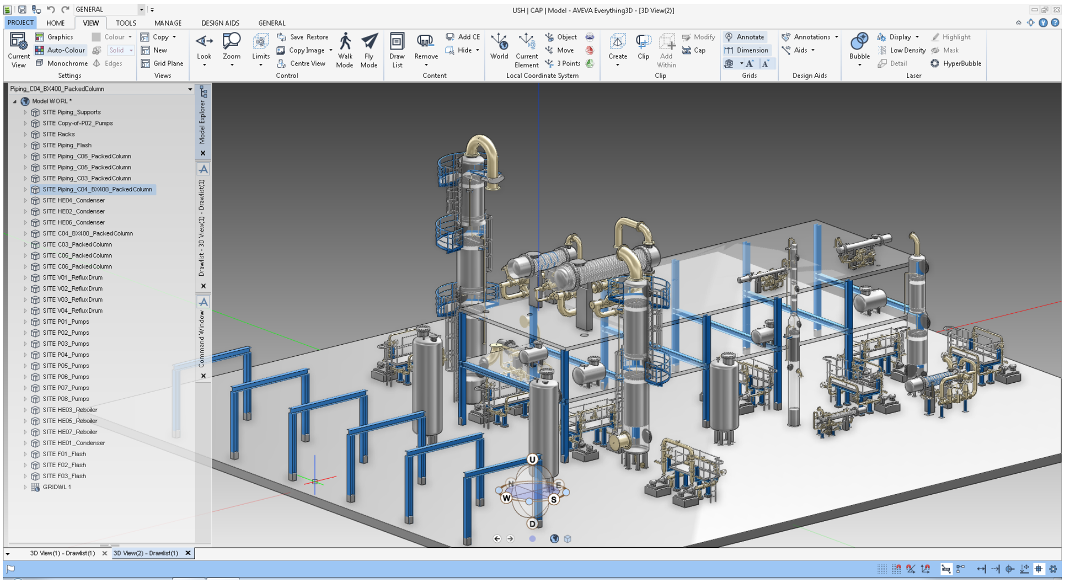


Figure 3.40: Generated 3D models of MPUs including adaptions of close piping and replaced MPUs, visualized in E3D™ 2.1

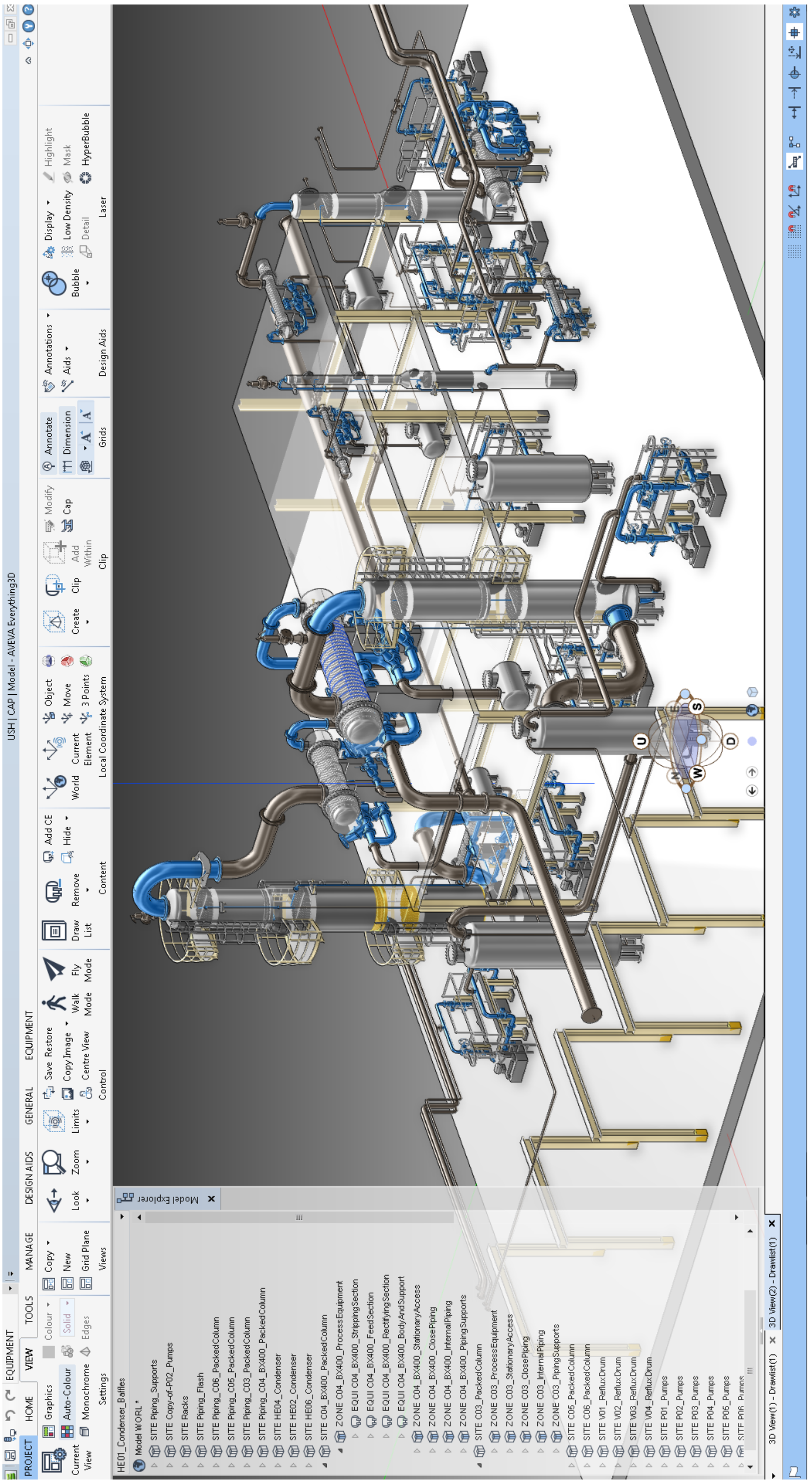


Figure 3.41: Global piping of MPUs (manually added piping is colored brown), visualized in E3D^{TM} 2.1 [**A3 version in appendix**]

Finally, the piping connection between the process units can be designed manually or by using auto-routing algorithms. The final 3D model including the equipment and the pipework is illustrated in figure 3.41. All manually added pipes are colored in brown, the automatically generated pipes are colored in blue.

3.4.3.4 Evaluation of the *PlantDesign* workflow

PlantDesign enables a faster constructive design and the creation of a representative 3D plant model for modular process units including the equipment, internals, supports, steelwork, close and internal piping with fittings and instrumentation. The level of detail of the 3D models of process units is much higher than within the 3D models typically used in process industries. This leads to a better as-built-modeling of the plant as well as less rework and improved conditions during the plant assembly due to the exact graphical representation of the equipment – especially with respect to the installation of internals, e.g. for welding operations. Typically, only the outer shell of equipment including connection points to the pipework, e.g. nozzles, are created within the classical planning procedure as basis for the pipework. Due to this, a direct comparison of the time expenditure between the *PlantDesign* and the classical planning workflow is not representative. The routing of the connecting pipes between MPUs is not included within the approach but there are tools available on the market, that apply an automatic, rule-based routing for an appropriate piping using optimization algorithms.

The significantly higher level of detail of the equipment design within *PlantDesign* provides the opportunity of a much more precise cost estimation. The prerequisite for this is the availability of specific component and material costs, which is typically available in engineering departments of chemical and plant design companies.
Furthermore, the better representation of the spatial design already in an early stage of the planning procedure results in important advantages during the risk assessment and safety analysis of (petro-)chemical plants (HAZOP – Hazard and Operability Study), which have a high impact in the planning procedure as well as during the operation period. The existing equipment and piping design allow for example a well-founded decision for a suitable positioning of feed and discharge pipes, a suitable infrastructure and the installation of cable trays/runs, to grant good accessibility for maintenance tasks. Further on, the development of analysis concept, e.g. the positioning of sampling points depending on the accessibility and the consideration of hazardous areas (hot surfaces, rotating parts) is beneficially affected.

The fast design of units with different design options (e.g. the choice of different internals) and the resulting module dimensions (total height and required floor space for the MPU) allow for an easy comparison of different engineering solutions. Especially if modules are integrated into existing plants (brownfield projects) this approach is advantageous with respect to the space management and installation. Here, a combination od laser scanning to get a 3D model of the existing plant elements (if not existing) as a basis for including additional 3D models is possible.

Adverse consequences of using a modular approach is, despite the several design options *PlantDesign* offers, to be limited regarding the possible engineering solutions. Nevertheless, the *PlantDesign* approach can easily be expanded to new constructive options and process units. A customization and extension of the module library with regard to standardized or even company-specific solutions has to be implemented only once and can be reused many times. The integration of this approach into the classical plant planning procedure, especially for frequently installed process units, guarantees proven engineering solutions and avoids extra work during the planning. It enables a central storage of engineering know-how for companies and can easily be adapted and extended by new solutions and design options.

Furthermore, a comprehensive documentation of the planning process can be realized automatically. The introduced data interfaces ensure an error-free and consistent data handover of the planning data between process simulation and 2D CAD tools. The availability of this data, as part of the plant life cycle data, offers great opportunities for the construction and assembly as well as the maintenance and turnaround management. A precise knowledge of the constructive design and the corresponding planning information improves the preparation of assemblies and installation tasks as well as during troubleshooting within plant startups.

4 Multidisciplinary data exchange for the life cycle of plants - interoperability of CAE-tools

The various dependencies regarding the data handover between the distinct disciplines and domains involved during the planning of process plants are illustrated in figure 1.1. Planning and plant information must be shared among the different stakeholders. Hereby, it has to be guaranteed, that the data is consistent, unambiguous, and at anytime up-to-date. Furthermore, the transfer of data has to be performed without losses of information – not only during the planning phases but also during the whole life cycle including operation, maintenance, modifications, and finally dismantling of plants. Due to the specific tasks of the single disciplines, the set of information that can be exchanged varies strongly. According to [Weber, 2014], there is a strong relation on the interfaces between basic and detailed engineering, since the commissioning companies typically consult contractors for the further planning steps.

Within industrial companies, a wide range of software tools including specialized features for similar or completely different functionalities are applied for plant design. Due to the various stakeholders the usage of different tools is practiced not only among diverse trades but even within single working areas. This procedure often requires a multiple manual input of the same specifications into different tools. This results in a higher expenditure of time for the conduction of the planning tasks as well as the maintenance of data integrity in case of occurring changes. A strong linkage between various fields of activity underlines the great importance of data exchange to achieve an intelligent connectivity of software tools applied in process industry.

Data exchange is strongly varying depending on the range of software used in the computational design of process plants. This chapter focuses on the investigation of data handover between different types of CAE software and the definition of data types associated with data exchange - primarily in the field of basic and detailed engineering. The investigation concentrates on three types of software applied in different disciplines of process industries, which are highly involved in the initial plant design, but also the later phases of a plant's life cycle: process simulation tools, 2D CAD tools for P&ID's as well as 3D CAD tools and the data associated with them.

The prototypical, proprietary data import interface for process simulation data to the *PlantDesign* tool has been introduced in the previous section. In this section, the interdisciplinary data exchange between 2D P&IDs and 3D plant models was investigated and a prototypical framework for the heterogeneous data exchange between the P&ID software X-Visual PlantEngineer, the integrated engineering tool MOSAIC-modeling *PlantDesign*, and the 3D CAD environment AVEVA PDMS™/E3D™ is presented for distillation columns.
The contents of this chapter refer in parts to the following publications [Fillinger, Bonart, et al., 2017], [Fillinger, Esche, et al., 2019] and [Fillinger, Seyfang, et al., 2020 (submitted)] as well as the master thesis of [Nowotnick, 2017], which was supervised in cooperation with the company X-Visual Technologies.

4.1 Multidisciplinary data exchange - general remarks

The large amount of different CAE systems results in a multitude of proprietary data formats and eco systems. The complex planning procedure, the great variety of engineering documents, the long-term operating times of plants and not at least the production guidelines ([DIN EN ISO 9001, 2015] or GMP [DIN EN ISO 15378, 2018] certificated) make the availability and compatibility of software and corresponding data formats mandatory. A change of tools in the software framework of chemical companies goes hand in hand with high efforts for e.g. the testing phase, the company-wide roll-out of a software, the training of employees, the customization of functionalities like reporting or company-specific implementations and the setup of connections to the existing software framework.
The diverse information content generated within the planning steps impede the exchange between different tools, especially beyond vendor-specific ecosystems. The high diversity of vendor-specific solutions makes it difficult to define and establish standardized data models and data exchange interfaces. Although non-standardized, customized data interfaces can be realized with comparatively little effort for certain use cases, they can only be used to a very little extent. A roll out of these interfaces to other applications and processes requires a high degree of customization and quickly revokes or eliminates the initial savings. Moreover, a reliable support of data formats and the warranty of compatibility in different software versions are important decision factors for software users. Standardized solutions increase the reliability for customers.

Consequently, several practical requirements have to be fulfilled for a suitable data exchange. Following [Kim et al., 2016], the used data model should have the «capability of representing and integrating the plant life cycle data» and it should be independent of the software and manufacturer. Referring to the definition of ISO 15926, a data model «defines the meaning of the life-cycle information in a single context supporting all views that process engineers, equipment engineers, operators, maintenance engineers and other specialists may have of a plant». Referring to the three-schema architecture [ISO/TR 9007, 1987], the structure of data within a data model is represented in a form independent of any physical storage or external presentation format.

The data should be stored in a platform independent format, which is extendable in both, size and structure. To ensure consistent and up-to-date data for every participating stakeholder, only one copy of data should be accessible concurrently by multiple systems for multiple purposes [Kim et al., 2016]. The objective of the Namur initiative [NAMUR, 2019] is the development of an interface for the semi-automated, bidirectional standardized data exchange between CAE tools and PSE engineering tools. Important requirements and conditions associated with the exchange of engineering data are practicality, vendor neutrality, data consistency, tool independency, continuous data synchronization, prevention of data-errors, and avoidance of transfer of redundant data. Furthermore, the effort for provision and maintenance of the import/export interface should be minimized.

A change in one software should spark a bi-directional information exchange in the other software's. To guarantee the reusability of data, a standardized data exchange format with a widespread usage is needed. Thereby, it is essential to determine and establish a universal, generally accepted standard due to the widespread usage of various company-specific guidelines and the differing interests of various stakeholders.

However, a data exchange meeting all demands is currently not possible in a straightforward way. Several attempts have been undertaken to fulfill parts of the requirements, as already pointed out in section 2.4.3.

One way to enable distinct software to exchange data is to define a data model which represents the whole design process of the chemical plant. For example, the ISO 15926 aims to «facilitate integration of data to support the life-cycle and processes of process plants» [ISO 15926-1, 2004]. In theory, applications implementing interfaces consistent with the standard can exchange data. Recently, [Kim et al., 2016] showed the exchange of geometrical data in an ISO 15926 conform way. However, the exchange of process data between heterogeneous software packages, which fulfill different tasks during the design of plants, is a lot more complex since new data is created based on the input data.

Depending on the specific view on interoperability in process industry there are several starting points for the development of approaches and strategies for an implementation. In this work, the initial base for developing a 2D-3D data exchange framework are detailed plant models from an application-oriented point of view, which have been created using the *PlantDesign* tool introduced in the former chapter. The objective target is to investigate data that can be transferred between software tools applied in several areas of work during the planning process as well as occurring limitations and challenges. The focus is on data exchange between 2D and 3D CAD tools. Special attention is addressed to the subject of standardization, which is a significant requirement to achieve feasibility in a wide field of application. Due to the importance of applying standards, the approach is inspired by the work of the DEXPI initiative, which deals with the development and the promotion of a general data exchange standard for the process industry, currently for P&IDs [DEXPI Initiative, 2019]. The investigations and the prototypical implementations performed in this work can be used as a starting point for the extension of the standardization work with respect to the heterogeneous data exchange between CAD environments and further disciplines in process industries.

4.1.1 Tool-specific data exchange

Apart from different types of data mentioned in section 2.4.1, the type of software, between which data is exchange is performed, also plays an important role. An overview for data handover between homo- and heterogeneous software is shown in figure 4.1.
Homogeneous data exchange can be applied between different software tools (from different software vendors) with a similar field of application as it is illustrated in the upper and lower boxes of figure 4.1. Homogeneous software tools fulfill in general the same purpose for the design of plants but in particular have special functionalities and features. It typically deals with the same information that needs to be transferred – under the assumption that the tools have similar functionalities. Tool-specific varieties or deviations regarding the internal processing of data, which are constituted by system architecture as well as programming logic, should not have any impact on the data transfer between these systems.
However, each software tool has a differing focus and perspective on the objects related to the process plants - as well as companies have. There are special features and functionalities with varying levels of detail regarding planning. This fact can partially lead to a different set of data that should be transferred among homogeneous tools.

For that reason, a bi-directional data exchange is feasible in general, if the set of data to be exchanged is defined and an appropriate data exchange format with a corresponding data interface is available. A successful development and implementation of homogeneous data transfer between different P&ID systems is realized by the DEXPI initiative.

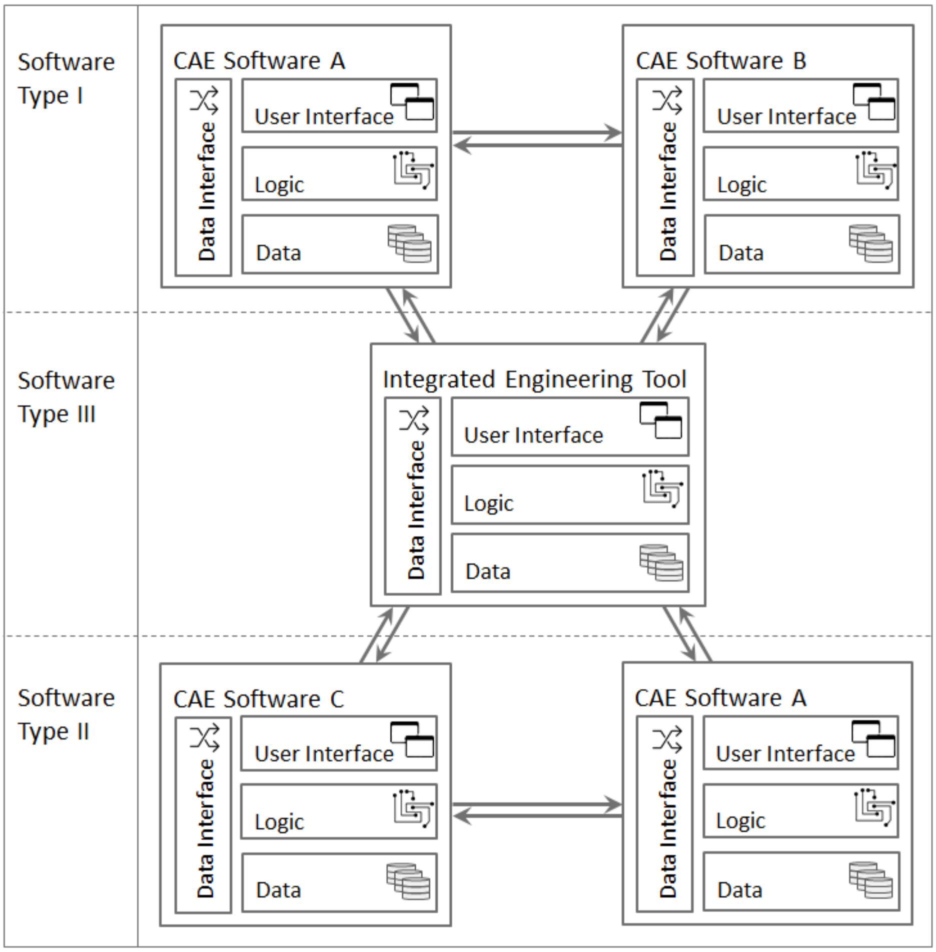


Figure 4.1: Data exchange between different CAE tools applied in process industries [Fillinger, Bonart, et al., 2017, p. 1457]

Development and implementation of data formats and interfaces between heterogeneous software tools is a more challenging area. As illustrated in figure 4.1, this case of data exchange can be performed either between middle and upper, or middle and lower box respectively. By contrast to the data transfer among homogeneous tools, those between heterogeneous software requires a separate analysis regarding the types of data, which should be exchanged. Hence, a particular challenge is handling different information occurring in respective applications due to varying sets of information in the corresponding data models. Exemplarily, CAD tools for the creation of P&IDs on the one and 3D plant models on the other hand have common information, but parts of the data set cannot be interpreted and processed within the respective other tool.

It is mandatory to define a process unit specific information set including characteristic information, which should be transferred between those tools. In that case, a direct transfer and processing of data within diverse applications is possible. Within this approach, based on the information of the P&ID, the generation and processing of data required for the 3D plant model is realized with MOSAICmodeling's *PlantDesign* feature. It serves as an integrated engineering tool, which realizes the linking between both CAD tools and furthermore has a linkage to process simulation as part of MOSAICmodeling.
Prerequisite for the 2D-3D data exchange framework is the development of a suitable 3D data model, whereby the focus is on the exchange of plant and process information, not on the exchange of information related to the graphical representation.

4.2 3D data models for industrial plants

A 3D data model for industrial plants should be able to handle all information related to a as-built-status of a plant, including all constructive elements, process information as well as the hierarchy related to the site-specific information of the plant components. For this reason, the starting point of the development of the 3D data model are the 3D plant models generated with *PlantDesign*. As shown in the section 3.1, these models show a particularly high level of detail, which is currently not the state of the art in the process industry, but should be covered in any case.

4.2.1 Exchange of geometric information

As already mentioned in section 2.4.2, graphical information between 3D CAD tools can be exchanged using formats like STEP or in an ISO 15926 conform way (as shown by [Kim et al., 2016]). An alternative approach has been presented in section 3.3 using *PlantDesign* for the automated generation of the 3D plant models for different 3D CAD environments with the help of the introduced source code converter framework. This enables a loss-free transfer of the information for the graphical representation as well as the further processing of the generated 3D model - a decisive advantage compared to the use of data exchange formats such as STEP.
It would be highly desirable to integrate a standardized intelligent data exchange format into the *PlantDesign* source code converter method library. This would allow an universal data exchange between different CAD tools without having to extend the method library with vendor-specific methods by adding proprietary programming languages that can be interpreted by the CAD environment.

Due to the different geometric representation of 2D and 3D plant models, the heterogeneous data exchange of geometric information between 2D and 3D CAD tools is not relevant. For the development of the prototypical 2D-3D data exchange framework the focus is on the exchange of process and plant information related with equipments. An extention related to pipework is still pending.

4.2.2 Hierarchical representation of plant structure

Referring to [DIN 28000-1, 2011, p. 5-7], process plants can be structured in a hierarchical way as illustrated in figure 4.2. The top levels of the hierarchy are related to the site-specific classification of a process unit, the lower box is referred to the equipment and piping structure. The underlying hierarchy for the equipment level is identical with the structure of the MPU shown in figure 3.1 of section 3.1. Hereby, the hierarchy level for a process unit is either suitable for a modular process unit or for a «normal» process unit, even if the representation in figure 3.1 only refers to MPUs. Beside constructive information, the equipment level includes also functional and structural hierarchy information, e.g. the subdivision into equipment sections, the internal and external piping, steel constructions or supports.
This structuring is related to a trade-specific view on the process unit and it can be easily extended to further trades like electrical or civil engineering - however, other trades were not taken into account within the scope of this work.

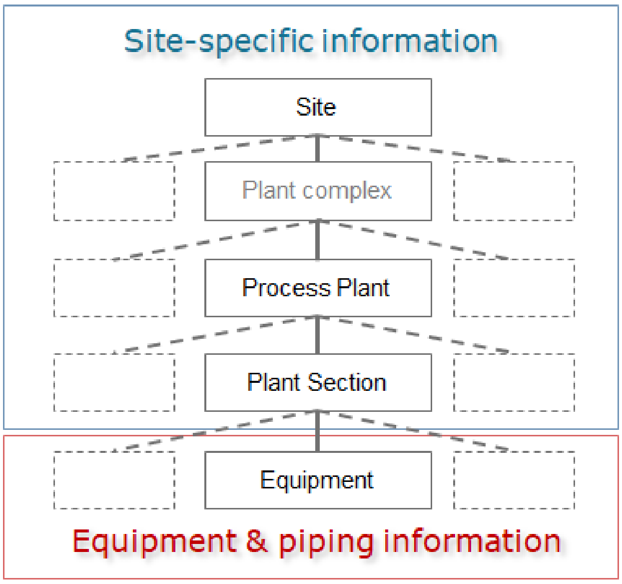


Figure 4.2: Hierarchical structure of process plants

4.3 Interdisciplinary data exchange - prototypical 2D-3D data exchange framework

The interdisciplinary data exchange between 2D P&IDs and 3D plant models has been investigated in [Fillinger, Bonart, et al., 2017]. As already mentioned in chapter 2, promising existing candidates for the exchange of 3D graphics are established formats like STEP, but an extension for the transfer of processing data without loss of information is mandatory. Moreover, subsequent processing or changing of the 3D model after data transfer into another CAD environment is strongly limited. Inspired by the investigation of the homogeneous data exchange of the DEXPI initiative and in absence of an appropriate established standard for the intelligent exchange of 3D plant model data (respectively not only the exchange of data for the graphical representation) DEXPI's P&ID schema [Proteus Schema, 2016] for the exchange of P&IDs was adapted and extended to enable the interdisciplinary heterogeneous data exchange between 2D P&ID and 3D plant models. The specification included in Fiatech's 3D model based on ISO 15926 [Laud, 2008] does not have the required level of detail but is taken into account for the developed extensions of the 3D data model in this work.

A prototypical 2D-3D data exchange framework between X-Visual's PlantEngineer [X-Visual Technologies, 2019], MOSAICmodeling's *PlantDesign* as an integrated engineering tool, and AVEVA PDMS™/E3D™ for the 3D visualization has been successfully implemented. Within *PlantDesign*, the generation of 3D plant models based on simulation results, heuristics, and standards for the constructive design is performed automatically. The resulting 3D model is the basis for the data exchange from the 3D perspective. The prototypical data interface allows for the transfer of equipment information, process conditions, functional as well as site-specific information, and procurement data.

During the investigation, different constraints for the standardized implementation of interdisciplinary data exchange are detected. One of the most relevant limiting factors is the set of object definitions with sufficient detail within the reference data library (RDL), which is incapable of representing the detailed constructive design of 3D models created with *PlantDesign*. Exemplarily, attributes referring to the internal piping, internals, or supports are currently missing in existing RDL's, e.g., PCA (POSC Caesar Association) RDL.

4.3.1 2D-3D data exchange framework

A feasibility study and prototypical implementation for interdisciplinary data exchange between P&ID and 3D data models for equipment information has been performed in cooperation with the software vendor X-Visual Technology. The software tools involved are the P&ID tool PlantEngineer, the 3D CAD tool AVEVA PDMS™/E3D™) and the intermediate integrated engineering tool *PlantDesign* for the automated generation of 3D models, as shown in the schematic overview in figure 4.3.

A characterization of data to be exchanged between different software has been performed in section 2.4.1 to enable a distinction for the different kinds of data transfer. An analysis of 2D and 3D data models establishes characteristic attributes of the considered process unit and the investigation of the intersecting set of information which can be exchanged. Based on this, a characteristic specification for distillation columns has been developed and a prototypical interface has been implemented and successfully tested.

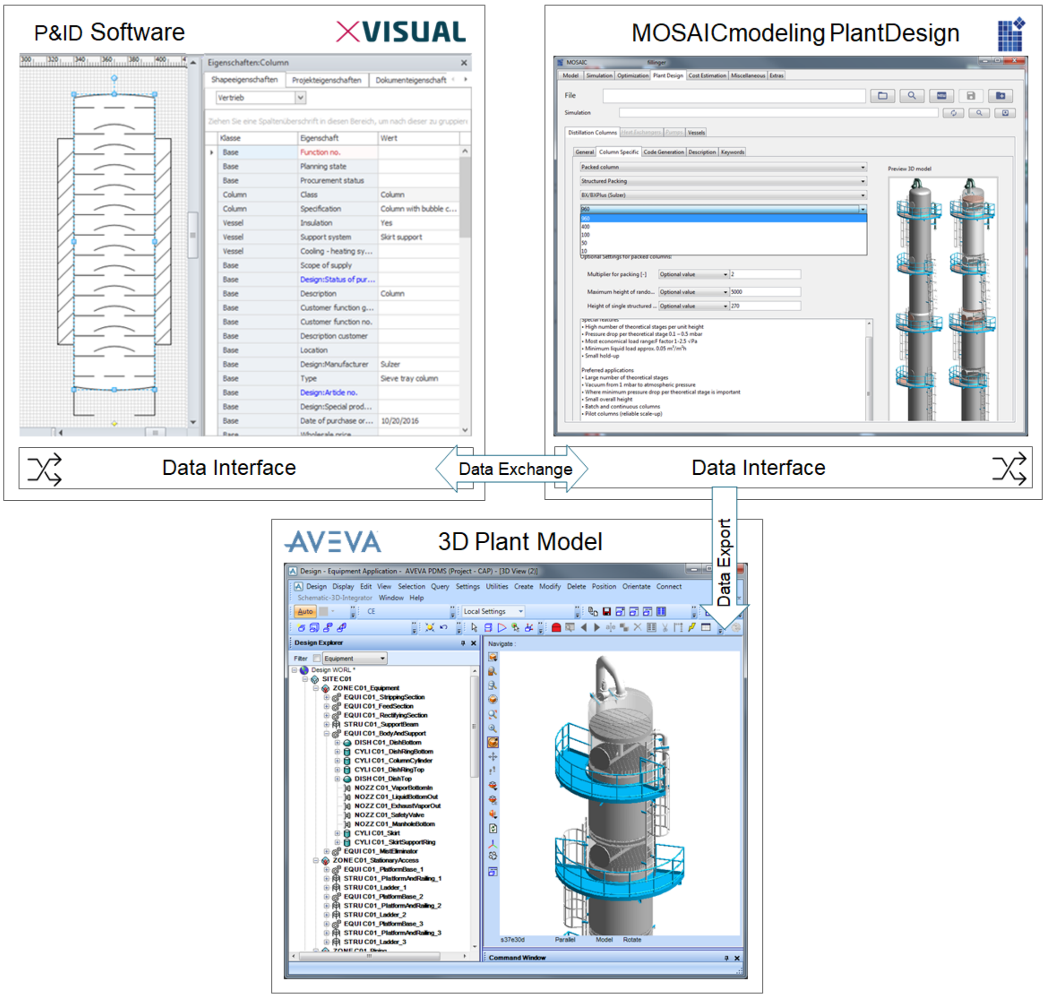


Figure 4.3: Overview of 2D-3D data exchange framework, exemplary for rectification columns

4.3.2 Information content of 2D- and 3D-plant models

To define base data for the exchange between both systems, information of 2D- and 3D-specific engineering and apparatus design have been examined and compared. Most relevant standards regarding plant design refer to two-dimensional representation, but there are no pertinent standards for 3D models and their contents. For this reason, the detailed 3D model developed within *PlantDesign* was the basis for the further investigations. A distillation column serves as an example for the case study. General commonalities and differences between both data models have been analyzed in detail and the specification of characteristic attributes for the data exchange has been developed for distillation columns. The heterogeneous data exchange of the different types of data with respect to distinct categories of information in plant design (e.g. general equipment data, functional information, process conditions etc.) between the 2D and the 3D data model is illustrated in figure 4.4.

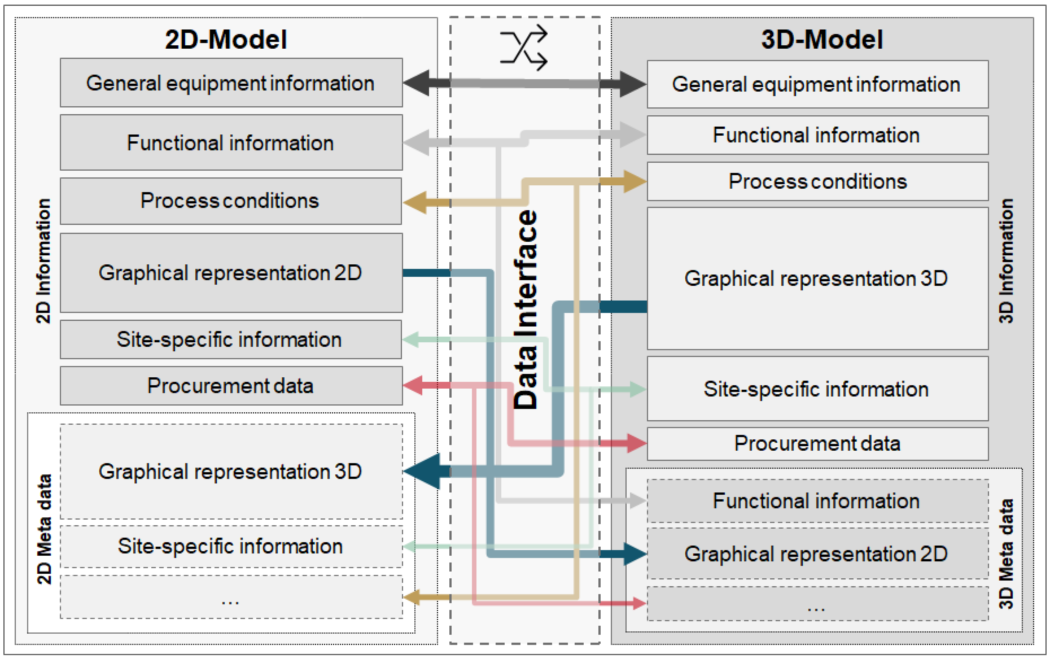


Figure 4.4: Schematic overview of heterogeneous data interface between 2D P&IDs and 3D CAD tools with respect to different categories of information in plant design

The exchange of invariant data that does not change during the planning is relatively easy to handle. For example tag numbers or equipment type information within the information category «general equipment data» or «site-specific information» such as the site and plant designation can be interpreted and used directly in the individual tools after the data exchange. This is illustrated by an bi-directional information arrow between the 2D and 3D model without branching arrow to the respective meta data section of the data models.
Intermediate and processed data of the respective tools require a different procedure depending on the type of information. These kinds of data cannot be interpreted completely by other tools after importing due to differing functionalities and purposes of each software.

As example, the exchange of data related to the category «functional information» between P&ID and 3D CAD systems can be mentioned. Within P&IDs, the information content of control structures is higher than in 3D models and transferred information cannot be used in a 3D CAD tool due to missing graphical and functional representation opportunities of signal lines. On the other hand, the 3D model includes spatial information for example about the detailed geometric characteristics of sensors or control valves that are not included in the P&ID model. Therefore, information, which are not part of the intersecting data set, can be transferred and stored as kind of tool specific meta information within the other tool. This is illustrated in the bottom boxes of the 2D and 3D models. This information is not further processed after data exchange.
Furthermore, some tool-specific information cannot be interpreted by another system at all. For example, data related to the category «graphical representation» of one system cannot be interpreted by the other. In 2D CAD tools symbols created out of lines, curves and points are used for the graphical representation of the plant elements, whereas in 3D CAD models a realistic representation of the elements created with other geometrical methods, as introduced in section 2.3.2. Meta information related to specific functionalities of single tools or further trades can also be transferred. This is illustrated through the bottom box within the meta data sections without specific information category.
A general overview of the intersection data set as well as differences between the 2D and 3D data models is given in table 4.1.

The set of characteristic attributes for the description of distillation columns has been defined during this investigation. An overview of the exchangeable attributes is given in figure 4.5. The specified column attributes are available in both tools, PlantEngineer and *PlantDesign* to enable the unambigious mapping of exchanged information during the data exchange. Information that is not included in the intersection data set of specified characteristic attributes can be transferred between both tools as additional attributes within the meta data information.

The essential prerequisite for doing so is that these additional attributes can be arranged into the structure of the data exchange format. The applied *XML* exchange format is well suited for this purpose since the hierarchical structure is easily extendable. Within the prototypical implementation, additional attributes exported from one tool are labeled with the respective tool name infront of the attribute naming. This proceeding enables receiving a full set of data without data loss - especially if data is modified after import from one tool and transferred back later.

Component Data:

- Component #
- Feed mole fraction #
- Distillate mole fraction #
- Bottom mole fraction #
- Medium group PED

Component index

Process conditions:

- Feed aggregate state
- Min. operating temperature
- Max. operating temperature
- Min. operation pressure
- Max. operating pressure
- F-Factor
- Liquid bottom level (max.)

Process Data:

- Feed flowrate
- Bottom liquid flowrate
- Reflux flowrate
- Bottom vapor flowrate
- Exhaust vapor flowrate

Apparatus design:

- Column material
- Number of stages
- Feed stages
- Ext. diameter rectifying section
- Ext. diameter stripping section
- Manhole diameter
- Position of feed connection
- Mist eliminator
- Height of mist eliminator
- Mist eliminator material
- Column end shape (top, bottom)

General equipment data:

- Tag name
- Equipment description
- Explosion protection (ATEX)
- Estimated overall costs

Column specific data:

- Column type (packed, tray)
- Internal type (packing, tray)
- Internal size (packing, tray)
- Max. height of packing

Piping and nozzles:

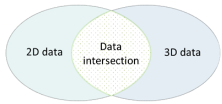
- Piping class
- Piping material
- Nozzle connection type
- Nozzle material
- Nozzle length
- Velocity feed
- Velocity relux
- Velocity liquid bottom
- Velocity vapor bottom
- Velocity exhaust vapor

Insulation:

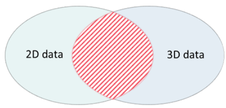
- Equipment insulation type
- Equipment insulation material
- Euipment insulation thickness
- Piping insulation type
- Piping insulation material
- Piping insulation thickness
- Feed pipe insulation
- Reflux pipe insulation
- Bottom liquid pipe insulation
- Bottom vapor pipe insulation
- Exhaust vapor pipe insulation

Figure 4.5: Exemplary characteristic attributes for the data exchange of distillation column models [Fillinger, Bonart, et al., 2017]

Table 4.1: Overview of data intersection between 2D and 3D data models



Properties (exemplary)	Attributes 2D/3D
Specific classification features	Name, tag name, description
Type of equipment	Column type, Type of internals
Main dimensions, weight	Diameter, length, height, empty weight
Process conditions	Temperature, pressure, throughput, concentrations
Procurement information	Order date, manufacturer, article number, price
Characteristic design features	Volume, material, isolation
Nozzles, piping	Pipe class, nominal diameter, material, sealing class



Properties (exemplary)	2D attributes	3D attributes
Scale, spatial representation	✗	✓
Functional representation	✓	✗
Location-related plant information	✗	✓
Operating states of MSR technology	✓	✗
Freespace volumes, traffic routes	✗	✓
Position of nozzles, auxiliary structures, steel construction, foundations	✗	✓
Representation of the flow paths/directions	✓	✗

4.3.3 Case study - 2D-3D data exchange for packed columns

With respect to the investigation of 2D and 3D data models, a prototypical data exchange framework between X-Visual's PlantEngineer, *PlantDesign* as integrated engineering tool, and AVEVA PDMS™/E3D™ for the 3D visualization has been implemented. As a case study, an industrial scale distillation column including internals has been used. The corresponding P&ID is shown in figure A.33 of section A.5, whereas the focus is on the distillation column $K100$.
The data transfer has been performed via *XML* files. The exported *XML*-files from the P&ID tool PlantEngineer are compliant with the Proteus Schema used by DEXPI initiative. Since distillation columns have not been on the focus of the DEXPI initiative during this investigation, the characteristics for these kind of process units have been developed within the work.

The specification of a set of characteristic attributes for distillation columns has been done based on the researched norm information content for P&IDs and the newly developed *PlantDesign* 3D model. The main column attributes are shown in figure 4.5. The specified column attributes are available in both tools, PlantEngineer and *PlantDesign*, to enable the mapping of exchanged information. Further information can also be transferred between both tools. As already mentioned, additional attributes exported from one tool are labeled with the respective tool name in front of the attribute naming.

After importing the P&ID *XML* file into *PlantDesign*, internal calculations (e.g. wall thickness or stress calculations) are performed based on the input data. The constructive design of the distillation column is performed automatically using the results. The generated information within *PlantDesign* includes mainly intermediate and processed data, e.g. the detailed constructive design including dimensions and spatial information of the equipment components. Within this prototype, process, apparatus, component, piping, nozzle and insulation data are exchanged. Currently, graphical representation data from P&ID and 3D model are not included within the transferred data set for the distillation column due to the lack of ability to interpret and process them from one tool to another. Nevertheless, an extension of these information to the respective *XML* transfer files is possible as shown in section 4.3.5.

4.3.4 *XML* structures - DEXPI P&ID and *PlantDesign* 3D plant model

The hierarchy of the DEXPI *XML* schema is similar to the *PlantDesign* transfer file, but there are some deviations which has been derived from the structure of the 3D model. Due to the higher degree of detail regarding constructions in comparison to P&IDs, the 3D *XML* schema has additional levels of hierarchy to represent site specific information as well as equipment sections and subsections. Especially in complex apparatus like distillation columns, equipment sections and subsections are important. Different internals in the rectifying or stripping section (type, size, material) or different types of collector-distributor systems (depending on the liquid and vapor loads) are only some examples which show the need for a more detailed hierarchy. Furthermore, internal piping information can be integrated within the equipment level. The DEXPI schema also has nested «equipment» hierarchy levels (instead of the equipment section and subsections), but with identical *XML* tag names. Nevertheless, an explicit mapping of attributes is possible since the number of nested levels is counted and stored in the *XML* file. The simplified equipment level hierarchies of the extended 3D *XML* schema (3D_PlantDesign_v0.8.xsd) and the DEXPI *XML* schema for P&ID's (XMpLantPIDProfileSchema_4.0.1.xsd) are shown in figure 4.6.

The attribute structure at the lower levels of both schemata is nearly identical. Both schemata contain «Name», «Value», «DefaultValue», «Units» and «Format» to describe the attributes. The only difference is the additional «Origin» statement within the 3D *XML* structure. It is used to store the origin or source of the data to improve the traceability of the decision-making process. Furthermore, Unified Resource Identifiers (URIs) for the Attributes, Values, and Units («AttributeURI», «ValueURI», «UnitsURI») are given, which refer to standardized definitions of plant objects stored in Reference Data Libraries (RDL), e.g. the POSC Caesar RDL [POSC Caesar Association, 2019]. An important requirement for data exchange in process industry is the extension of standardized object definitions in sufficient detail within the RDLs.

4.3.5 Possible extensions of *XML* structure

The prototypical 2D-3D data exchange framework focuses on the exchange of equipment information. Beside this, the DEXPI P&ID schema also includes other hierarchy levels to store further information. Following possible extensions of the *XML* structure for 3D models with respect to these levels are evaluated. However, no implementation has been done within the scope of this work.

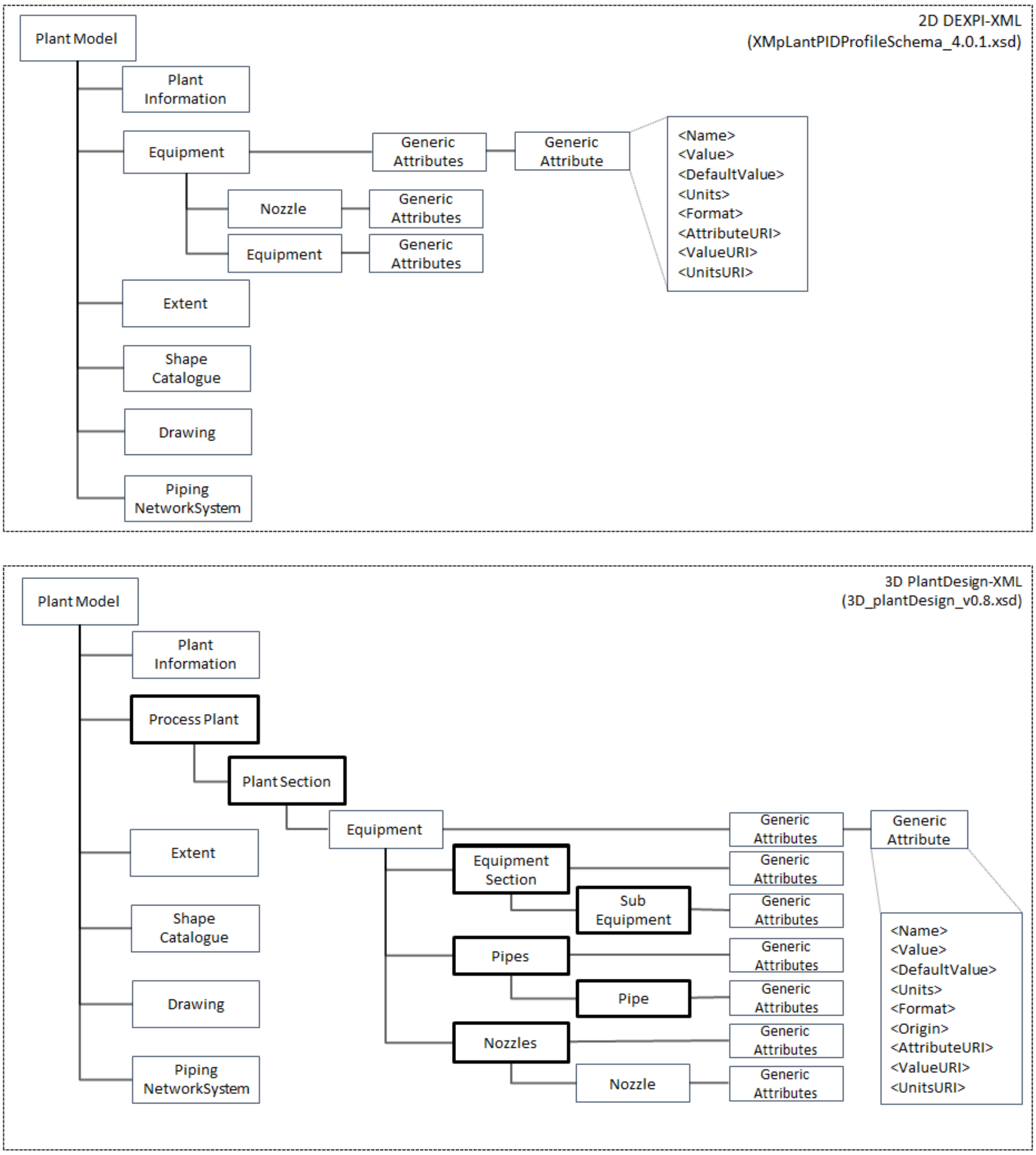


Figure 4.6: Comparison of *XML* structure between DEXPI data exchange format (XMpLantPIDProfileSchema_4.0.1.xsd) for P&IDs (upper box) and (3D_plantDesign_v0.8.xsd) *PlantDesign XML* structure for 3D models (lower box) [Fillinger, Bonart, et al., 2017]

The breakdown of the structure of the «PlantInformation» and «Extent» hierarchy levels of the DEXPI schema are shown in figure 4.7. All information related to the «PlantInformation» level are available in the 2D P&ID as well as in the 3D plant model. The level elements marked with a star (∗) even contain the same information in both models. The «Extent» section in the schema contains information about the sizing of the 2D model. With respect to 3D models this information is related to the minimal and maximal spatial dimensions of the 3D model and the third space coordinate Z has to be specified for 3D models ($Z \neq 0$). The meaning of the extent information varies due to the different geometrical information given in the two CAD models.

Figure 4.8 illustrates the information levels «ShapeCatalogue» and «Drawings». The «ShapeCatalogue» level contains information about the graphical representation of equipment and piping components for P&ID symbols. It should be also possible to define 3D models, but the current structure is not able to handle the description of 3D geometries. The «Drawings» level contains information about the 2D drawing, e.g. the label, title, size and the orientation. An extension to handle 3D information is possible, but instead of a drawing information the dimension and coordinate information of the 3D model have to be stored.

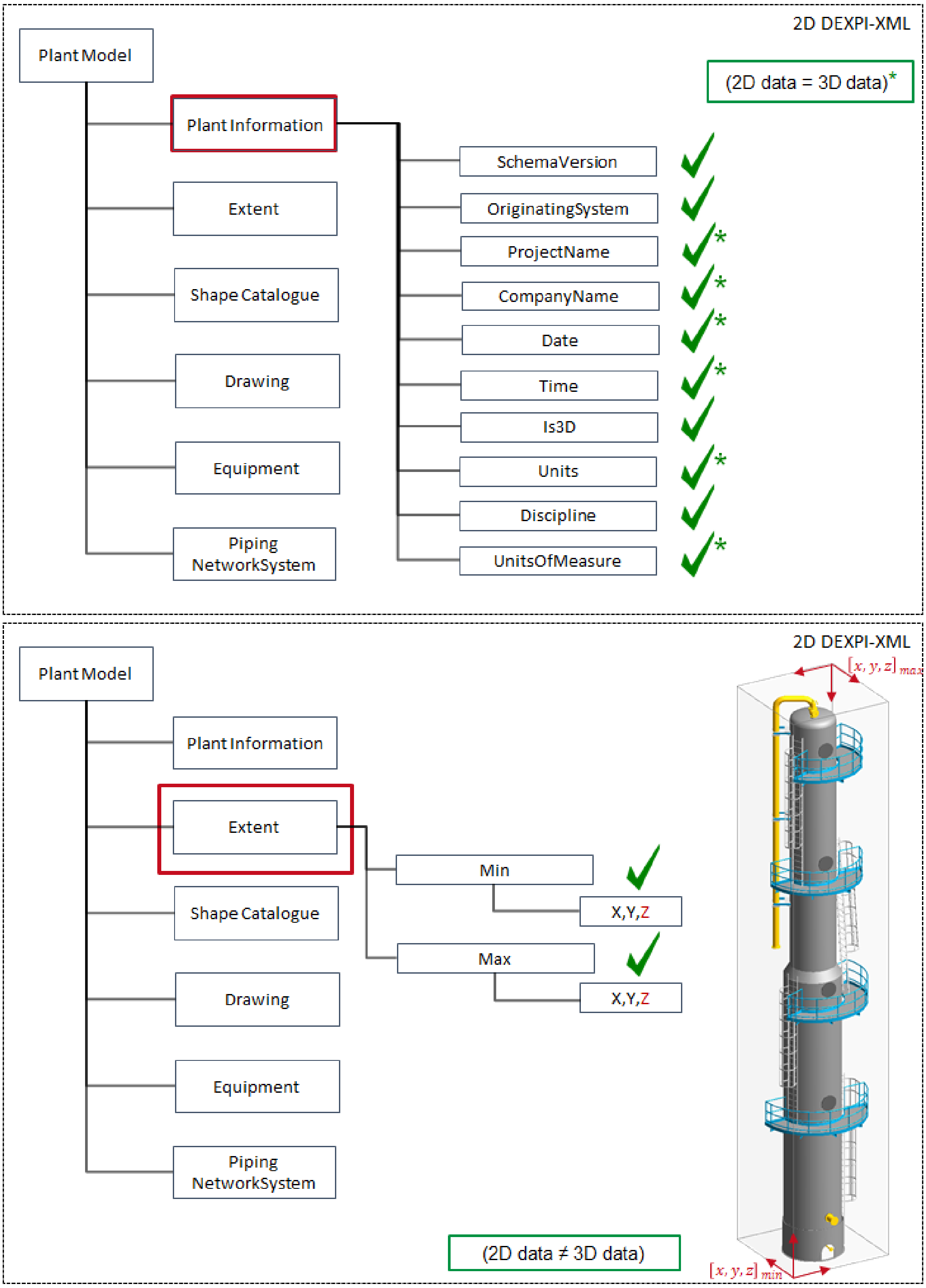


Figure 4.7: Applicability and extensibility of 3D *PlantDesign-XML* schema with respect to 2D DEXPI-*XML* schema - «PlantSection» and «Extent» levels

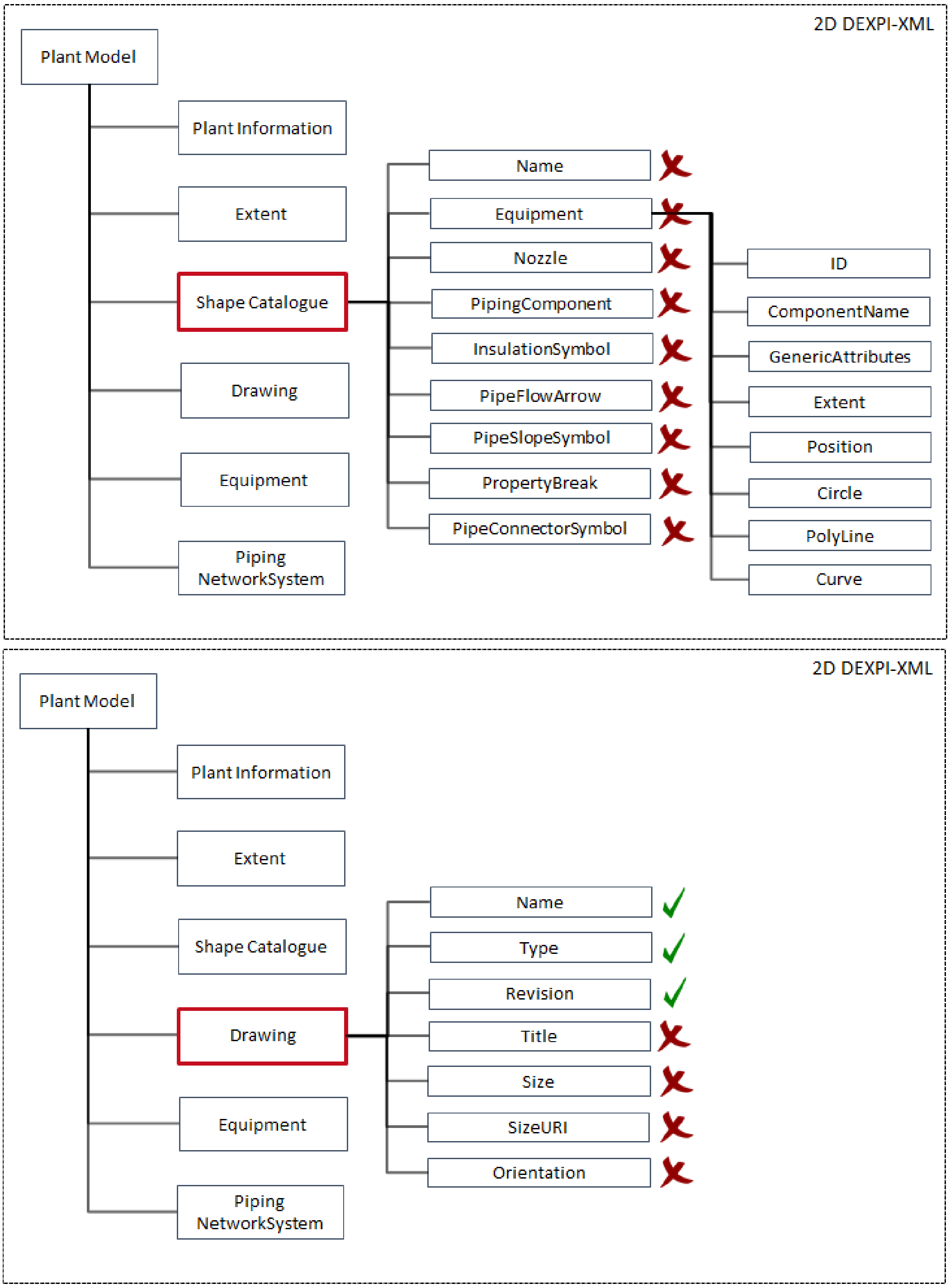


Figure 4.8: Applicability and extensibility of 3D *PlantDesign-XML* schema with respect to 2D DEXPI-*XML* schema - «ShapeCatalogue» and «Drawing» levels

4.3.6 Conclusions and evaluation of the 2D-3D data exchange framework

The interoperability between software tools strongly depends on their communication capabilities. Providing standardized data exchange formats as well as the implementation, provision and maintenance of corresponding data interfaces from CAE vendors is the prerequisite for acceptance, wide applicability and practicability in the industrial praxis. The different stakeholders in process industries are faced with various challenges – different applied standards, technical recommendations or company guidelines for plant design, various requirements and application perspectives of plants to special points in time, standardized descriptions of plant objects as well as uniform data exchange formats and interfaces - to mention only a few.
The presented 2D-3D data exchange framework is a first successful step for the data exchange between heterogeneous CAD software tools of different eco systems. The prototype includes the exchange between the P&ID software X-Visual PlantEngineer, MOSAICmodeling *PlantDesign* as intermediate software tool for the generation of detailed 3D plant models and the 3D CAD tool AVEVA PDMS™/E3D™.

The approach includes currently the transfer of equipment data. The framework has been successfully tested for industrial scale distillation columns, whereby the characteristic attribution has been developed within the framework of this work.

In order to enable a full data exchange between 2D and 3D CAD environments, some enhancements are still pending. Of particular importance is the extension of the exchange of information on pipelines, instrumentation and piping components. Furthermore, the portfolio of process units must be expanded, since the prototype investigation only considers columns with a comparatively high degree of complexity. An important prerequisite for the efficient data exchange of equipment and piping information is that the information can be clearly integrated into and interpreted by the respective target system. This requires fundamentally similar functionalities and, in the case of piping, an extensive database of pipe classes in the tools. For example, the exchange of 3D models within the same software is only possible if the pipe classes used in the source system are also stored in the database of the target system. However, this prerequisite is often not guaranteed. In the context of a master thesis, which was supervised in cooperation with the company UNISON Engineering [UNISON Engineering, 2019], the automated creation of project piping class databases was investigated [Schoele, 2017].

A successful prototype implementation for AVEVA PDMS™ was carried out, which is now used and extended in the company. The feasibility of the automated creation offers the potential for a simultaneous transfer of the required or missing pipe class information with the exchange of 3D plant information.

However, the approach would have to be developed in such a way that the information can be exchanged between different tools. In the case of equipment information, besides the geometric creation of the components, only the creation of the plant hierarchy must be possible.

Furthermore, it is highly desired to extend the 2D-3D data exchange framework regarding further trades, e.g. civil, automation or electrical engineering. To achieve that, the suitability of a centralized data model approach for the storage and exchange of plant and process information of the whole life-cycle should be investigated. This possible approach for the creation of a multidisciplinary data exchange framework is briefly discussed in the following section.

4.4 Concept of central data models for chemical plants

Achieving a consistent multidisciplinary data exchange for the life cycle of plants is a major challenge for the process industry. Requirements are the platform independence of the formats, scalability and extensibility regarding size and structure, possibilities to reliably track changes to ensure life cycle capabilities as well as inherent data consistency, i.e., no two datasets should have the possibility to be actively contradicting [Kim et al., 2016]. Various groups are working on different solutions to improve data exchange in individual disciplines, but a holistic approach is still lacking.
A possible starting point for this is a data centering and a draft of a central, standardized data model for the storage and exchange of process data as well as the provision of manufacturer-neutral interfaces for the import and export of information. A common hierarchy structure for all tools has to be designed in order to structure the affiliation of data and models to specific sections in the process. In order to achieve continuous data consistency, the software must signalize any data changes that occur during the planning process and transfer them to the other tools as a revision request. Thus, the first requirements for the design of complete, intelligent plant models and the linking of real plants with virtual plants have been created.

To allow for communication between more than two different tools from different disciplines or domains, there are various strategies to align the multitude of data formats or to define interchange formats in between. The presented approach is a first starting point for improving multidisciplinary data exchange – an extension to other disciplines and data sources used in the industrial environment is inevitable.

The consideration of a few disciplines initially enables the development of methods, which can then be used for further investigations. Figure 4.9 depicts three fundamentally different approaches to the alignment of the three types of data structures and domains. An overarching data format could be defined (figure 4.9 I.), which is able to handle all data required by all software from all domains. This can be considered as highly desirable, but at the same time as difficult to realize due to the large diversity of software and existing solutions out there for each domain and the various data not required to be exchanged between different tools. The opposite situation is shown on the right hand side (figure 4.9 III.), in which the data of all three domains remains completely separated. The data formats are aligned in such a manner that data exchange will be feasible by design, but this approach is unrealizable as shown in this previous section.
As an alternative to these two extremes, the solution in (figure 4.9 II.) would create an additional, central data specification, which serves as a handler between all three domains and holds the information necessary to facilitate the exchange (interchange data). From a standpoint of practicality, this might be the only feasible approach, given the complexity of the standardization processes in each domain. However, it comes at the cost of additional effort to derive such an interchange format and to determine which data to store therein.

A concept of a central data model for the multidisciplinary data exchange in process industries has been derived based on the investigations and implementations within this work. Parts of this concept are elaborated in cooperation with the Technical Research Centre of Finland VTT [VTT, 2019], which are members of the DEXPI initiative. Furthermore, a feasibility study with resepect to interoperability in plant design funded by the Transfer BONUS program [IBB, 2019] has been initiated in cooperation with X-Visual Technologies, but the execution has not been part of this work. The investigation has focused on the exchange between process simulation, P&ID's as representative for the 2D CAD planning and 3D CAD models based on a central data model approach.

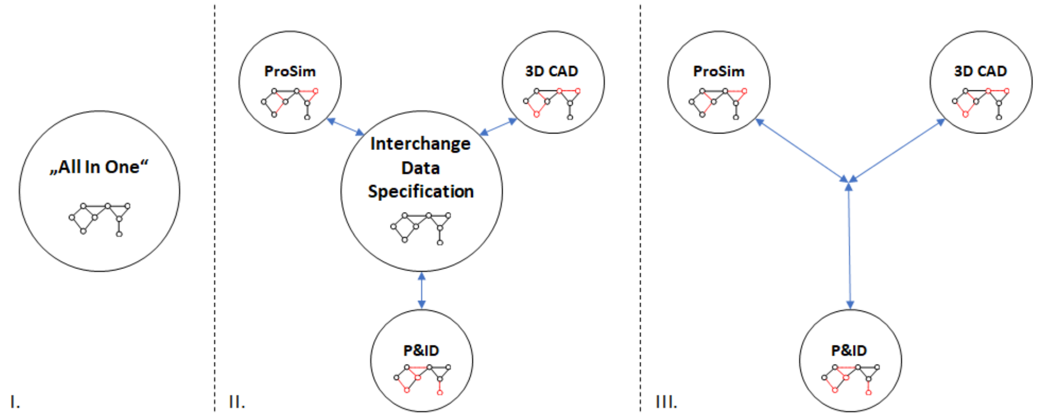


Figure 4.9: Different options to align data models from different disciplines, exemplary for P&ID, 3D CAD, and process simulation. Option I. refers to an overarching data format for all disciplines, option II. shows a central data specification to handle different formats of different disciplines and in option III. data models of all domains are perfectly aligned and data can be stored independently. The small figure in each data model (represented by the bubble) is a graph-like representative of the parts of the topology stored within (black: stored; red: not stored)

Figure 4.10 depicts the central data model approach. Central point is the inner core of the graphic called the «*OPEN Database*» (Open Process ENgineering), which is representative for the central data exchange model for process industries. Within this central data model common data to characterize process plants as well as a collection of corresponding «bridging» mappings are specified. The specifications have to be developed together with experts from the different trades or disciplines (e.g. process simulation, 2D and 3D planning, automation or electrical engineering), which are schematically illustrated by the grey circles. The extensibility by a flexible connection of further disciplines (represented by the circle with «...») is an important prerequisite of the concept.

The blue and red circle segments represent data interfaces - the blue one illustrates an existing, appropriate standardized data interface or data format, the red one characterizes disciplines where currently no appropriate standard is available. In case of the red circle segments an investigation of existing standards and an extension to fulfil the requirements should be conducted.

A similar procedure has been performed during the development of the prototypical 2D-3D data exchange framework. The DEXPI exchange standard for P&ID's has been extended to been able to handle also 3D plant model information.

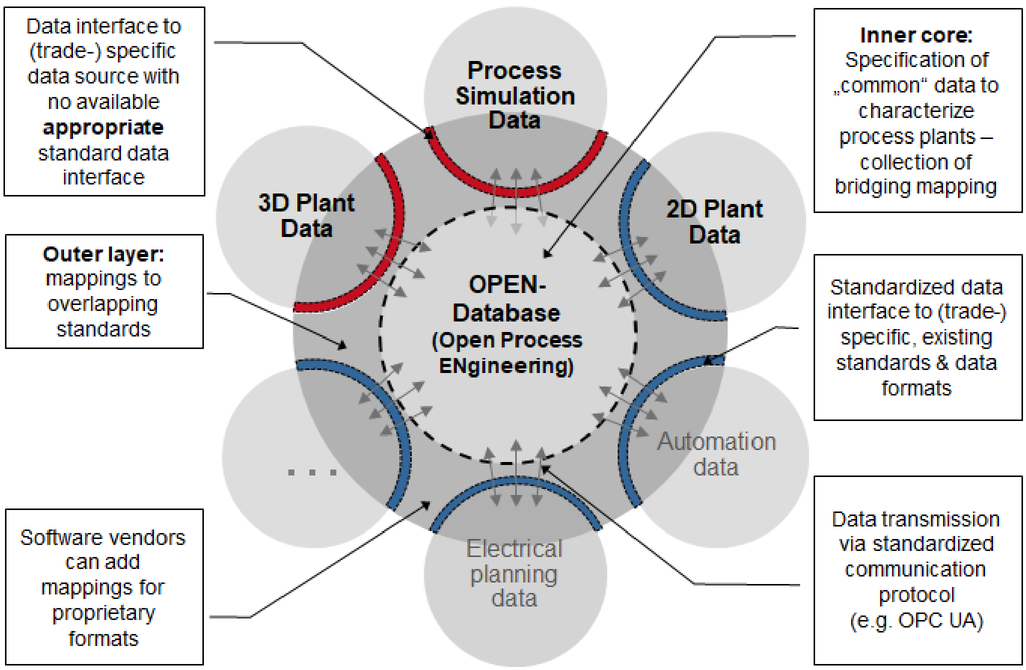


Figure 4.10: Concept of central data model for the multidisciplinary data exchange in process industries

The exchange of geometric information can be performed with existing standards like STEP. As shown within this work this procedure is generally feasible, but the extension of an standard couldn't be performed within an academic investigation since a committee for standardization (e.g. the European Committee for Standardization CEN) is required.
The outer layer of the *OPEN Database* illustrates the mapping to overlapping standards, which can also include mappings for vendor-specific proprietary formats. This procedure enables a significant reduction of effort with respect to maintaining data interfaces. The data transmission, represented by the grey bi-directorial arrows between the discipline-specific data interface and the *OPEN database*, should be performed using a standardized communication protocol e.g. OPC UA (Open Platform Communications Unified Architecture).

5 Summary & outlook

5.1 Summary

Ensuring the economic success of chemical, pharmaceutical and petrochemical companies is associated with various challenges and requires a flexible adaptation of corporate strategies to the current global economic situation. In this thesis, a combined approach for more efficient plant design in the process industry is developed and the prototypical integrated engineering tool *PlantDesign* is successfully implemented within the MOSAICmodeling environment.

The developed approach is divided into two parts. On the one hand, a flexibly adaptable modular concept for the automatic creation of the detailed constructive design of process units is implemented, which combines an enormous time saving for planning as well as the reuse and knowledge storage of proven engineering knowledge. The decision-making process regarding different constructive alternatives and arrangements of components based on best-practice engineering solutions is supported by the assistant system.
The design of the MPUs is individually adaptable to the process data, operating conditions, material selection and constructive design requirements and heuristic rules. This is especially beneficial as support for engineers with limited practical experience in order to obtain best-practice engineering solutions. Also, the documentation of reasons that lead to the choice of an constructive design should allow for comprehension and reproduction of the decision-making process at any time of the life cycle of plants. An integration of this approach into the classical engineering workflow is possible, as shown within the presented case studies. The higher level of detail of the construction leads to various advantages during the planning, for example within the safety analysis as well as during the operation phase, for example for maintenance tasks, turnarounds or plant refits. The enhancement of transparency in plant design due to the documentation of the decision-making process of the plant design and a centralized storage of the data models enables an efficient workflow and the continuity of data transfer during planning and throughout the life cycle of the plant is improved.

Despite of the flexible modeling options, the modular approach enables less possibilities than the classical one, where typically tailored solutions are developed. The implementation of modular concepts in the manufacturing industry is easier to implement and therefore much more widespread. However, the thriving implementation in *PlantDesign* also shows the potential for improvement in the process industry, where much higher demands are placed on flexibility and tailored adaptation of the design.

On the other hand, the developed approach enables cross-discipline interoperability by developing and providing various data exchange interfaces to different CAE tools applied in plant design. The goal of the fourth industrial revolution is, among other things, the digitalization of industrial processes and the associated utilization of available data during the process life cycle. A major obstacle here at the present time is the heterogeneity of tools and data formats in industrial use. Currently, there are no exchange formats to link the above mentioned tools with each other and to achieve a comprehensive virtual representation of process plants.
In this work, the interoperability between different CAE software tools has been investigated and the prototypical integrated engineering tool *PlantDesign* has been successfully implemented. The tool enables a linking of tools from the early beginning of planning to the detailed engineering. The resulting 3D models created with this tool represent the as-built-status of modular process units and can be used during the further life cycle of the plant. The data interfaces to software for process simulation, 2D planning and 3D CAD tools reduce the error susceptibility of the previously manual data transmission, accelerate the engineering phase and increase the overall safety of plant operation through consistent digitalization. The presented 3D data model developed for the heterogeneous data exchange between 2D and 3D CAD tools bases on the data exchange format for the homogeneous exchange between P&ID tools provided by the DEXPI initiative. Extension and harmonization of existing data exchange standards drom different trades and disciplines provides a promising opportunity to achieve a higher-level, cross-discipline data exchange framework for the entire life cycle of process plants.

This approach has a strong focus on the process engineering point of view on the planning procedure and the investigations and prototypical implementations are realized from an academic perspective. In practice, the various existing software implementations and legacy formats further constraint compromises on standardized data exchange formats. In addition, the size and scope of the overall data exchange problem cannot be addressed in such a scientific investigation alone – the technical expertise, practical example data from large-scale chemical plants, and knowledge of the needs of industrial partners is essential for finding a practical solution.

Also, in cooperation with an industrial consortium, it is to be expected that there are strong differences in the existing solutions of the companies, e.g. different company-internal guidelines, country-specific standards, and in-house software developments. Consequently, a defined consensus can only be achieved with corresponding effort on all sides. The implementation of the approaches in commercial tools by software vendors is also complex and an implementation does not always go hand in hand with the vendor-specific developments and business concepts. Nevertheless, the challenge of this topic should be faced and it should be strived for first solutions for a harmonization of the different needs and conceptions.

5.2 Outlook

An extension of the PlantDesign approach with regard to the implementation of further constructive design options for the existing MPUs as well as the design of further frequently used process units is desirable in order to enable a more extensive and flexible usability of the presented concept. A more intensive use and integration into the classical plant planning increases the efficiency and the potential for savings. In particular, the extension of the code generator framework by additional target programming languages enables a broader applicability to new CAD environments. The extension by standardized formats would be the most suitable and preferred choice to maximize the usability with the most resource-saving effort for the creation and maintenance of the method library.
In addition, the automated documentation of plant and process information should be enabled, since the documentation is the prerequisite for every single step during the whole plant life cycle and the potential for savings is enormous.

Improving the interoperability between software tools and the permeability between software and process data is of great importance for the digitalization in process industries. This leads to an acceleration of the design and planning process for plants and makes them more sustainable and more cost-effective. For this reason, future research of the Process Dynamics and Operation Group at TU Berlin is dedicated to the development of platform-independent, standardized plant life cycle data management and data exchange platform between different domains and disciplines within process industries. Thereby, the focus is on harmonizing existing standards which are already established in the domains as well as the consistent change management in a multidisciplinary heterogeneous software framework.

The existence of structured and in particular linked plant information of all departments and trades in a digital form has not yet been achieved in industrial practice. A stronger use of modern methods and approaches such as artificial intelligence offers the possibility to map and use a combination of facts, the interpretation of data by an assignment of meaning and a rule-based conclusion. The utilization and reuse of engineering knowledge for design processes offers not only enormous savings potentials, but also an opportunity to safeguard expert knowledge. The high complexity of plants and processes in an industrial environment poses a great challenge and requires profound interdisciplinary knowledge in the areas of process technology as well as information and software technology.

5.3 Publications

Table 5.1: Publication list

Authors	Title, Journal, Year
S. Fillinger, B. Seyfang, G. Wozny and J.-U. Repke	*PlantDesign - prototypical implementation of an integrated engineering tool*, Computers & Chemical Engineering, submitted 01/2020
S. Fillinger, E. Esche, G. Tolksdorf, W. Welscher, G. Wozny and J.-U. Repke	*Data Exchange for Process Engineering - Challenges and Opportunities*, Chemie Ingenieur Technik, DOI:10.1002/cite.201800122, **01/2019**
S. Fillinger, H. Bonart, W. Welscher, E. Esche and J.-U. Repke	*Improving Interoperability of Engineering Tools - Data Exchange in Plant Design*, Chemie Ingenieur Technik, DOI:10.1002/cite.201700032, **10/2017**
S. Fillinger, J. Talaga, M. Dyląg, G.Wozny and J.-U. Repke	*Automatic Equipment Design for Modular Process Units*, Chemical Engineering and Equipment, **10/2017**
S. Fillinger, G. Tolksdorf, H. Bonart, E. Esche, G. Wozny and J.-U. Repke	*Linking Process Simulation and Automatic 3D Design for Chemical Plants*, Symposium on Computer Aided Process Engineering - ESCAPE 27, Barcelona, Spain, DOI:10.1016/B978-0-444-63965-3.50387-1, **10/2017**
H. Bonart, S. Fillinger, E. Esche, G. Wozny and J.-U. Repke	*Source Code Generation for Parallelized Simulations of Large-Scale Nonlinear Equation Systems on a Supercomputer using MOSAIC, PETSc, and ADOL-C*, Symposium on Computer Aided Process Engineering - ESCAPE 27, Barcelona, Spain, DOI:10.1016/B978-0-444-63965-3.50349-4, **10/2017**

Continuation table 5.1 of previous page

Authors	**Title, Journal, Year**
E. Esche, G. Tolksdorf, S. Fillinger, H. Bonart, E. Esche, G. Wozny and J.-U. Repke	*Support of Education in Process Simulation and Optimization via Language Independent Modeling and Versatile Code Generation*, Symposium on Computer Aided Process Engineering - ESCAPE 27, Barcelona, Spain, DOI:10.1016/B978-0-444-63965-3.50490-6, **10/2017**
E. Esche, C. Hoffmann, M. Illner, D. Mueller, S. Fillinger, G. Tolksdorf, H. Bonart, G. Wozny, and J.-U. Repke	*MOSAIC - Enabling Large-Scale Equation-Based Flow Sheet Optimization*, Chemie Ingenieur Technik, DOI:10.1002/cite.201600114, **04/2017**
V.A. Merchan, E. Esche, S. Fillinger, G. Tolksdorf and G. Wozny	*Computer-Aided Process and Plant Development. A Review of Common Software Tools and Methods and Comparison against an Integrated Collaborative Approach*, Chemie Ingenieur Technik, DOI:10.1002/cite.201500099, **12/2015**
M. Fedorova, G. Tolksdorf, S. Fillinger, G. Wozny, M. Sales-Cruz, G. Sin and R. Gani	*Development of Computer Aided Modelling Templates for Re-use in Chemical and Biochemical Process and Prodict Design: Import and export of models*, Symposium on Computer Aided Process Engineering - ESCAPE 25, Copenhagen, Denmark, DOI:10.1016/B978-0-444-63577-8.50004-8, **06/2017**
G. Tolksdorf, S. Fillinger, G. Wozny, F. Manenti, F. Rossi, G. Buzzi-Ferraris, Sauro Pierucci, M. Fedorova and R. Gani	*A Posteriori Integration of University CAPE Software*, Chemical Engineering Transactions, DOI:10.3303/CET1543225, **05/2015**

Continuation table 5.1 of previous page

Authors	**Title, Journal, Year**
R. Kraus, S. Fillinger, G. Tolksdorf, Duc H. Minh, Victor A. Merchan-Restrepo and G. Wozny	*Improving Model and Data Integration Using MOSAIC as Central Data Management Platform*, Chemie Ingenieur Technik, DOI:10.1002/cite.201400007, **06/2014**

5.4 Presentations

Table 5.2: Presentation list

Authors	Title, Conference/meeting, Year
S. Fillinger, G. Wozny and J.-U. Repke	*Software-Interoperabilität in der Anlagenplanung - Pototyp eines Engineering Tools zur Apparateauslegung*, Jahrestreffen der Fachgemeinschaft Prozess-, Apparate- und Anlagentechnik, Würzburg, Germany, **11/2017**
S. Fillinger, G. Tolksdorf, H. Bonart, E. Esche, G. Wozny and J.-U. Repke	*Linking Process Simulation and Automatic 3D Design for Chemical Plants*, Symposium on Computer Aided Process Engineering - ESCAPE 27 Barcelona, Spain, **10/2017**
S. Fillinger, J. Nowotnick, W. Welscher, G. Wozny and J.-U. Repke	*2D-3D Exchange Framework*, DEXPI Meeting, Frankfurt a.M., Germany, **12/2016**
S. Fillinger, J. Nowotnick, E. Esche, W. Welscher, G. Wozny and J.-U. Repke	*Automatisierte 3D-Modellierung und standardisierter Datenaustausch in der Anlagenplanung*, Jahrestreffen der Fachgemeinschaft Prozess-, Apparate- und Anlagentechnik, Karlsruhe, Germany, **11/2016**
S. Fillinger, G. Tolksdorf, E.Esche and G. Wozny	*Automatisierte 3D-Visualisierung und standardisierter Datenaustausch in der Anlagenplanung*, Jahrestreffen der Fachgemeinschaft Prozess-, Apparate- und Anlagentechnik, Bruchsal, Germany, **11/2015**
S.Fillinger and G.Wozny	*Prozesssimulation und automatisierte 3D-Visualisierung in MOSAIC*, BASF, Schwarzheide, Germany, **08/2015**
S.Fillinger, G.Wozny	*Modulare Anlagen in der Prozesstechnik*, Temporärer Arbeitskreis Modulare Anlagen, Frankfurt a.M., Germany, **04/2015**

Continuation table 5.2 of previous page

Authors	**Title, Conference/meeting, Year**
S. Fillinger and G. Wozny	*Prozesssimulation und 3D-Visualisierung in der Modellierungsumgebung MOSAIC*, Jahrestreffen der Fachgemeinschaft Prozess-, Apparate- und Anlagentechnik, Lueneburg, Germany, **11/2014**
S. Fillinger, G. Tolksdorf and G. Wozny	*Austausch von Modellen in der Prozesssimulation unter Verwendung standardisierter Schnittstellen*, ProcessNet AA Modellgestützte Prozessentwicklung und -optimierung, Hanau, Germany, **05/2014**

5.5 Supervised Masters & Bachelor Thesis

Table 5.3: Supervised Masters & Bachelor Thesis

Name	**Title, Thesis, Year**
S. Weidemann	*Smart Dow - Evaluierung und Pilotierung von Industrie 4.0 Lösungsansätzen von Engineering bis zur digitalen Baustelle*, Masters Thesis in cooperation with Dow Olefinverbund GmbH, **02/2018**
H. Richter	*Inbetriebnahme einer Vakuumrektifikationskolonne*, Masters Thesis, **08/2017**
A. Brodowska	*Automatisiertes Apparatedesign fuer Rektifikationskolonnen*, Masters Thesis, **05/2017**
L. Schoele	*Generische Erstellung von Projektdatenbanken für 3D-Rohrleitungskomponenten*, Masters Thesis in cooperation with UNISON Engineering GmbH, **04/2017**
J. Nowotnick	*Entwicklung eines Datenaustausch-Frameworks für 2D-3D-Anlagenmodelle*, Masters Thesis in cooperation with X-Visual Technologies GmbH, **03/2017**
S. Bublitz	*Konvergenzanalyse eines Nichtgleichgewichtsmodells für Rektifikationsprozesse*, Masters Thesis, **11/2016**
K. Koczy	*Design and automated generation of three-dimensional models of rectification tray columns*, Masters Thesis in cooperation with Technical University of Cracow, **08/2016**
S. M. Menschikowski	*Modellierung von Rektifikationsprozessen unter Verwendung von MOSAIC*, Bachelor Thesis, **04/2016**
M. Jurga	*Design and automated generation of three-dimensional models of process units*, Masters Thesis in cooperation with Technical University of Cracow, **12/2015**
H. Bonart	*Source code generation for parallelized simulations of a dynamic non-equilibrium separation unit using MOSAIC*, Masters Thesis, **11/2015**

Continuation table 5.3 of previous page

Name	**Title, Thesis, Year**
B. Behl	*Stationäre Modellierung des Ethenkältekreislaufs eines Steamcrackers zur Entwicklung von Verbesserungstrategien der Betriebsfahrweise der Ethen/Ethan-Trennkolonne*, Masters Thesis in cooperation with LyondellBasell Industries Basell Polyolefine GmbH, **08/2015**
D. Orlando	*Modeling, simulation,and optimization of a cruide oil distillation unit*, Masters Thesis in cooperation with Politecnico di Milano, **06/2015**
P. Schulz	*Aufbau einer Vakuumdestillationsanlage - Neuaufbau nach Umbauarbeiten*, Bachelor Thesis, **03/2015**
M. Gracjas	*Design and automated generation of three-dimensional models of rectification packed columns*, Masters Thesis in cooperation with Technical University of Cracow, **09/2014**
D. Seidl	*Dynamische Simulation und Validierung einer Vakuumrektifikation mit Seitenentnahme*, Bachelor Thesis, **04/2014**
A. Borowiec	*Design and automated generation of three-dimensional models of process units*, Masters Thesis in cooperation with Technical University of Cracow

A Appendix

A.1 CAPE- and CAE-software in basic and detailed engineering

A.1.1 Process simulation tools

Table A.1: Overview of frequently used process simulation & optimization environments in process industries (incomplete)

Software	Application	Remarks	Vendor
Aspen Plus (Dynamics)	SS, DS, O, FS	ACM for user-specific modeling	Aspentech Aspen Plus, 2019
Aspen HYSIS (Dynamics)	SS, DS, EO	Hydrocarbon processes	Aspentech, 2019
Chemasim	SS, DS, EO	In-house tool	BASF AG, 2019
Chemcad (CC-Dynamics)	SS, DS, O, FS		Chemstations, 2019
DYNSIM	DS, FS	Operator training	AVEVA, 2019c
gPROMS	SS, DS, O, EOF		Process System Enterprise gPROMS, 2019
Matlab	SS, DS, O, EO		Mathworks Matlab, 2019
MOSAICmodeling	SS, DS, O, EO	In-house web application TU Berlin	MOSAICmodeling, 2019
PRO/II	SS, FS	Hydrocarbon processes	AVEVA, 2019d

Continuation table A.1 of previous page

Software	Application	Remarks	Vendor
ProSimPlus (Batch Column)	SS, DS, FS	Dynamic batch processes	ProSim, 2019
ROMeo	EO, O	Hydrocarbon processes	AVEVA, 2019d
SimCentral	SS, DS, EOS		AVEVA, 2019e
Unisim	SS, DS, FS		Honeywell Unisim, 2019
VT Plan	SS, DS, EO	In-house tool	Bayer AG, 2019

SS: Steady-state process simulation
DS: Dynamic process simulation
O: Process optimization

EO: Equation-oriented approach
FS: Flowsheeting environment (no access to equation models)
EOF: Equation-oriented flowsheeting environment

A.1.2 CAD tools

Table A.2: Overview of frequently used of 2D and 3D CAD environments in process industries (incomplete)

Software	Application	Vendor
AutoCAD	2D, 3D	Autodesk, 2019a
Autodesk® Fusion 360/Inventor	3D	Autodesk, 2019b
AutoPlant Modeler	3D	Bentley, 2019
AVEVA P&ID	3D	AVEVA Engineering Software, 2019
CADISON P&ID Designer	2D	ITandFactory GmbH, 2019b

Continuation table A.2 of previous page

Software	Application	Vendor
CADISON 3D Designer	3D	ITandFactory GmbH, 2019a
Hexagon Intergraph Smart 3D	3D	Hexagon, 2019
PDMS™/Everything3D™	3D	AVEVA Engineering Software, 2019
PlantEngineer	2D	X-Visual Technologies, 2019
Solid Edge	2D, 3D	Siemens, 2019b
SolidWorks	3D	Dassault Systèmes, 2019
Visio	2D	Microsoft, 2019
2D: 3D:	2D CAD environment 3D CAD environent	

A.2 Appartus design of process units

A.2.1 Fundamentals of calculation for constructive elements

Table A.3: Wall thickness calculation for cylinders under internal and external pressure [Klapp and Lambrecht, 1981]

Pressure	Diameter ratio	Calculation formula	Notes
$> 1atm$	$\frac{D_o}{D_i} < 1,2$	$s = \frac{D_o \cdot p}{2{,}0 \cdot \frac{K}{S} \cdot \nu + p} + c_1 + c_2 + c_3$	$\nu = 0,8 \ldots 1,0$
$> 1atm$	$1,2 < \frac{D_o}{D_i} \leq 1,5$	$s = \frac{D_o \cdot p}{2{,}3 \cdot \frac{K}{S} - p} + c_1 + c_2$	$S = 1,1$ for testing, $S = 1,5$ for operating pressure

Table A.4: Standards for the dimensioning of constructive components and the design of process units applied in PlantDesign

Plant components & process units	**Applied standards**
Column cylinders, support rings	DIN 28015, 1987
Torispherical and ellipsoidal heads	DIN 28011, 2012, DIN 28013, 2012
Flanges	DIN 28030-1, 2013, DIN 28031, 2013, DIN 28033, 2013, DIN 28034, 2013 DIN EN 1092-1, 2013
Nozzles	DIN 28025, 2003
Manholes	DIN 28124-1, 2010 DIN 28124-2, 2010 DIN 28124-3, 2013 DIN 28124-4, 2010
Skirt supports	28082-1, 2016
Tubular supports	DIN 28081-1, 2015
Bracket supports	DIN 28083, 2017
Torispherical heads	DIN 28011, 2012
Ellipsoidal heads	DIN 28013, 2012
Platforms and ladders	DIN 28017-1, 2014 DIN 28017-2, 2012 DIN 28017-3, 2012 DIN 28017-4, 2012
Insulations	DIN 4140, 2014 DIN EN 14303, 2016 DIN EN 14309, 2016 DIN EN 14313, 2016 DIN EN 14314, 2016
Material properties	DIN EN 10028-2, 2009 DIN EN 10028-3, 2009 DIN EN 10028-7, 2013 DIN EN 10216-1, 2014

Continuation table A.4 of previous page

Plant components & process units	**Applied standards**
	DIN EN 10216-2, 2014 DIN EN 10216-3, 2014 DIN EN 10216-4, 2014 DIN EN 10216-5, 2014
Distillation columns	DIN 28015, 1987 DIN 28016, 1987 DIN 28007-1, 2009 DIN 28007-2, 2017
Shell and tube heat exchangers	DIN 28183, 2007 DIN 28184-1, 2009 DIN 28184-1, 2010 DIN 28191, 2009 DIN 28179, 2007 DIN 28185, 2007 DIN 28008, 2010 DIN EN ISO 16812, 2007 DIN 2413, 2011 DIN 2510-5, 1971
Pumps	DIN 24250, 1984 DIN EN 733, 1995 DIN EN 2858, 2011 DIN 24259, 1979
Pressure vessels	DIN 28019, 2016 DIN 28020, 2007 DIN 28021, 2006 DIN 28022, 2006 DIN 28050, 2009 DIN 13445-3, 2018

A.2.2 Design of distillation columns

Variable list for the constructive design of distillation columns

Table A.5: User-specific variables for the constructive design of distillation columns - General apparatus information

Variable name	Description	Column*
!dRectSecColumn	Column diameter rectifying section [mm]	P,T
!dStripSecColumn	Column diameter stripping section [mm]	P,T
!feedStage	Separation stage with feed inlet [$-$]	P,T
!numberOfTrays	Theoretical number of separation stages [$-$]	P,T
!pressure	Maximum allowed operating pressure [bar]	P,T
!temperature	Maximum allowed operation temperature [°C]	P,T
!materialTypeColumn	Apparatus material [$-$]	P,T
!supportTypeColumn	Choice of supporting element of column [$-$]	P,T
!bottomHighLiquidLevel	Maximum liquid level in column bottom [mm]	P,T
!isRectColumn	Rectifying column [$-$]	P,T
!isStripColumn	Stripping column [$-$]	P,T
!minNumberOfTrays-Manholes	Minimum number of separation stages between two manholes	T
!processType	Vacuum, amospheric or pressure distillation [$-$]	
!FFactor	F-Factor representing the gas load [$\sqrt{Pa}$]	P
!feedInletDesign	Design option of the feed section [$-$]	P

Continuation table A.5 of previous page

Variable name	**Description**	**Column***
* P: Packed column,	T: Tray column	

Table A.6: User-specific variables for the constructive design of distillation columns - Internals, Manholes and Nozzles

Variable name	**Description**	**Column***
!hweir	Height of the weir [mm]	T
!isMistEliminatorRequired	Decision variable for demister [$-$]	P,T
!isBedLimiterViewDetailed	View option for detailed or simplified 3D view of bed limiter [$-$]	
!sizePacking	Size of selected packing [$-$]	P
!typePacking	Type of selected packing [$-$]	P
!hMaxRandomPacking-NoCrush	Maximum height of unstructured packing section, to prevent crushing [mm]	P
!hLayerStructuredPacking	Height of single structured packing section [mm]	P
!multiplierPackingHeight	Multiplier for calculation of packing height [$-$]	P
!hDistributor	Height of liquid distributor [mm]	P
!dManhole	Manhole diameter [mm]	P,T
!hNozzle	Length of nozzle [mm]	
!QExhaustVaporOut	Volumetric flow exhaust vapor outlet [$\frac{m^3}{s}$]	P,T
!QFeedIn	Volumetric flow feed inlet [$\frac{m^3}{s}$]	P,T
!QLiquidBottomOut	Volumetric flow bottom liquid outlet $\frac{m^3}{s}$]	P,T
!QRefluxIn	Volumetric flow reflux inlet [$\frac{m^3}{s}$]	P,T
!QVaporBottomIn	Volumetric flow vapor bottom inlet [$\frac{m^3}{s}$]	

Continuation table A.6 of previous page

Variable name	**Description**	**Column***
!velocityExhaustVaporOut	Velocity exhaust vapor outlet $[\frac{m}{s}]$	P,T
!velocityFeedIn	Velocity feed inlet $[\frac{m}{s}]$	P,T
!velocityLiquidBottomOut	Velocity bottom liquid outlet $[\frac{m}{s}]$	P,T
!velocityRefluxIn	Velocity reflux inlet $[\frac{m}{s}]$	P,T
!velocityVaporBottomIn	Velocity vapor bottom inlet $[\frac{m}{s}]$	P,T

* P: Packed column, T: Tray column

Computation algorithms for the constructive design of distillation columns

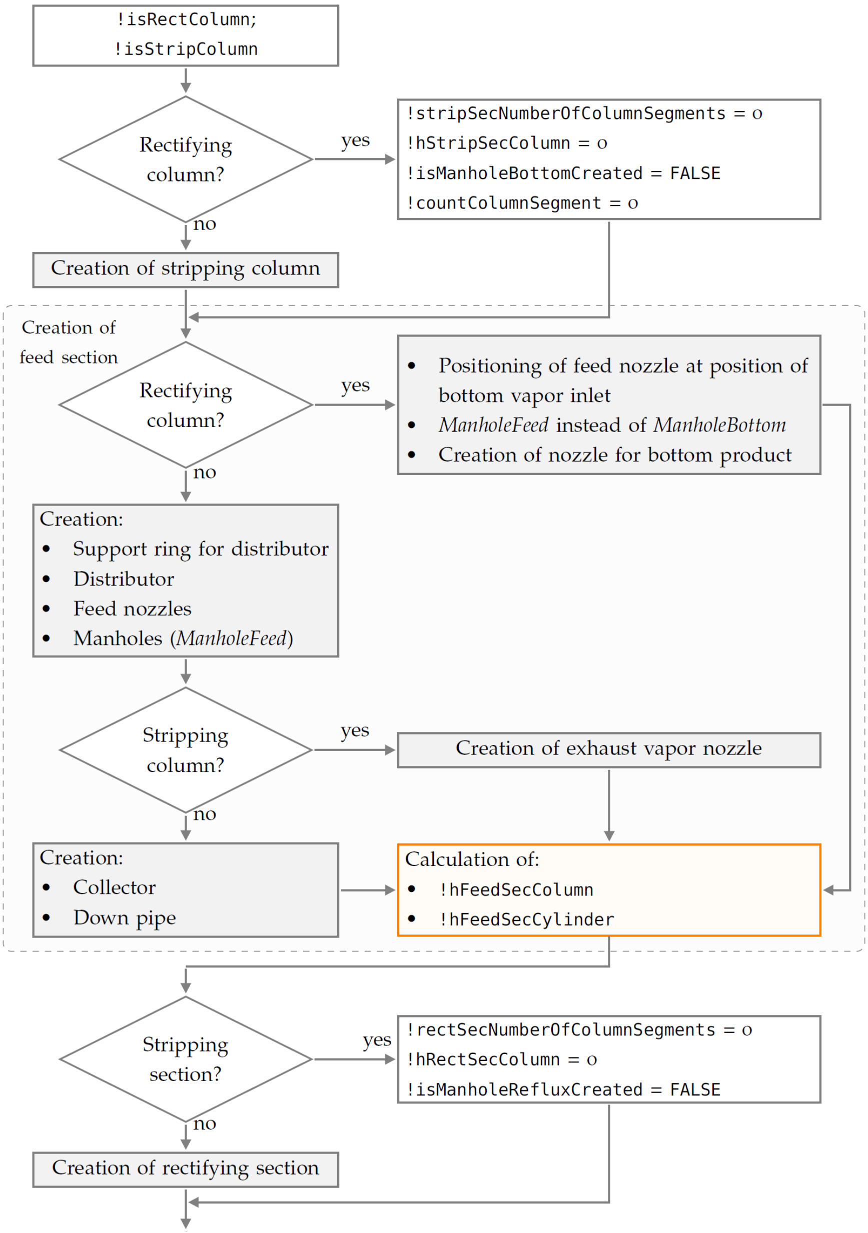


Figure A.1: Algorithm for overall design of internals for packed columns with different configurations

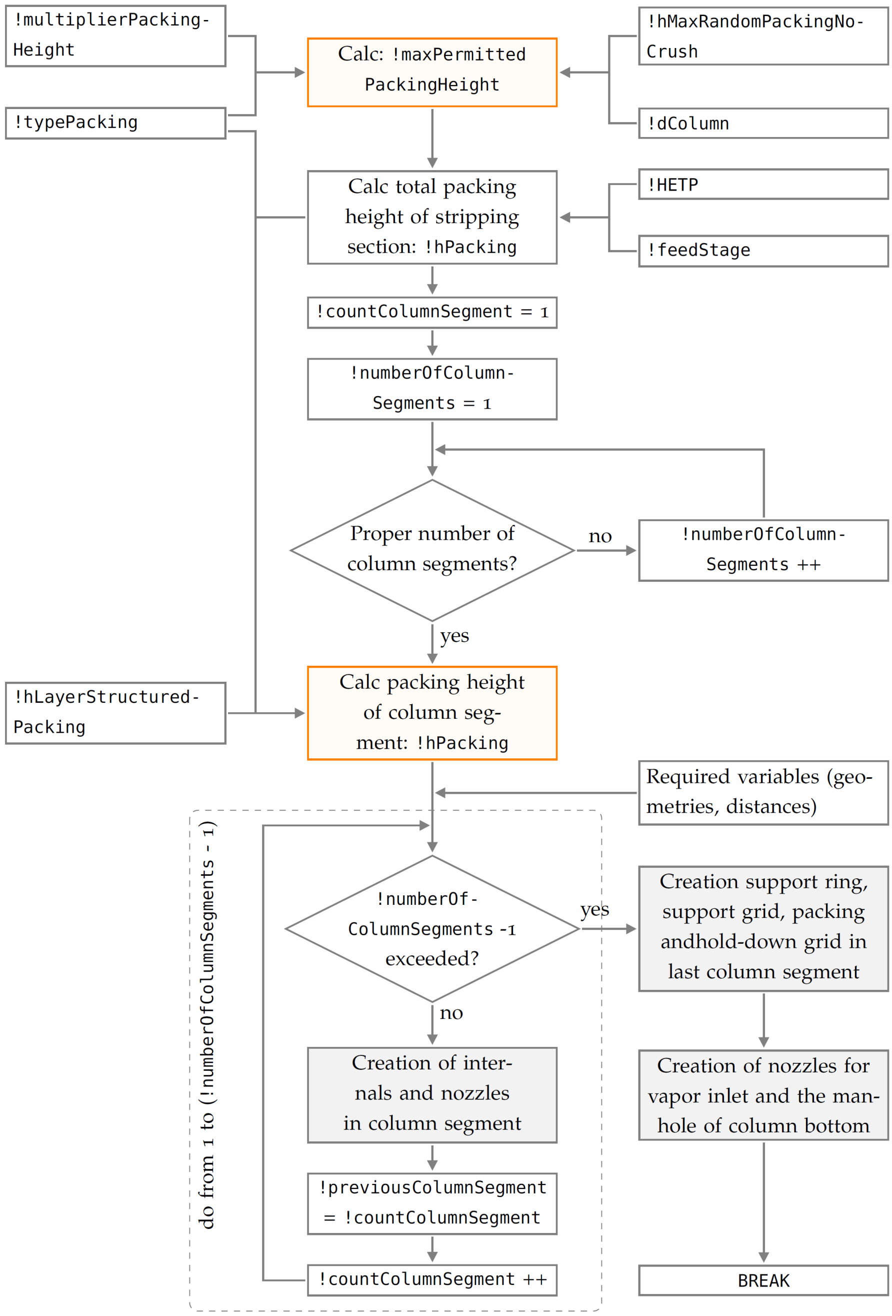


Figure A.2: Algorithm for constructive design of stripping section of packed columns

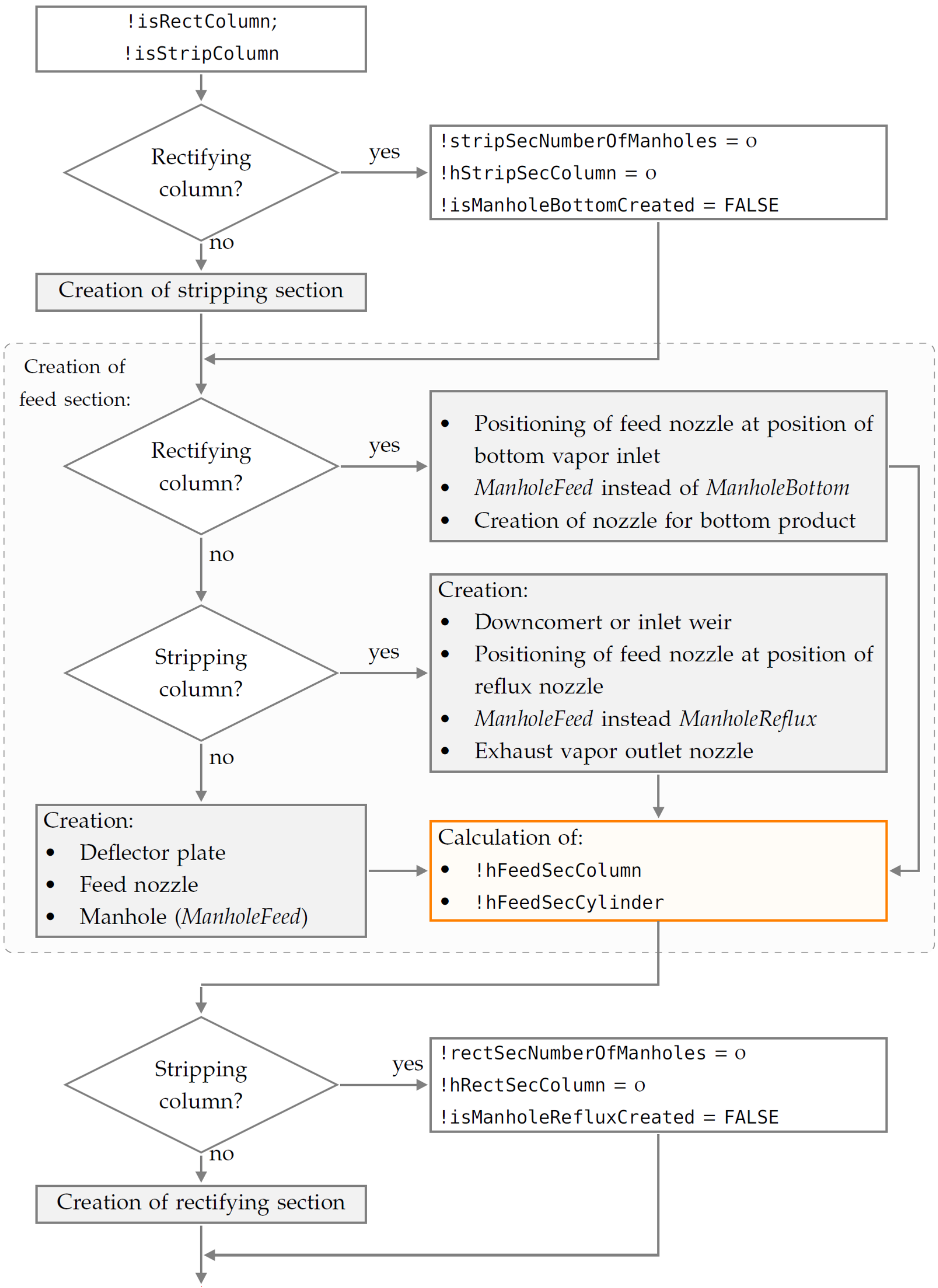


Figure A.3: Algorithm for overall design of internals for tray columns with different configurations

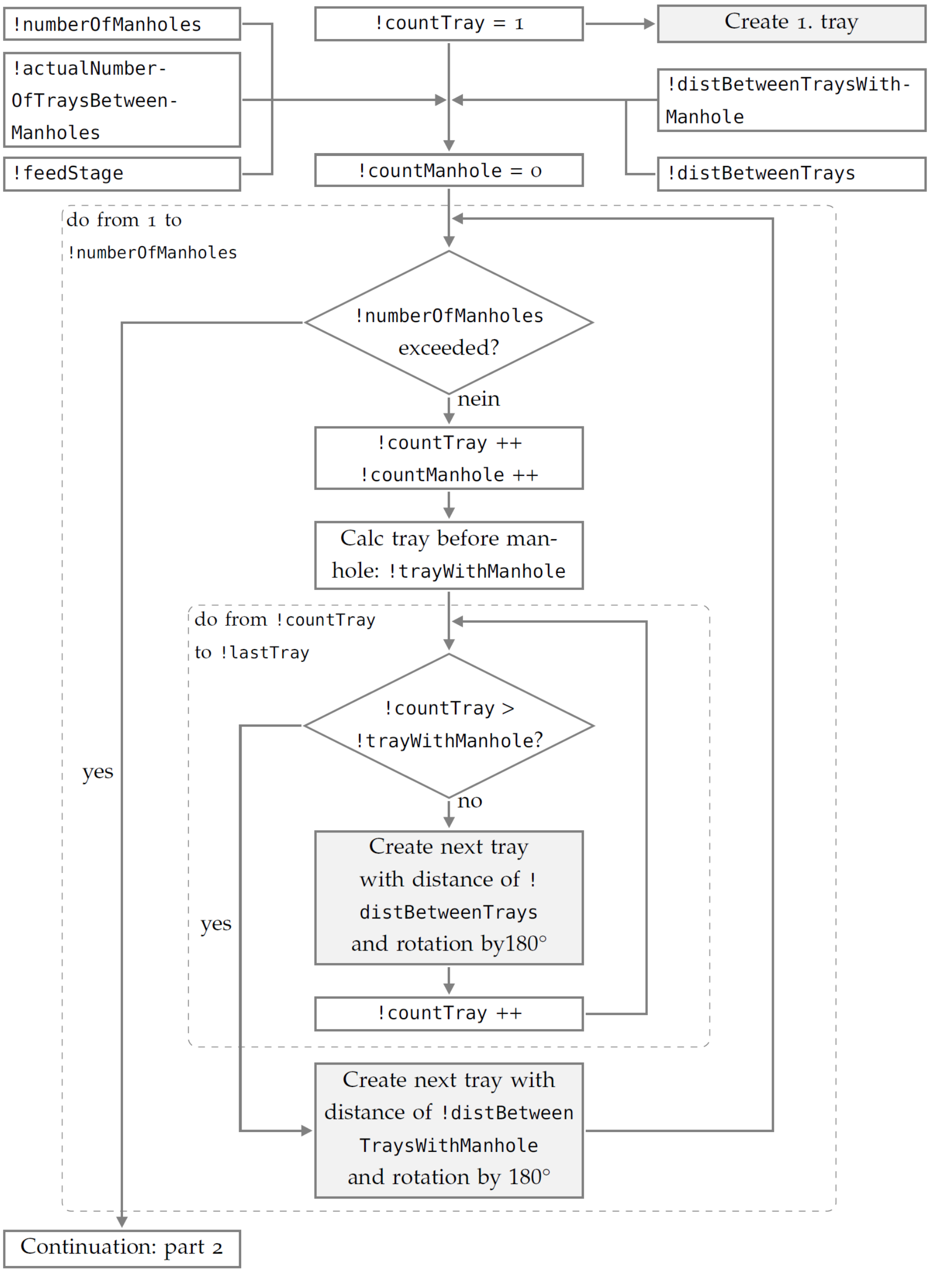


Figure A.4: Creation of trays and support rings in tray columns depending on the manhole arrangement - Part 1

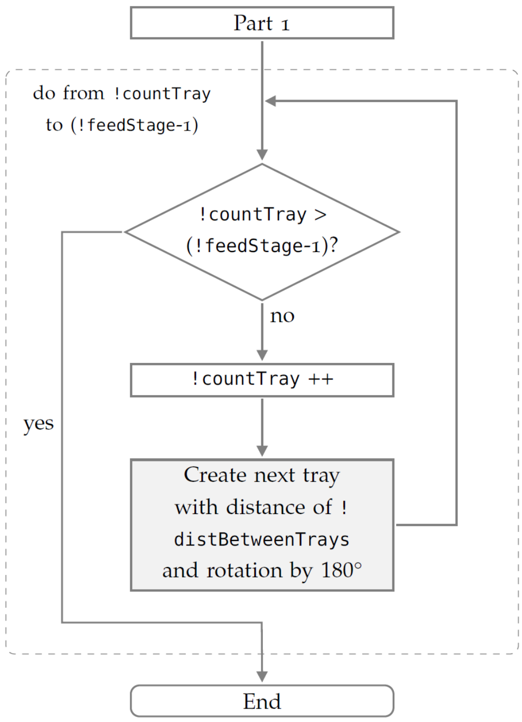


Figure A.5: Creation of trays and support rings in tray columns depending on the manhole arrangement - Part 2

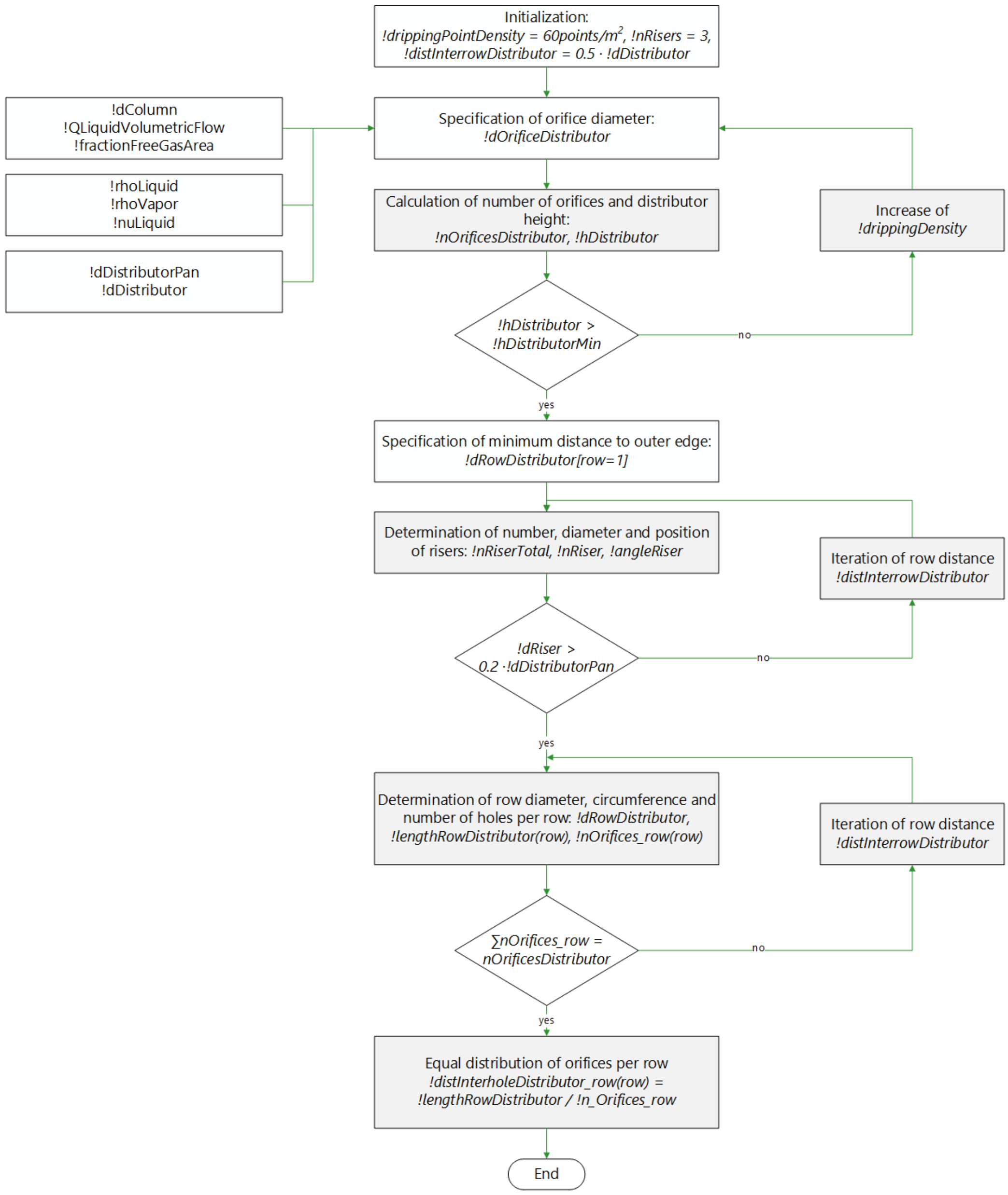


Figure A.6: Algorithm for the design of orifice pan distributor

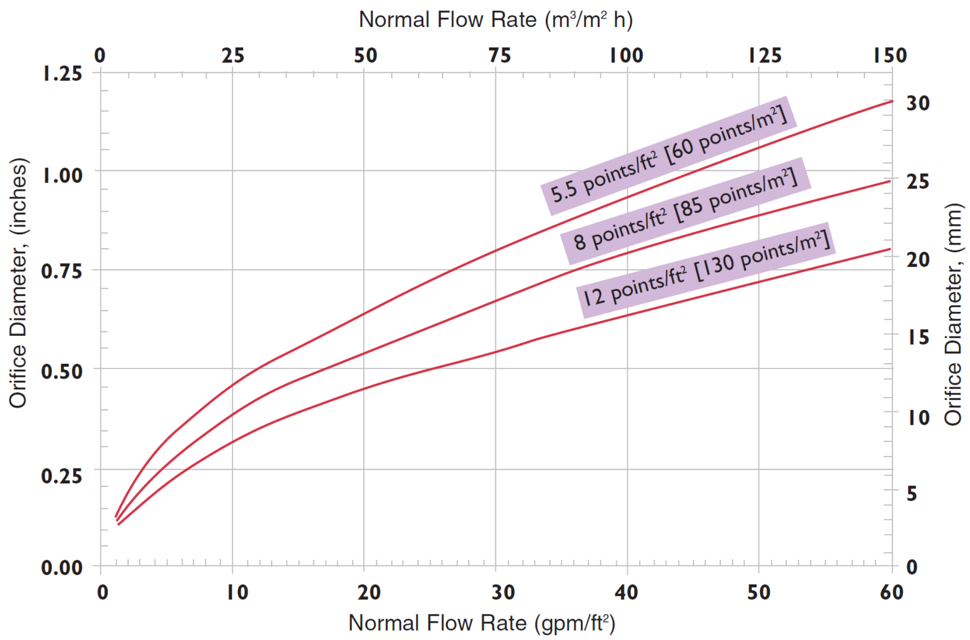


Figure A.7: Approximate orifice size for gravity flow distributors, applied for iteration of dripping density (see figure A.6) [Koch-Glitsch, 2010a, p.6]

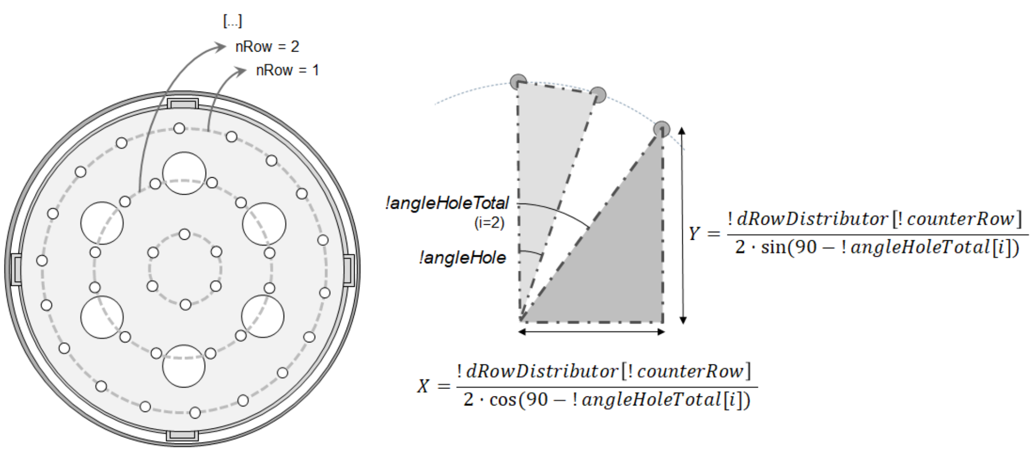


Figure A.8: Orifice pan distributor design variables for equal positioning of orifices

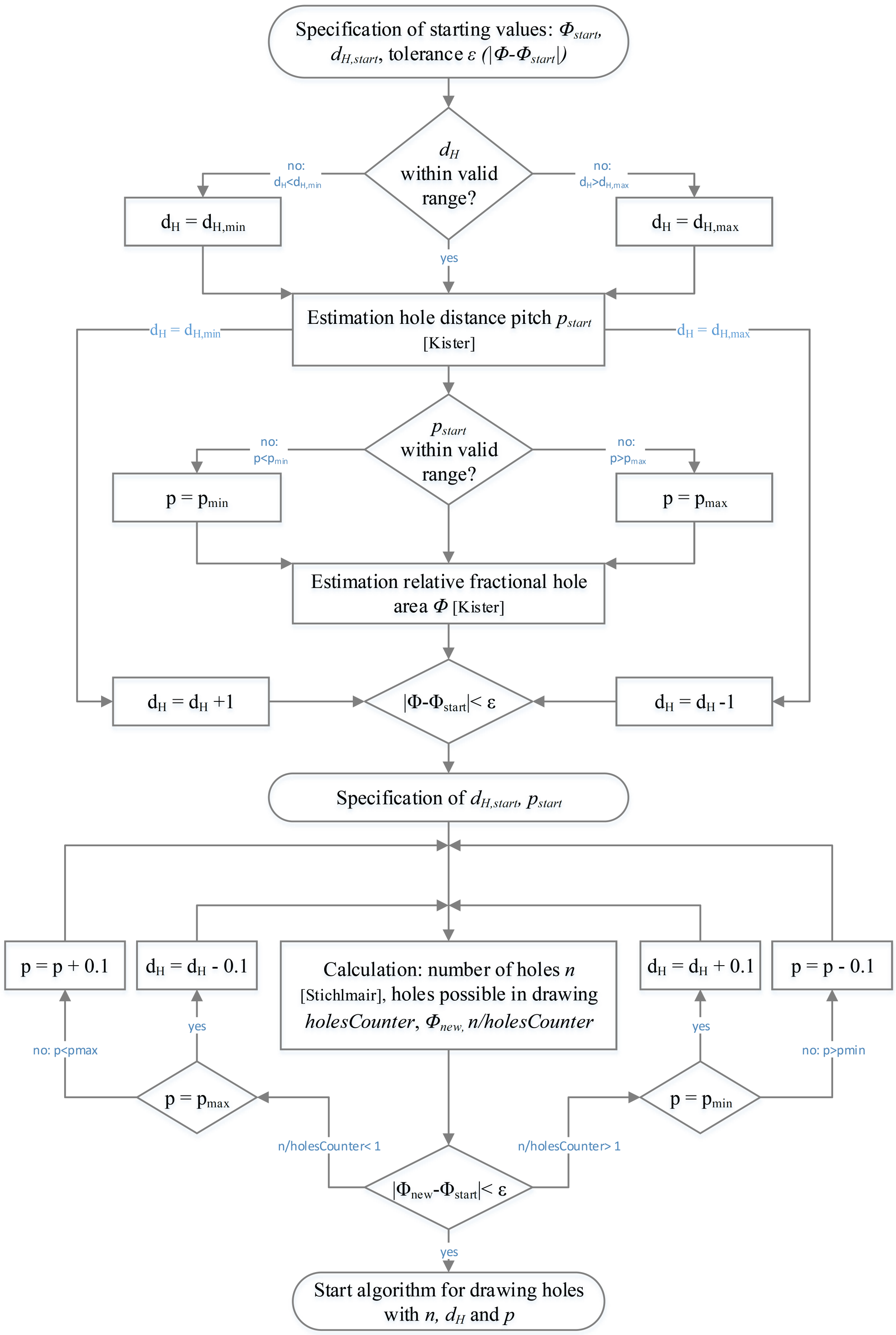


Figure A.9: Algorithm for determination of constructive design of sieve trays

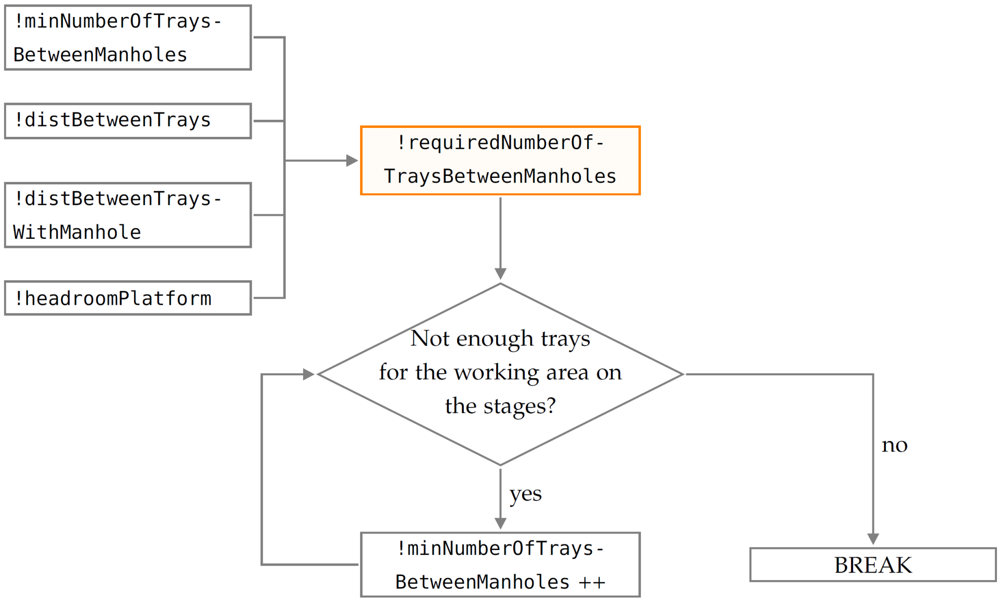


Figure A.10: Algorithm for determination of the minimum number of trays between two manholes in tray columns

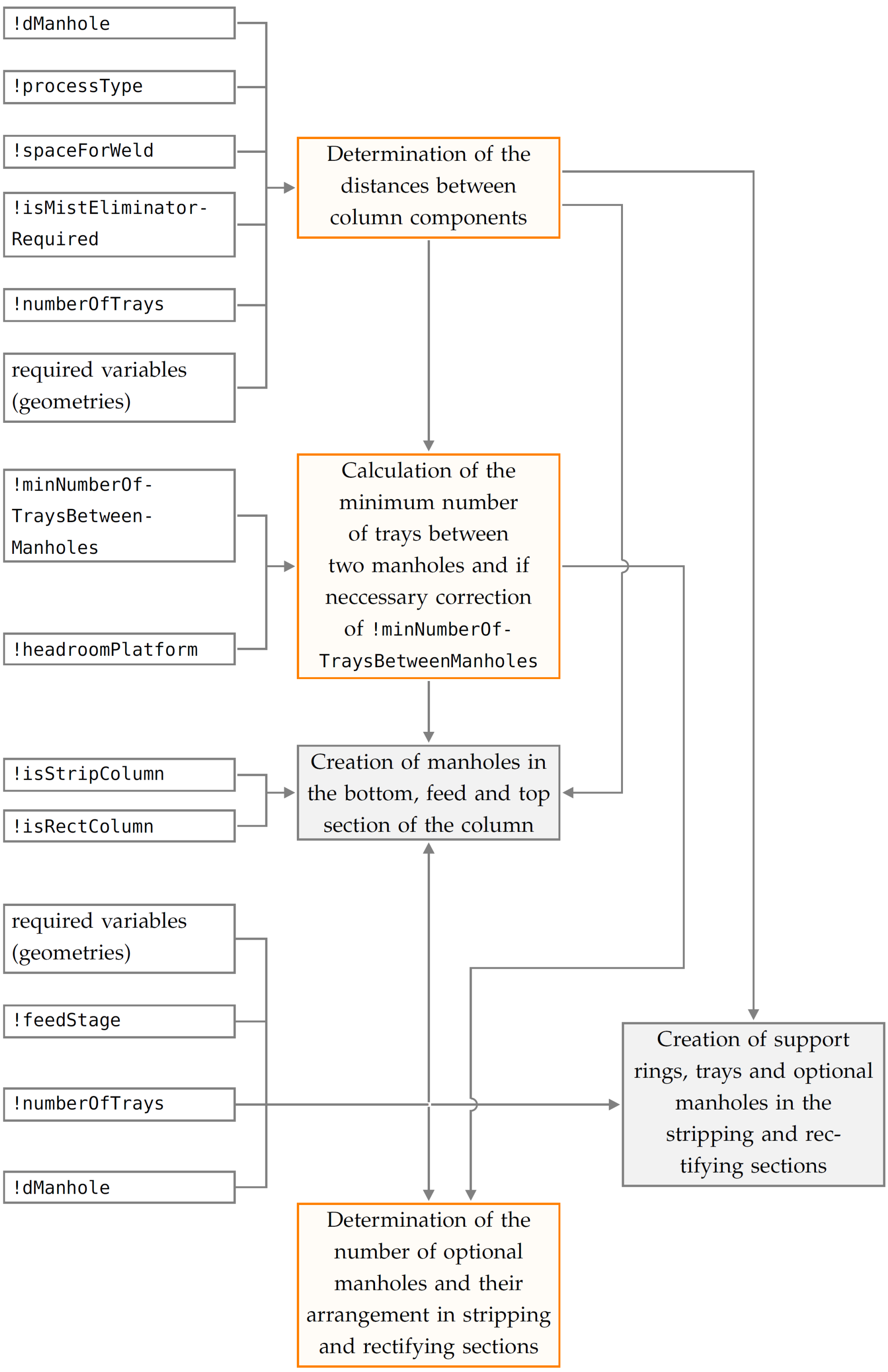


Figure A.11: Overall algorithm for the determination of the tray, manhole and support ring arrangements in trays columns

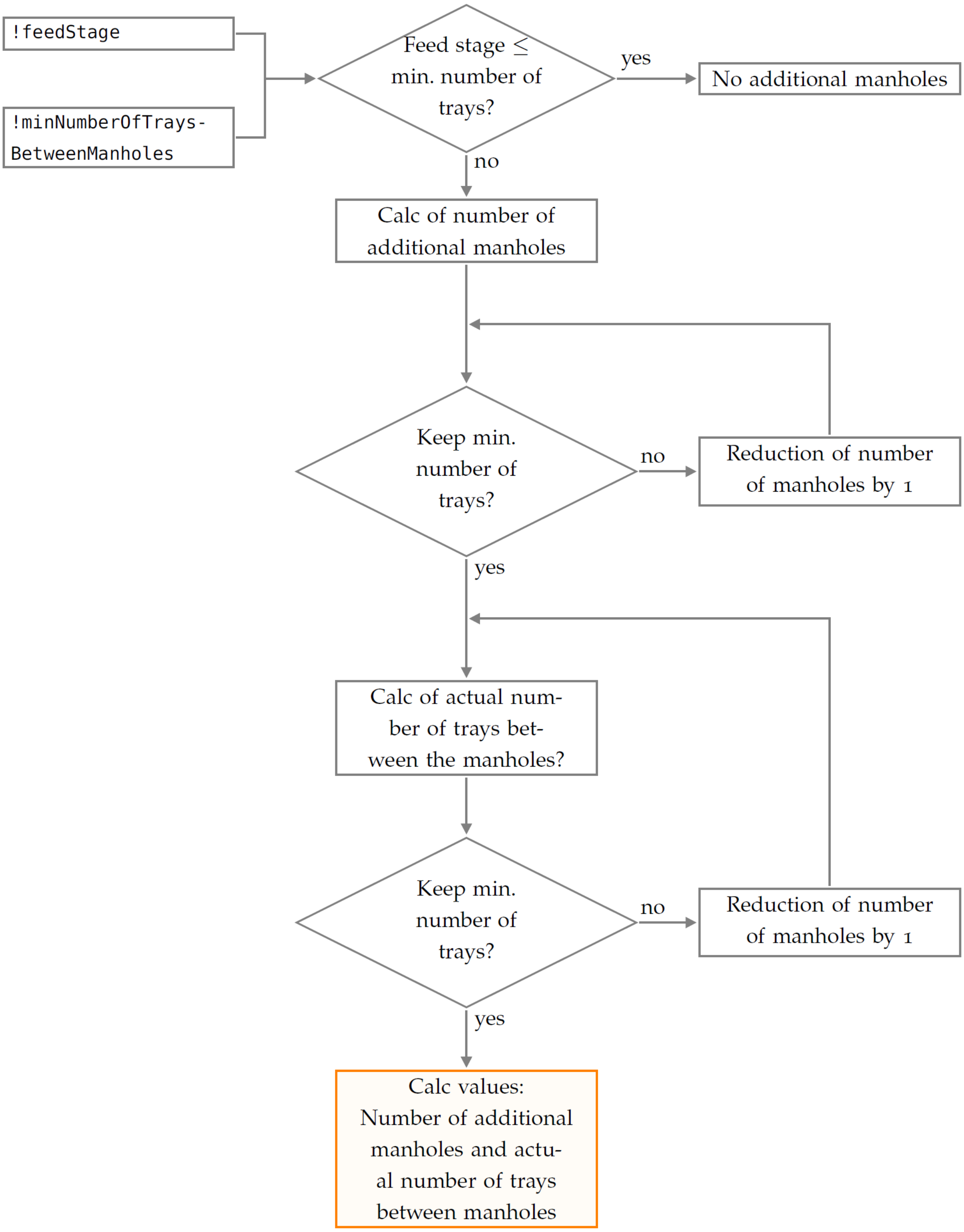


Figure A.12: Algorithm for determination of additional manholes in the stripping section of tray columns (referring to bottom box in figure A.11)

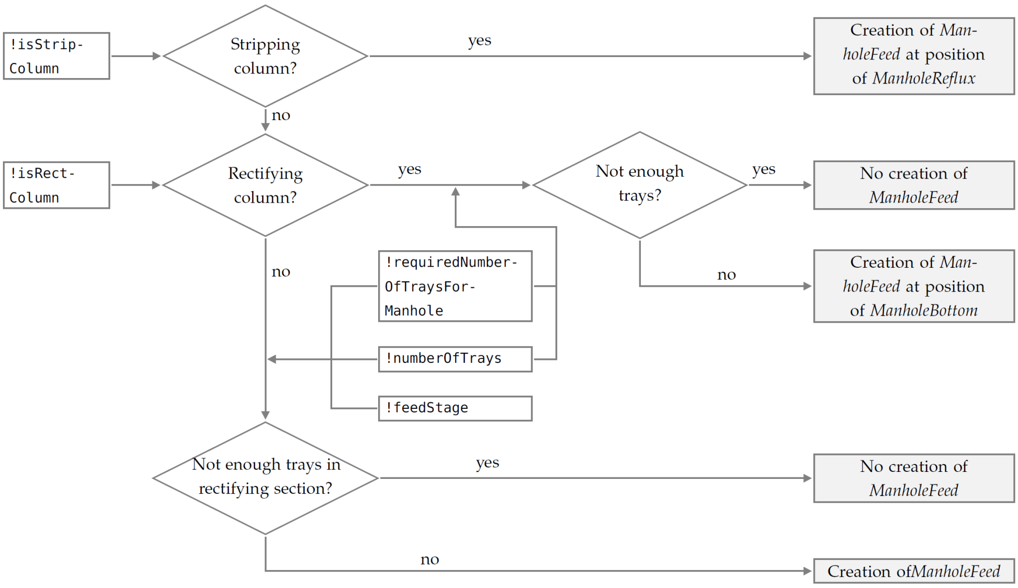


Figure A.13: Verification of installing of manhole in stripping sections / columns for tray columns

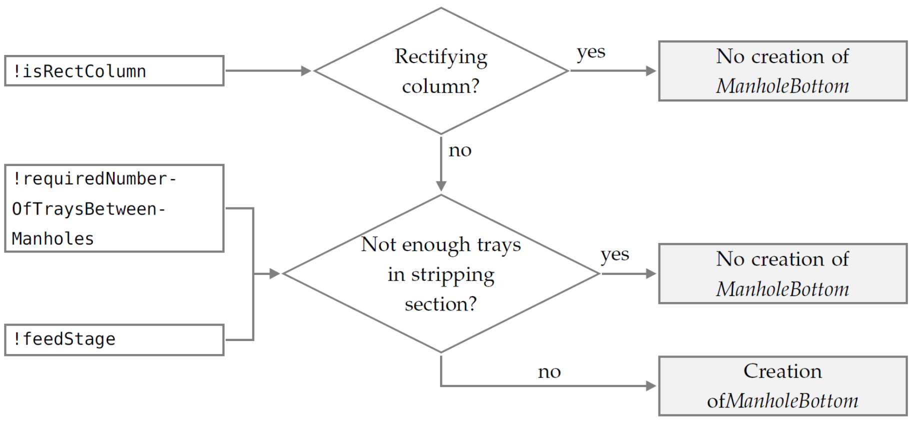


Figure A.14: Verification of installing of manhole in rectifyinging sections / columns for tray columns

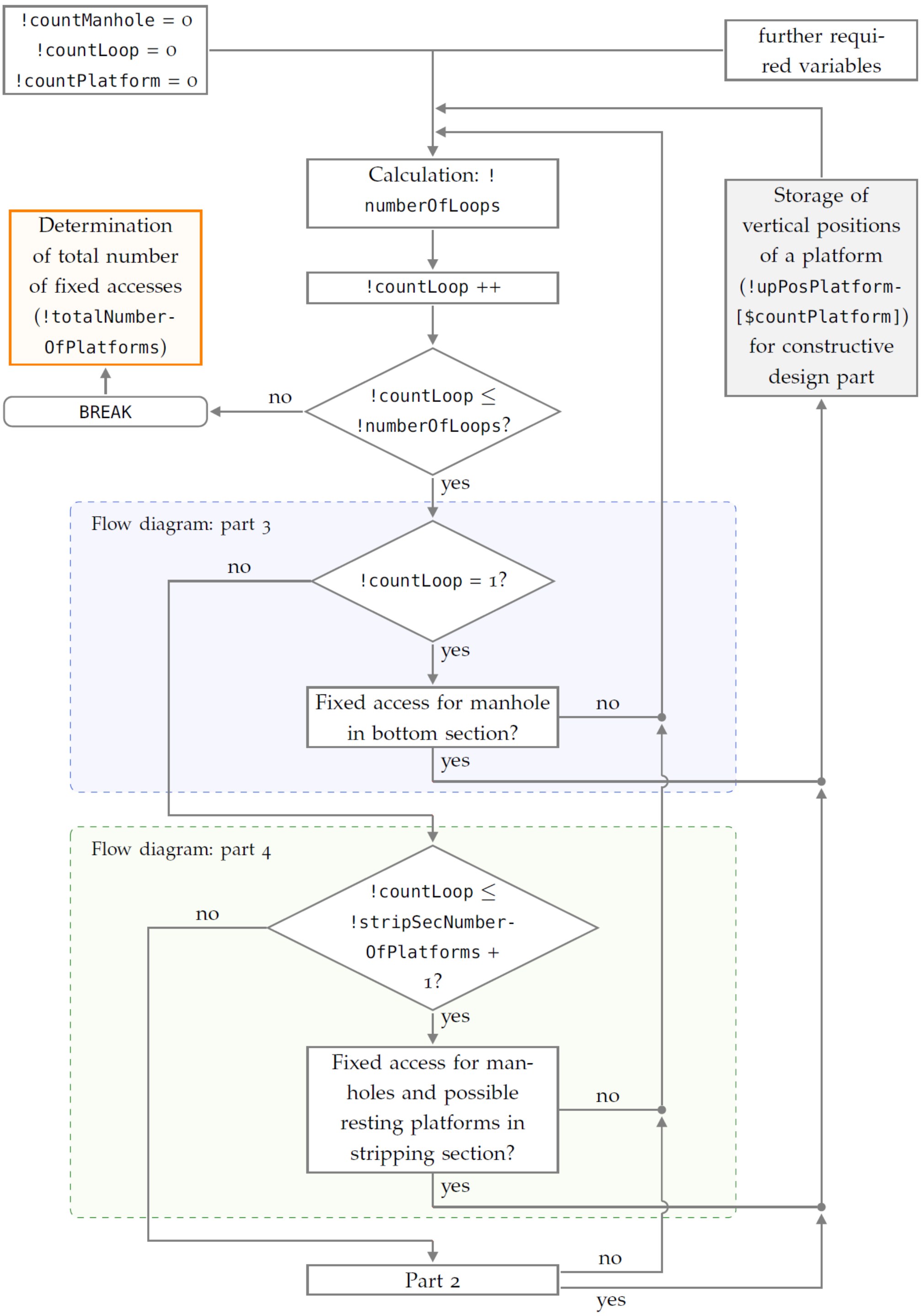


Figure A.15: Algorithm for creation of permanent means of access - part 1

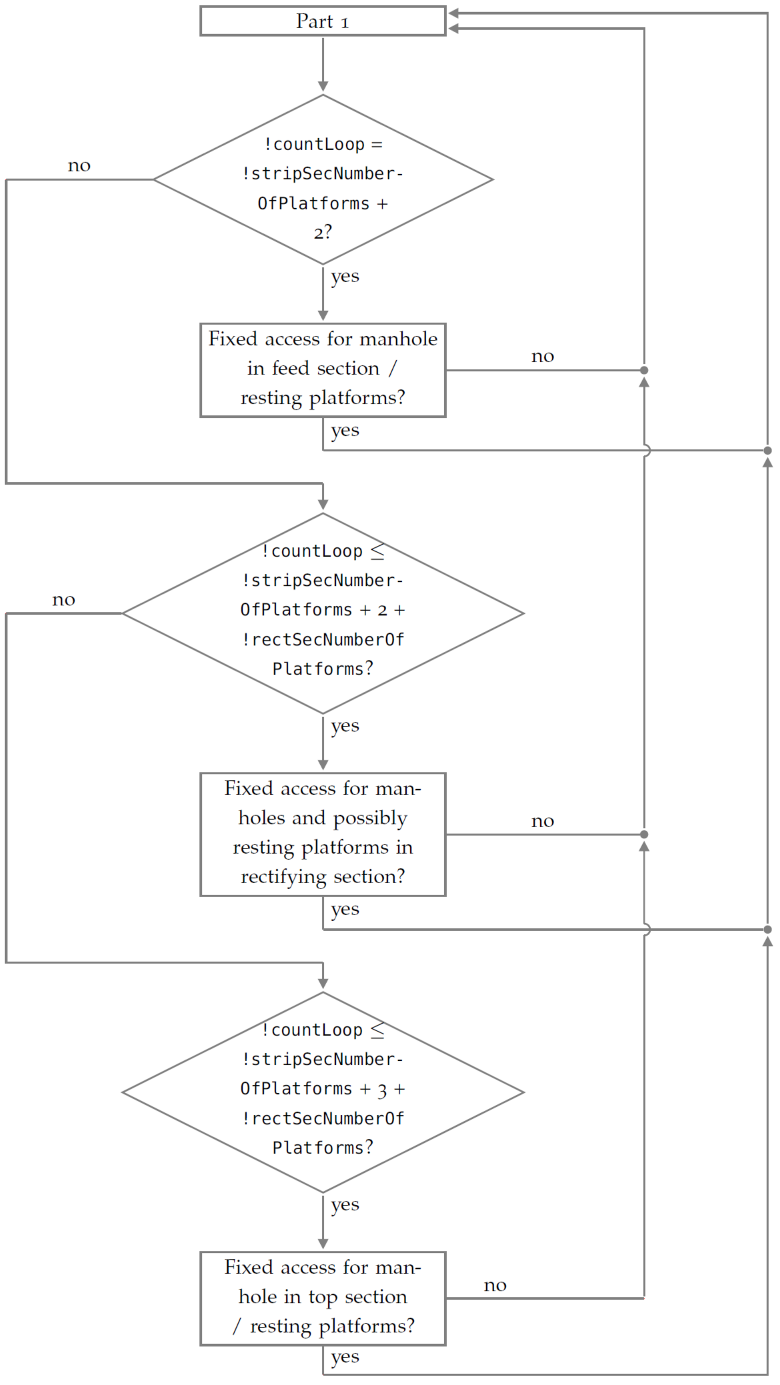


Figure A.16: Algorithm for creation of permanent means of access - part 2

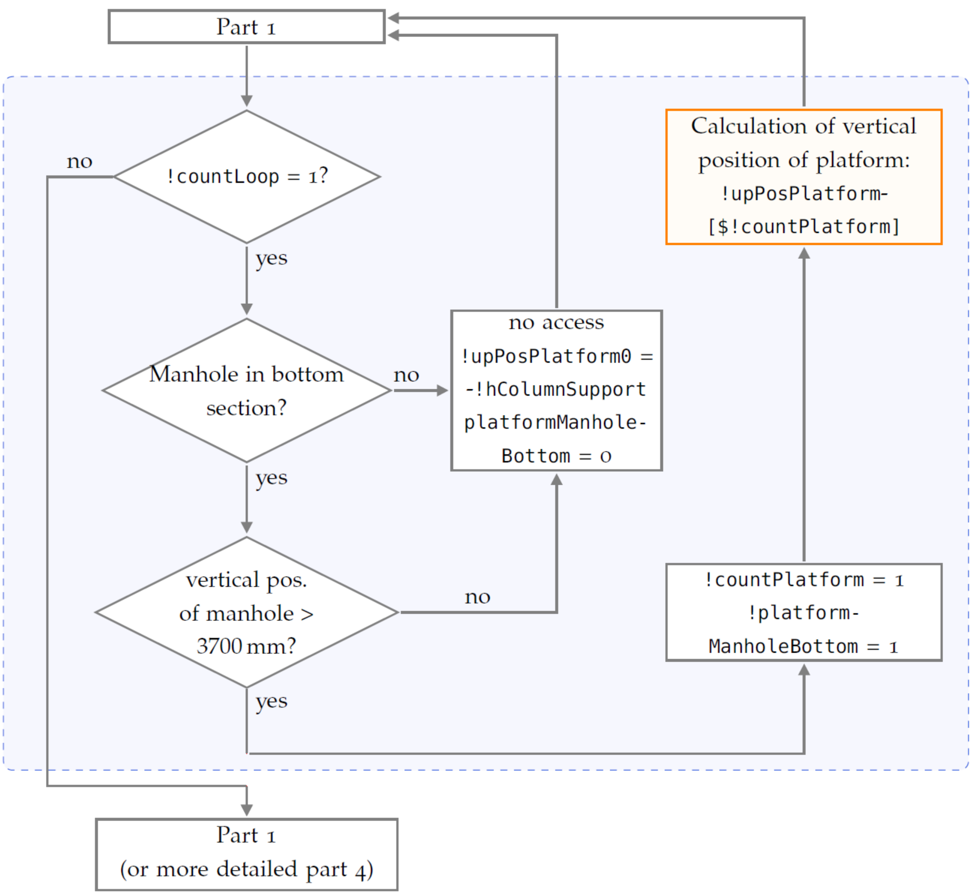


Figure A.17: Algorithm for creation of permanent means of access - part 3

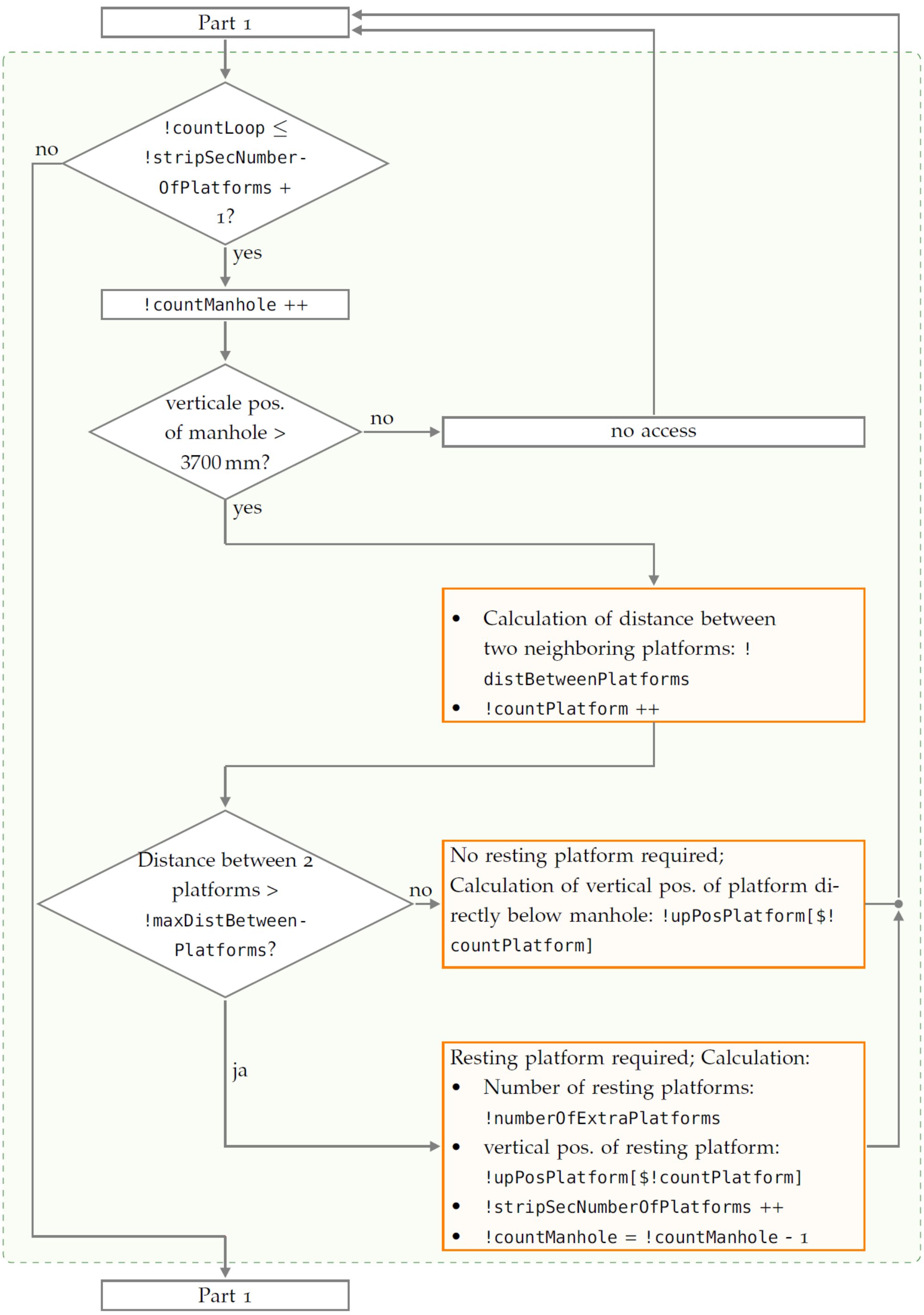


Figure A.18: Algorithm for creation of permanent means of access - part 4

Heuristics for constructive design

Table A.7: Selected heuristics for the constructive design of distillation columns

Variable name	Description	Source	Recommended values
!distVapor-BottomIn-NozzleTo-BottomDish	Distance between high liquid bottom level and bottom part of vapor inlet nozzle $[mm]$	Kister, 1992, p. 83-87	$> 12in \approx 300mm$
		Branan, 2005, p. 97	$> 12in \approx 300mm$ above high liquid level $> 18in \approx 460mm$ above normal liquid level
	Distance between high liquid bottom level and centre of vapor inlet nozzle $[mm]$	Saint-Gobain NorPro, 2001, p. 50, G-1	Small columns: $450mm + \frac{D_{vapBotIn}}{2}$, Large columns: Maximum value $(500mm; 2 \cdot D_{vapBotIn})$
!distSupport-RingToVapor-BottomIn-Nozzle	Distance between top part of bottom vapor inlet nozzle and bottom tray or packed support plate $[mm]$	Kister, 1992, p. 84-86	$> 15 - 18in \approx 380 - 460mm$
		Branan, 2005, p. 88-97	Maximum value $(18in \approx 460mm;$ 12in $+ D_{vapBotIn} \approx 300mm + D_{vapBotIn})$
	Using steam feed pipe opened at the bottom	Correspondence with Sulzer 2017	$> D_{col}$

Continuation table A.7 of previous page

Variable name	Description	Source	Recommended values
!multiplier-PackingHeight	Multiplier for max. packing height until redistribution (random packing) [mm]	Christen, 2010, p. 441	$3...6 \cdot D_{col}$
		Hobler, 1966, p.227	$\leq 7 \cdot D_{col}$
		Woods, 2007, p. 97 $< 6m$	$5...10 \cdot D_{col}$
		Treybal, 1981, p. 193 $< 6...7m$	$3...10 \cdot D_{col}$
		Hobler, 1966, p.227	$\leq 7 \cdot D_{col}$
		Sattler and Feindt, 1995, p. 198	$\leq 10 \cdot D_{col}$
!dist-Redistributor-ToPacking	Distance between (re)-distributor and packing [mm]	Kolev, 2006, p. 489	$D_{col} \leq 700mm$: $100 - 150mm$, $D_{col} > 700mm$: $150 - 250mm$, general:$150 - 300mm$
		Kister, 1990, p. 65-66	$> 6 - 12in \approx 150 - 300mm$, Spray distributors: $> 8 - 24in \approx 200 - 300mm$, Kister prefers: $6 - 8in \approx 150 - 200mm$ to avoid entrainment, frothing and splashing

Continuation table A.7 of previous page

Variable name	Description	Source	Recommended values
		Koch-Glitsch, 2010b, p.3	$0-8in \approx 0-200mm$
!hMax-Random-Packing NoCrush	Max. height random packing to prevent from crushing $[mm]$	Kister, 1992, p. 564	$< 20ft \approx 6m$, $N^{bed} < 10 \cdot N$
-	Distance between centre of feed inlet nozzle and collector above $[mm]$	Koch-Glitsch, 2010d, p. 20-21	$D_{col} \leq 710mm$: $100mm + D_{manhole} + \frac{D_f}{2}$ $D_{col} > 710mm$: $150mm + D_{manhole} + \frac{D_f}{2}$
!hMist-Eliminator	Heigth of mist eliminator (mesh wire) $[mm]$	Nitsche, 2014, p. 375-403	$100 - 300mm$
!hSpaceMist-Eliminator	Distance between mist eliminator and exhaust vapor nozzle $[mm]$	GEA Heat Exchangers/Enexio Group, 2014	Minimum value $(\frac{D_{col} D_{vapBotIn}}{2} + 100mm; 300mm))$
!hTotalColumn	Maximum tower heights due to wind load and foundation considerations m	KLM Technology Group, 2013, p. 28	$53m$
	Tower length to tower diamter ratio $[-]$	KLM Technology Group, 2013, p. 28	$\frac{l_{col}}{D_{col}} < 30$, preferably < 20
!distFeedIn-NozzleTo(Re)-Distributor	Distance between feed or reflux inlet nozzle to the top of the (re)-distributor $[mm]$	Kolev, 2006, p. 489	$100 - 300mm$

Continuation table A.7 of previous page

Variable name	**Description**	**Source**	**Recommended values**
		Billet, 1995, p. 237	$100 - 300mm$
		Saint-Gobain NorPro, 2001, p. 50, G-1	$150mm + 0.5 \cdot D_{f,in}$
!dist-CollectorTo-Redistributor, !distBetween-TraysWith-Manhole	Tray spacing at manhole $[mm]$	Kister, 1992, p.138	$> 35in \approx 915mm$
!hBedLimiter	Heigth of the hold-down grid	Kolev, 2006, p.499	$500 \leq D_{col} < 800$: $50mm$, $800 \leq D_{col} < 1500$: $60mm$, $1500 \leq D_{col} < 3000$: $80mm$
!spaceForWeld	Space for welding $[mm]$	Workship expertise	$> 50mm$
!headroom-Platform	Minimum working area under platforms (stationary access) $[mm]$	Kern, 1977b, p.123-129	$6.75ft \approx 2060mm$

Table A.8: Dimensioning for tray column internals

Variable	**Vacuum**	**Atmospheric**	**Pressure**	**Source**
Sieve trays				
Hole diameter	0.004 – 0.013	0.004 – 0.013	0.004 – 0.013	1
d_h $[m]$	0.004 – 0.013	0.004 – 0.013	0.004 – 0.013	2
	0.0159 – 0.03 for all pressures			3
Hole pitch	$2.5 - 3 \cdot d_h$	$3.5 - 4 \cdot d_h$	$3.5 - 4.5 \cdot d_h$	1
p $[m]$	$2.5 - 3 \cdot d_h$	$3 - 4 \cdot d_h$	$3.5 - 4.5 \cdot d_h$	2
Relative fractional	10 – 15	6 – 10	4.5 – 7.5	1
hole area Φ [%]	12 – 20	8 – 15	6 – 10	2
	$K \cdot (\frac{d_h}{p})^2$, $K_{triangular} = 0.905, K_{square} = 0.785$			3
	usually: 5 – 15, optimal: 8 – 12			3
Tray distance $!distBetweenTrays$	500 – 800	400 – 600	300 – 400	2
Valve trays				
Valve diameter	0.04 – 0.05	0.04 – 0.05	0.04 – 0.05	1
d_v $[m]$	0.05 – 0.15	0.05 – 0.15	0.05 – 0.15	2
Hole pitch	$1.5 \cdot d_v$	$1.7 - 2.2 \cdot d_v$	$2 - 3 \cdot d_v$	1
p $[m]$	$1.5 - 3 \cdot d_v$	$1.7 - 2.2 \cdot d_v$	$2 - 3 \cdot d_v$	2
Tray distance $!distBetweenTrays$	500 – 800	400 – 600	300 – 500	2
Bubble cap trays				
Bubble cap	0.08 – 0.15	0.08 – 0.15	0.08 – 0.15	1
diameter d_{bc} $[m]$	0.08 – 0.16	0.08 – 0.16	0.08 – 0.16	2
Bubble cap	$1.25 \cdot d_b c$	$1.25 - 1.4 \cdot d_b c$	$1.5 \cdot d_b c$	1
pitch t $[m]$	$1.25 \cdot d_b c$	$1.25 - 1.4 \cdot d_b c$	$1.5 \cdot d_b c$	2
Tray distance $!distBetweenTrays$	500 – 800	400 – 600	300 – 400	2

1: J. G. Stichlmair and Fair, 1998
2: Sattler and Feindt, 1995
3: Kister, 1990

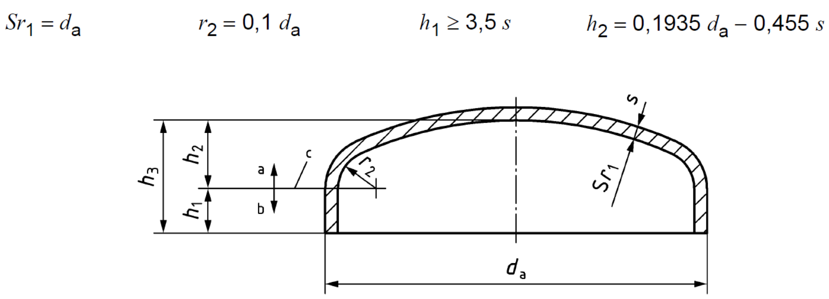


Figure A.19: Geometries for torispherical heads applied for the design of the bottom section of columns [DIN 28011, 2012, p.5]

Control schemes for distillation processes

Table A.9: Mass balance control configurations for distillation columns [related to Kister, 1990, p. 497]

Type	**Level reflux drum**	**Bottom level**	**Compo-sition**	**Free**	**Pressure control**	**Usage**
Ind	D	B	H	R	C	Most
Ind	D	B	R	H	C	common
Dir	R	B	D	H	C	
Dir	D	H	B	R	C	
Dir	D	R	B	H	C	Not
Dir	H	B	D	R	C	common
Dir	C	B	D	R	H	

Legend
B: Bottom
C: Condensation
D: Distillate
R: Reflux
Dir: Direct material balance
H: Heating medium
Ind: Indirect material balance

Table A.10: Pros and cons of common control schemes for distillation columns [related to Kister, 1990, p. 500]

Control scheme	**Figure 3.21 a**	**Figure8 3.21 b**	**Figure 3.21 c**	**MB control**
Type	**Indirect**	**Indirect**	**Direct**	**Direct**
Stream used for composition control	Reboil	Reflux	Top product	Bottom product
Top product for which scheme works	Liquid or vapor	Liquid or vapor	Liquid only	Liquid or vapor
Favored when more important product purity is:	Bottom	Top	Top	Bottom
Favored when smaller product flow is:	Bottom	Top	Top	Bottom
Favored when better control tray temperature is in:	Bottom	Top	Top	Bottom
Speed of response in large tray column	fast	slow	slow	reasonable fast
Suitability for essentially stripping columns	Excellent	Least satisfactory	Least satisfactory	Good
Response to disturbances in heating medium system	Reasonable	Least satisfactory	Least satisfactory	Excellent
Effect of small distillate flow	Reflux drum level drifts; mass balance poor	Reflux drum level drifts; mass balance poor	Loose composition control	Reflux drum level drifts; mass balance poor
Suitability to handly low reflux flows	Excellent	Good	Poor; reflux fluctuation likely	Excellent

A.3 Design of associated apparatus

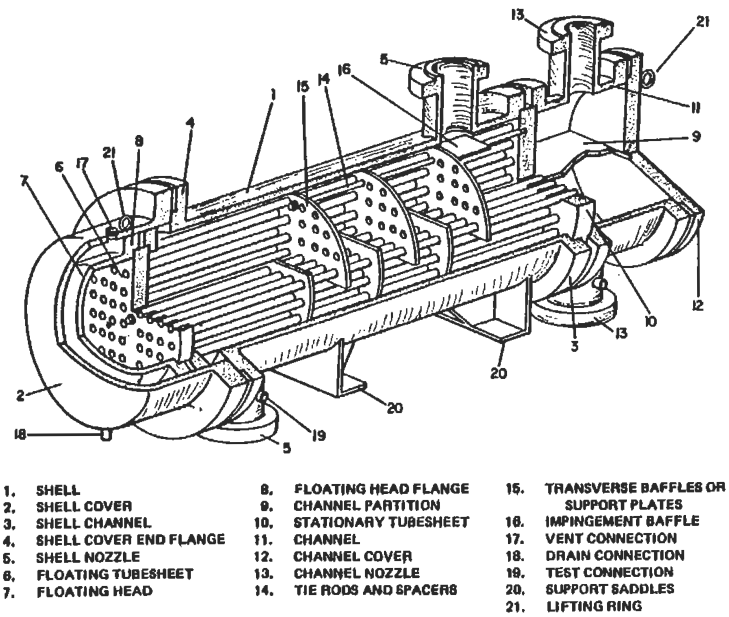


Figure A.20: Schematic overview of a shell and tube floating head heat exchanger [Pope, 1997, p. 34, figure 19]

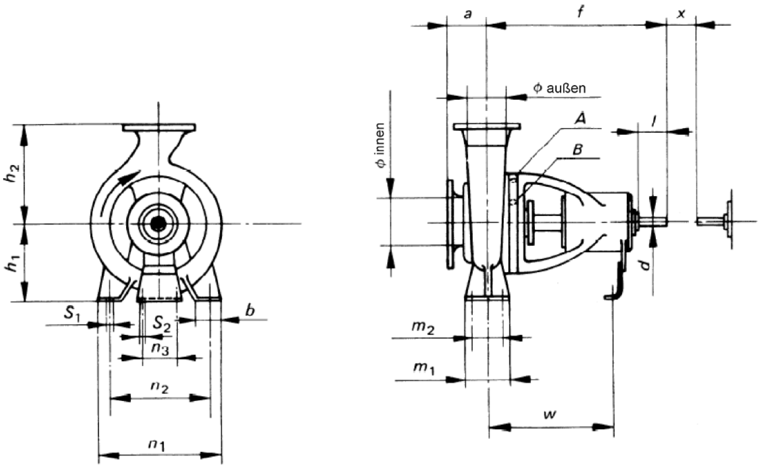


Figure A.21: Sketch for the dimensioning of centrifugal pumps (rating 16bar) based on [DIN EN 2858, 2011, p. 6]

A.4 MOSAICmodeling PlantDesign

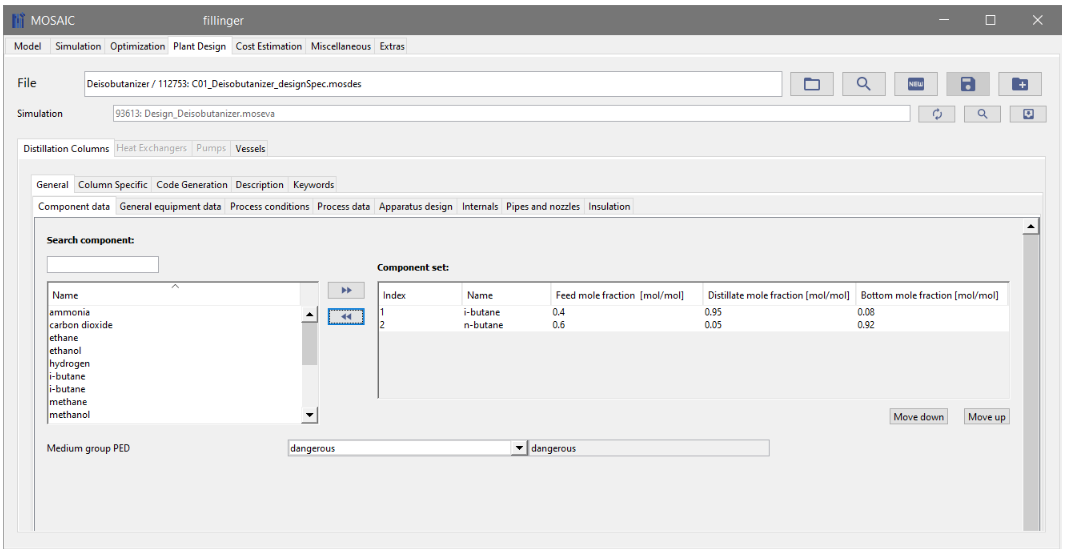


Figure A.22: GUI of *General / Component data* tab in MOSAICmodeling *PlantDesign*

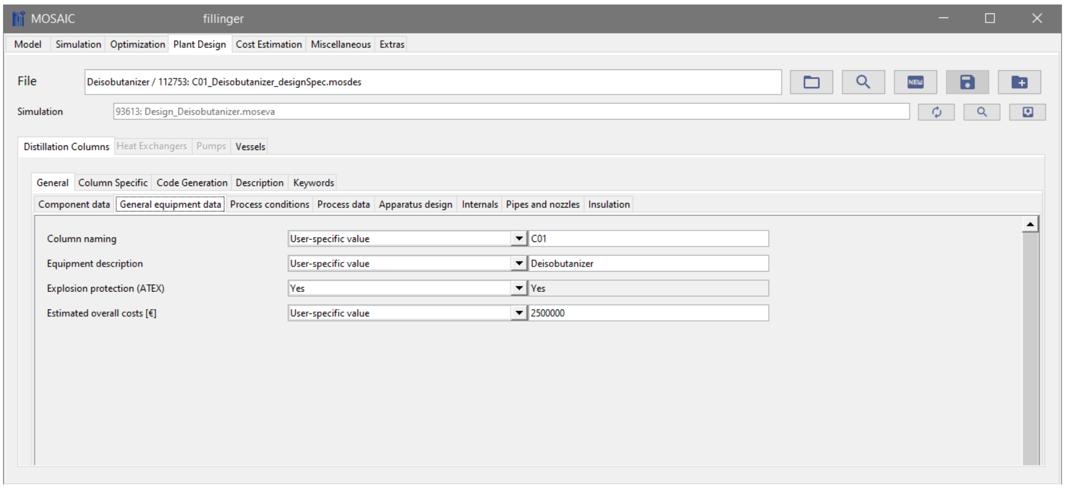


Figure A.23: GUI of *General / General equipment data* tab in MOSAICmodeling *PlantDesign*

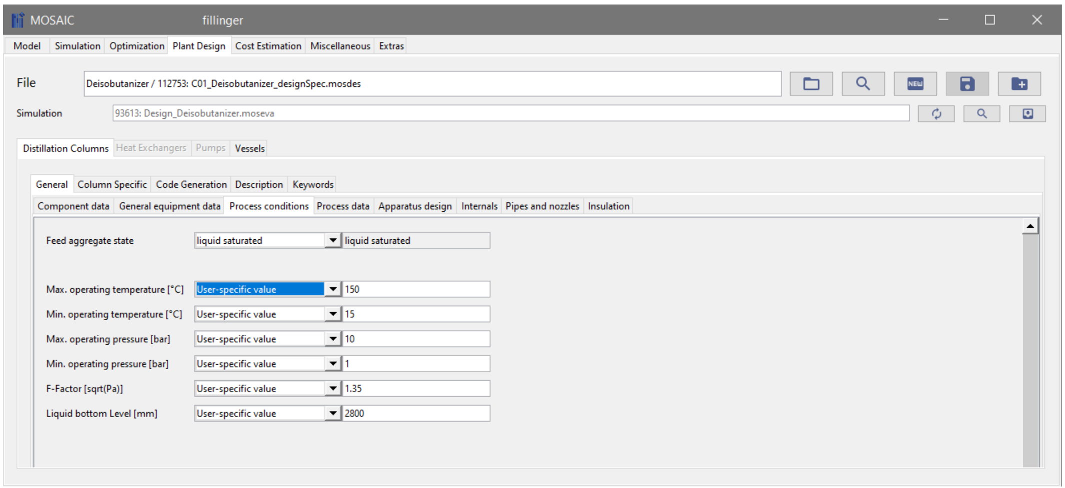


Figure A.24: GUI of *General / Process conditions* tab in MOSAICmodeling *PlantDesign*

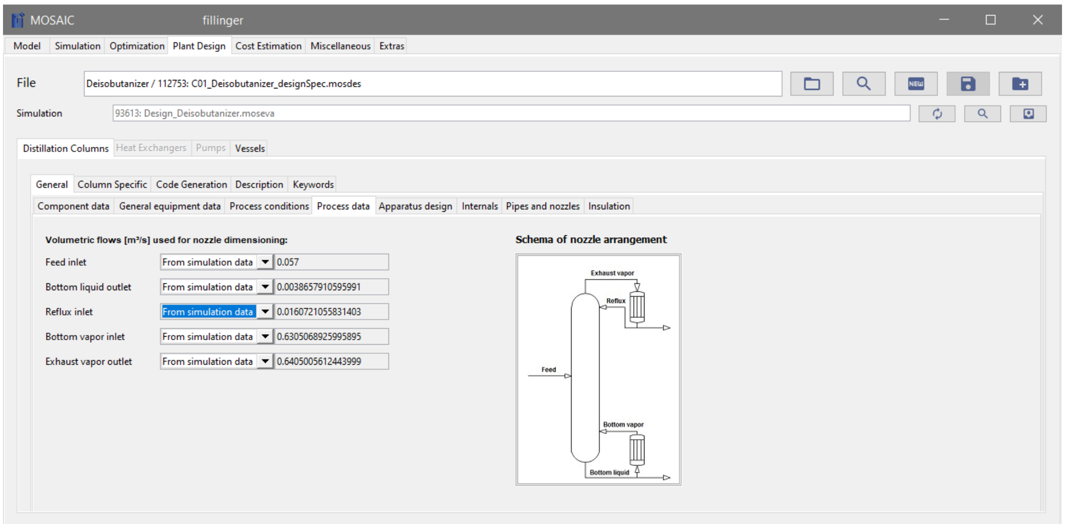


Figure A.25: GUI of *General / Process data* tab in MOSAICmodeling *PlantDesign*

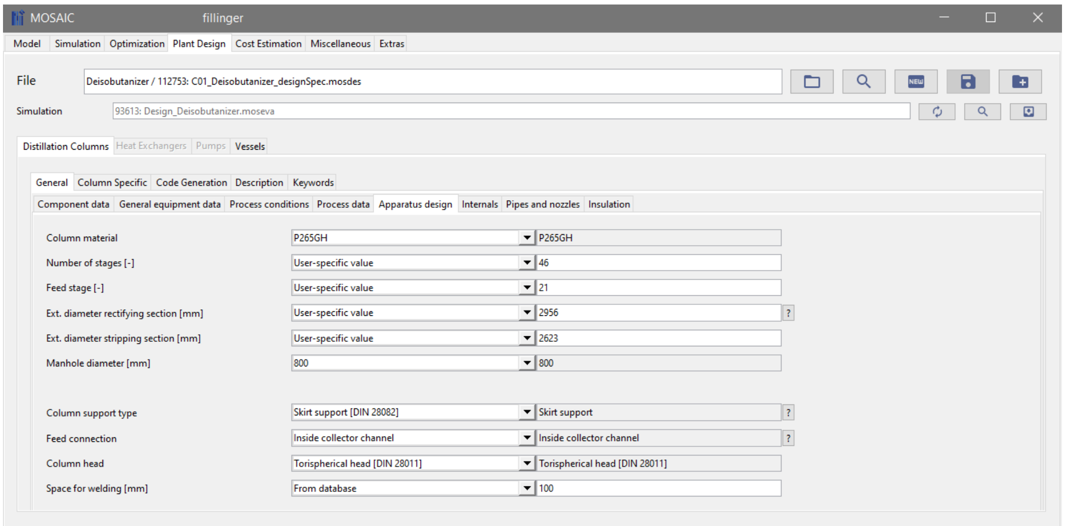


Figure A.26: GUI of *General / Apparatus design* tab in MOSAICmodeling *PlantDesign*

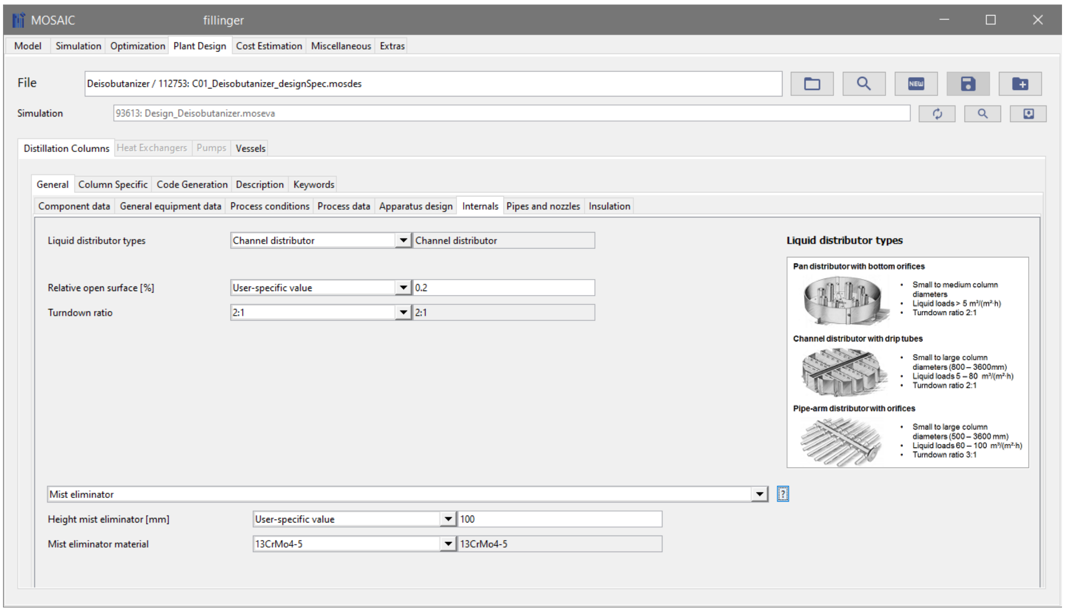


Figure A.27: GUI of *General / Internals* tab in MOSAICmodeling *PlantDesign*

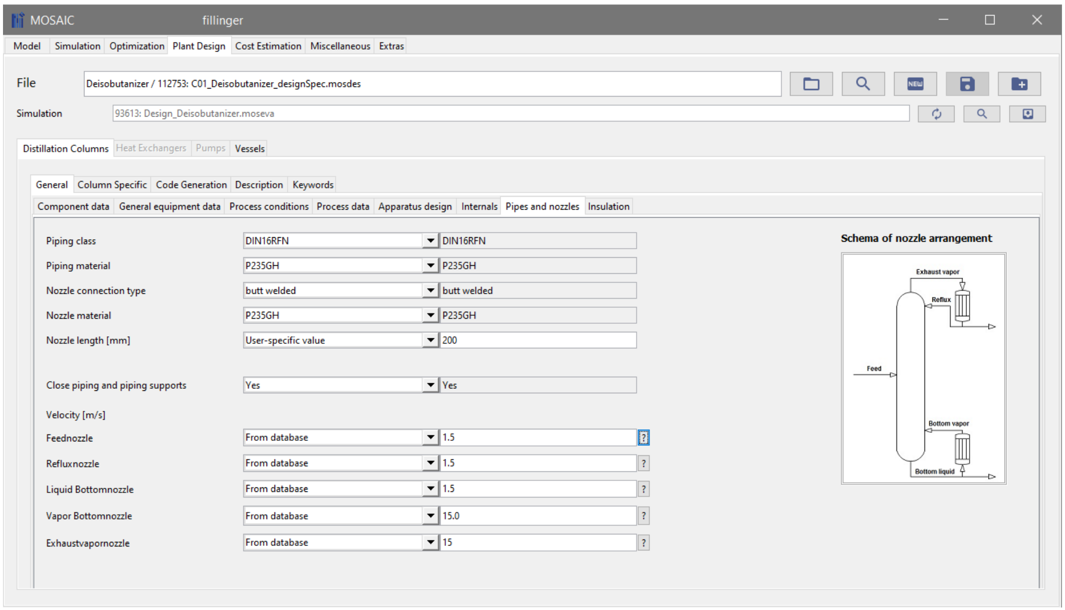


Figure A.28: GUI of *General / Pipes & nozzles* tab in MOSAICmodeling *PlantDesign*

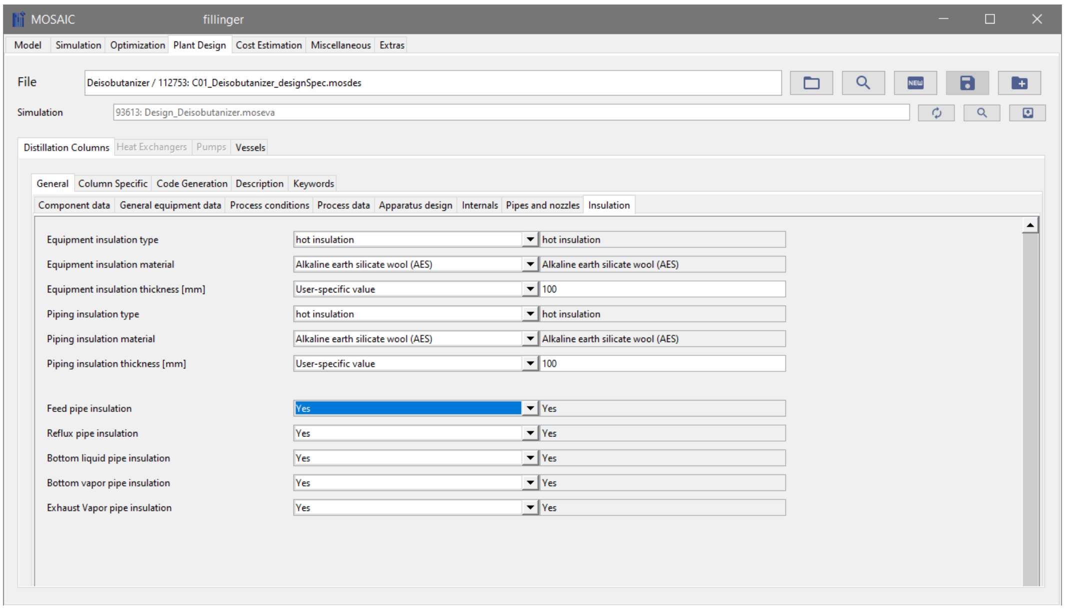


Figure A.29: GUI of *General / Insulation* tab in MOSAICmodeling *PlantDesign*

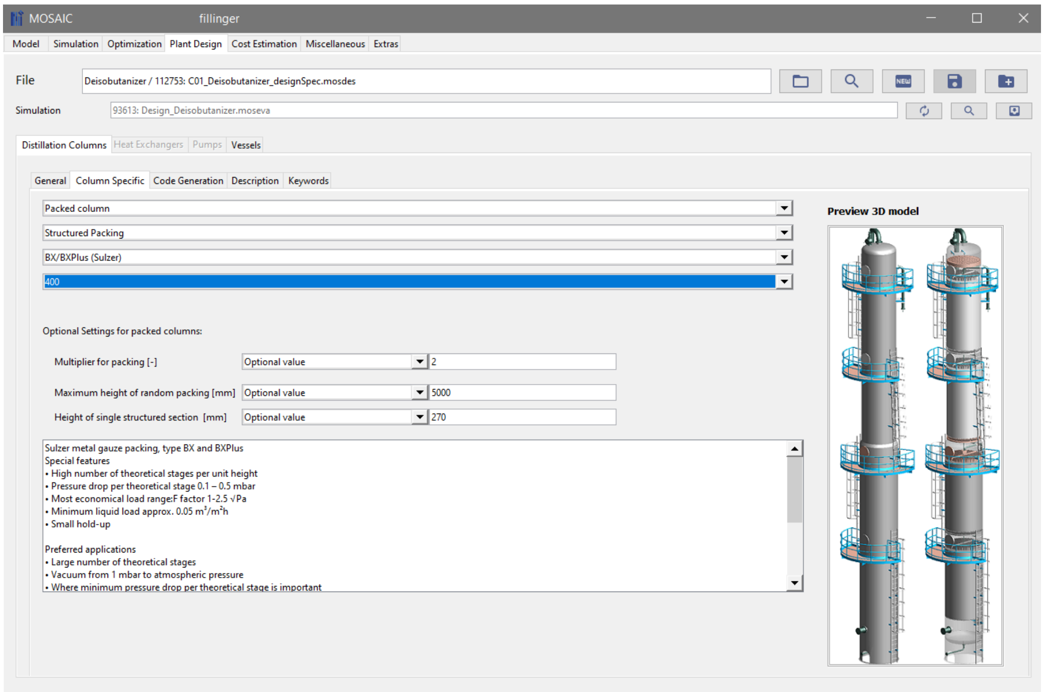


Figure A.30: GUI of *Column specific* tab in MOSAICmodeling *PlantDesign*

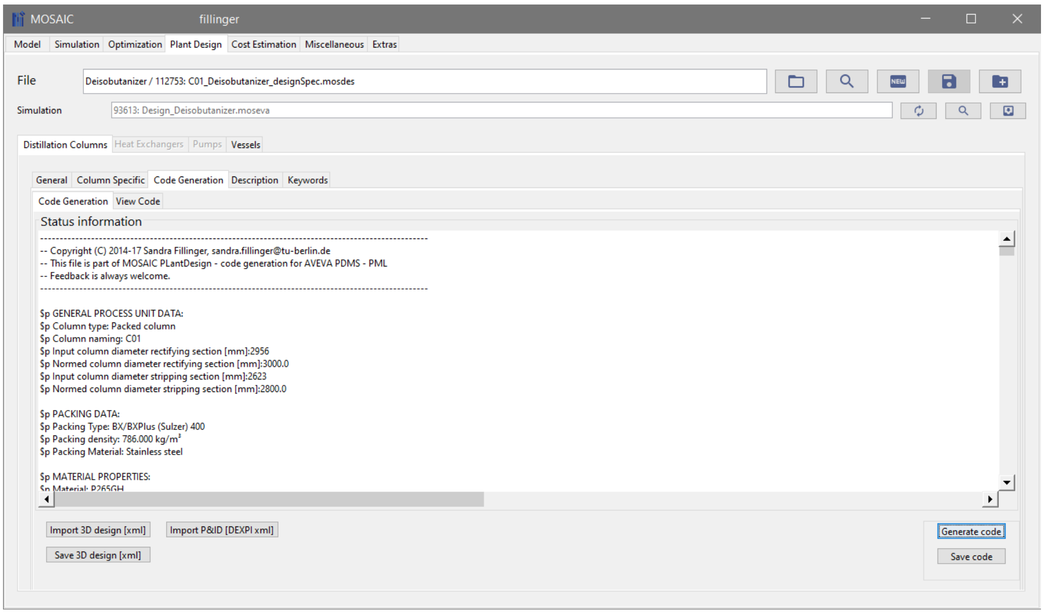


Figure A.31: GUI of *Code generation* tab in MOSAICmodeling *PlantDesign*

Appliance of *PlantDesign*

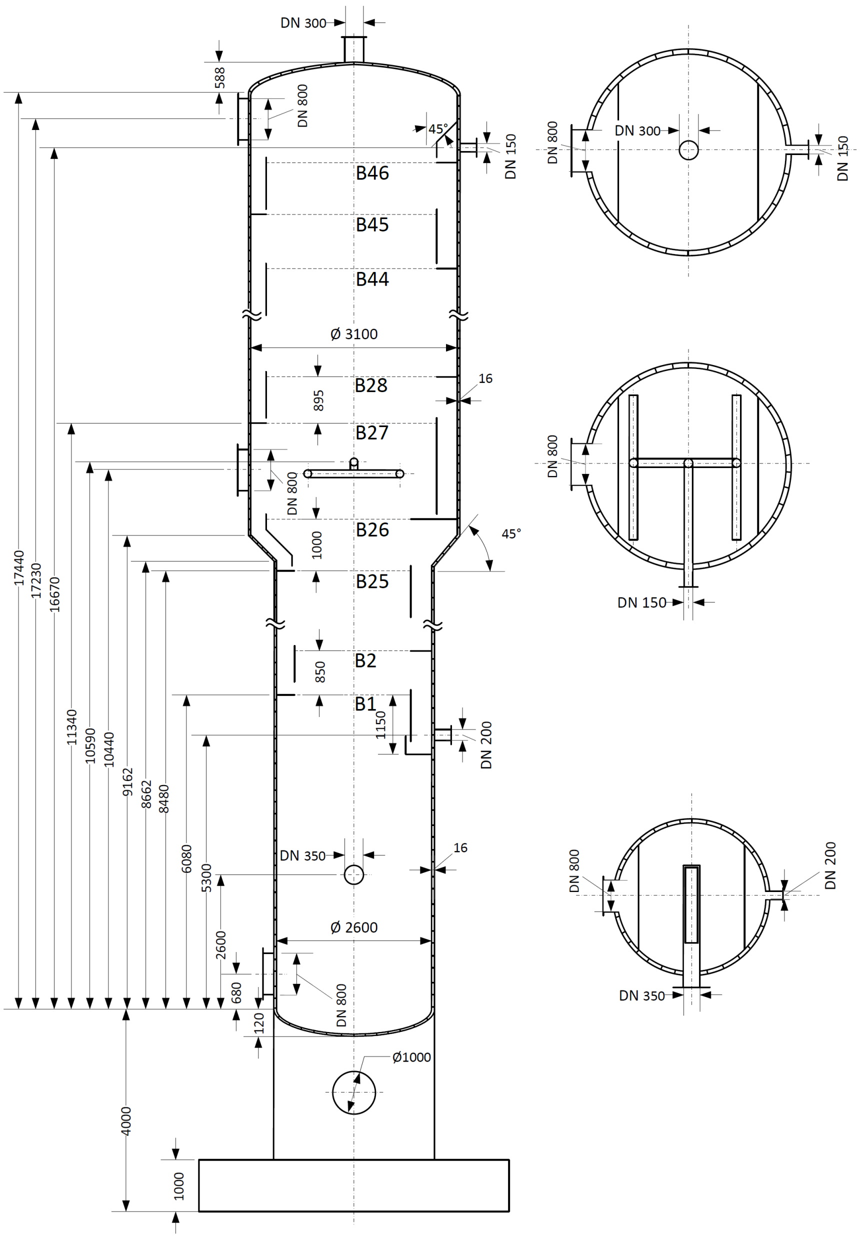


Figure A.32: Exemplary hand sketch of distillation column, drawn within the lecture CAP

A.5 2D-3D data exchange framework - case study

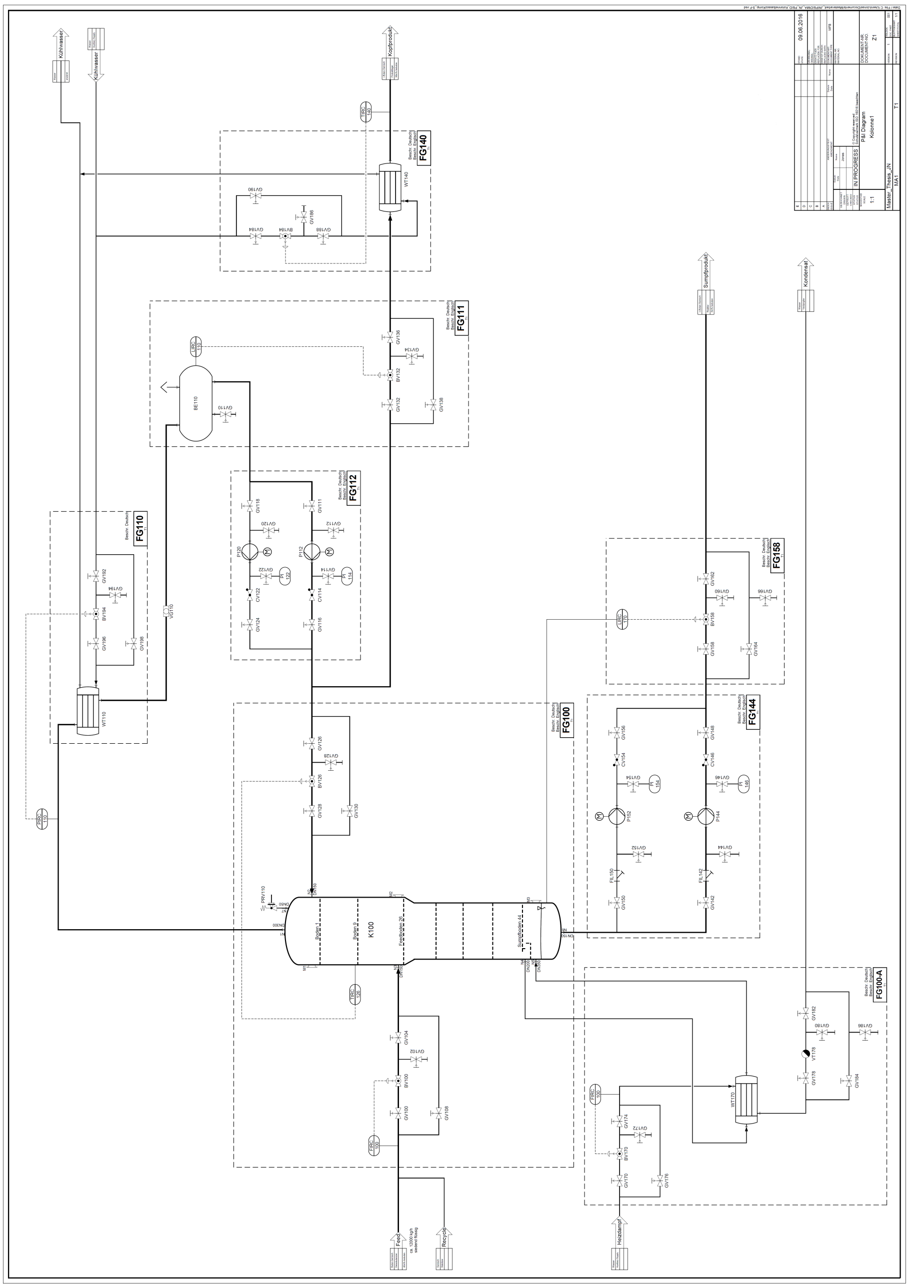


Figure A.33: P&ID of distillation column created with X-Visual PlantEngineer

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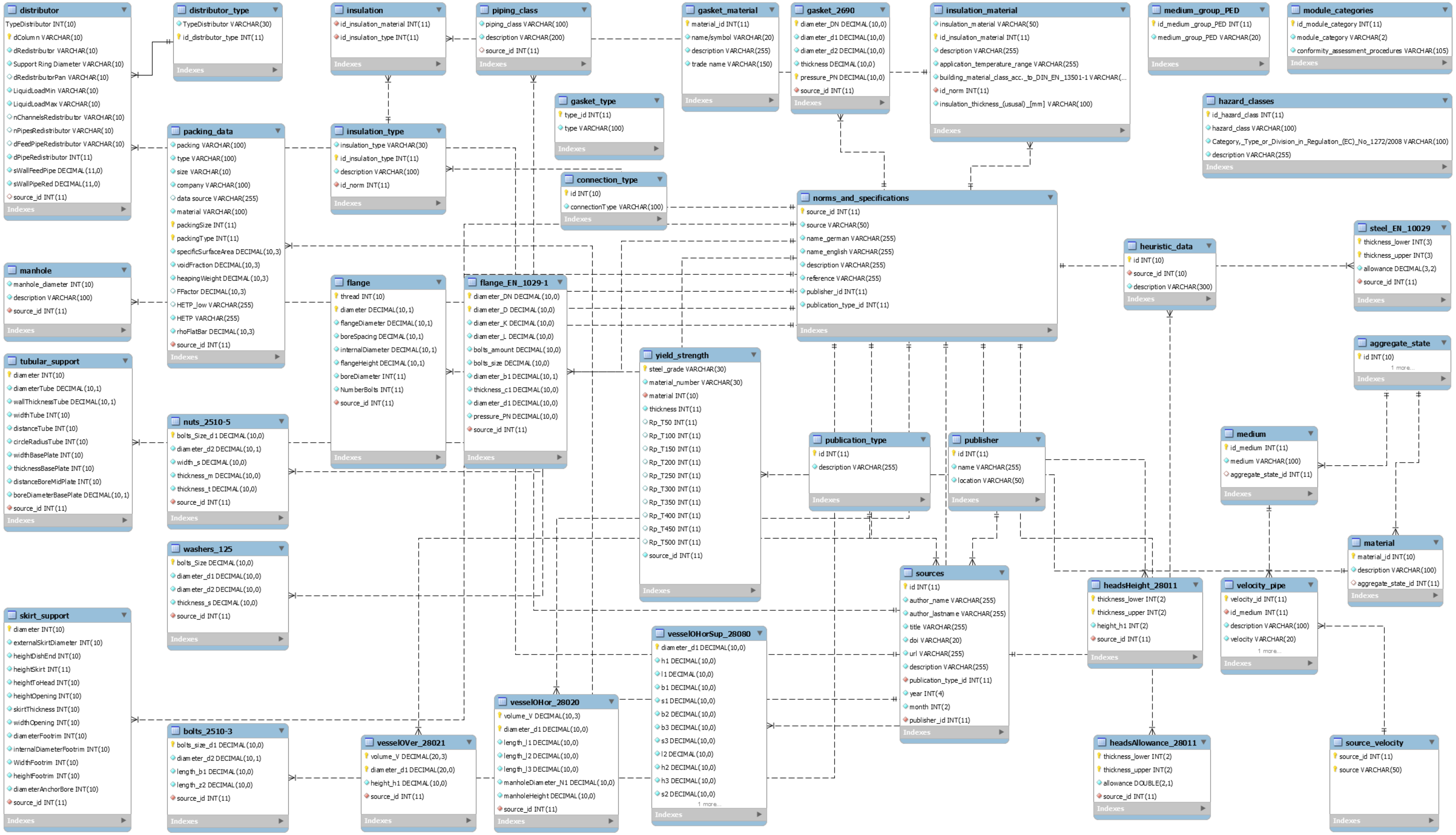
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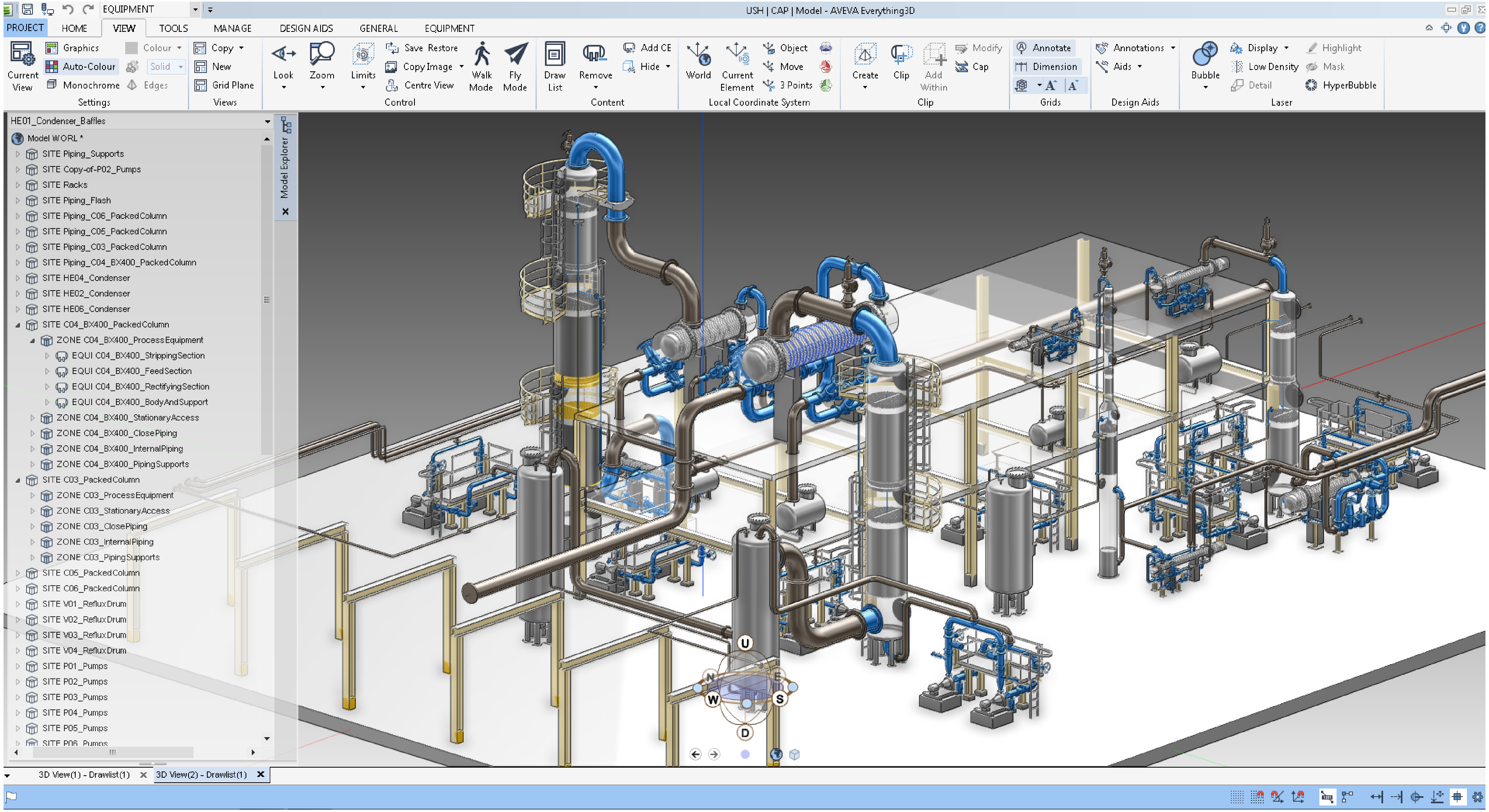
h3 DECIMAL(10,0)
s2 DECIMAL(10,0)
1 more...
vesselOHor_28020
volume_V DECIMAL(10,3)
diameter_d1 DECIMAL(10,0)
length_l1 DECIMAL(10,0)
length_l2 DECIMAL(10,0)
length_l3 DECIMAL(10,0)
manholeDiameter_N1 DECIMAL(10,0)
manholeHeight DECIMAL(10,0)
source_id INT(11)
bolts_2510-3
bolts_size_d1 DECIMAL(10,0)
diameter_d2 DECIMAL(10,1)
length_b1 DECIMAL(10,0)
length_z2 DECIMAL(10,0)
source_id INT(11)
vesselOVer_28021
volume_V DECIMAL(20,3)
diameter_d1 DECIMAL(20,0)
height_h1 DECIMAL(10,0)
source_id INT(11)
headsAllowance_28011
thickness_lower INT(2)
thickness_upper INT(2)
allowance DOUBLE(2,1)
source_id INT(11)
source_velocity
source_id INT(11)
source VARCHAR(50)


EQUIPMENT
USH | CAP | Model - AVEVA Everything3D
PROJECT
HOME
VIEW
TOOLS
MANAGE
DESIGN AIDS
GENERAL
EQUIPMENT
Current View
Graphics
Auto-Colour
Monochrome
Colour
Solid
Edges
Settings
Copy
New
Grid Plane
Views
Look
Zoom
Limits
Save Restore
Copy Image
Centre View
Walk Mode
Fly Mode
Control
Draw List
Remove
Add CE
Hide
Content
World
Current Element
Object
Move
3 Points
Local Coordinate System
Create
Clip
Add Within
Modify
Cap
Clip
Annotate
Dimension
Grids
Annotations
Aids
Design Aids
Bubble
Display
Low Density
Detail
Highlight
Mask
HyperBubble
Laser
HE01_Condenser_Baffles
Model WORL *
SITE Piping_Supports
SITE Copy-of-P02_Pumps
SITE Racks
SITE Piping_Flash
SITE Piping_C06_PackedColumn
SITE Piping_C05_PackedColumn
SITE Piping_C03_PackedColumn
SITE Piping_C04_BX400_PackedColumn
SITE HE04_Condenser
SITE HE02_Condenser
SITE HE06_Condenser
SITE C04_BX400_PackedColumn
ZONE C04_BX400_ProcessEquipment
EQUI C04_BX400_StrippingSection
EQUI C04_BX400_FeedSection
EQUI C04_BX400_RectifyingSection
EQUI C04_BX400_BodyAndSupport
ZONE C04_BX400_StationaryAccess
ZONE C04_BX400_ClosePiping
ZONE C04_BX400_InternalPiping
ZONE C04_BX400_PipingSupports
SITE C03_PackedColumn
ZONE C03_ProcessEquipment
ZONE C03_StationaryAccess
ZONE C03_ClosePiping
ZONE C03_InternalPiping
ZONE C03_PipingSupports
SITE C05_PackedColumn
SITE C06_PackedColumn
SITE V01_RefluxDrum
SITE V02_RefluxDrum
SITE V03_RefluxDrum
SITE V04_RefluxDrum
SITE P01_Pumps
SITE P02_Pumps
SITE P03_Pumps
SITE P04_Pumps
SITE P05_Pumps
Model Explorer
U
N
E
W
S
D
3D View(1) - Drawlist(1)
3D View(2) - Drawlist(1)