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Visual Environment for Editing and Solving Flowsheets

Konstantinos Raptis
September 2017

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Visual Environment for Editing and Solving Flowsheets

Design and implementation of a visual environment for editing and solving flowsheets to produce heat and material balances for urea plant designs

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Stan Ackermans Institute / Software Technology

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Date	**September 2017**	
Document Status	Public	
PDEng report no.	**2017/043**	

The design described in this report has been carried out in accordance with the TU/e Code of Scientific Conduct.

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Published by	Eindhoven University of Technology Stan Ackermans Institute
Printed by	Eindhoven University of Technology *UniversiteitsDrukkerij*
PDEng report no.	2017/043
Abstract	Urea is an organic compound that is used widely as a fertilizer to increase the crop size and the yield. Urea is produced from ammonia and carbon dioxide in urea plants. Stamicarbon's main activity is designing and licensing urea plants. An important activity of the process engineers at Stamicarbon consists of the design of the flowsheet and the calculation of the solution of the heat and material balances for the urea plant. Improving the productivity of the process engineers and shortening the learning curve of the new process engineers is of great importance to Stamicarbon. Stamicarbon's vision is to the change the flowsheet design from text-based to graphics-based. This project aimed to implement a graphics-based solution that would increase the comprehension of the structure and the state of the flowsheet design. This project also aimed to enable the process engineers to visually merge plant sections that could be reused in flowsheet designs. Finally, a part of this project involved the integration of the graphics-based editor and the flowsheet solver into one tool. The three major design criteria are usability, navigability, and extensibility. The main tools used for the implementation of this project are the Eclipse Modeling Framework (EMF) and the Eclipse Sirius. The domain model is designed with EMF. The visual representations are created with Eclipse Sirius. The architecture of the system is plug-in based. The final prototype is deployed as an RCP outside the Eclipse IDE.
Keywords	Flowsheet, heat and material balances, EMF, Eclipse Sirius, Stamicarbon, TUE, PDEng, software technology
Preferred reference	Visual environment for editing and solving flowsheets: Design and implementation of a visual environment for editing and solving flowsheets to produce heat and material balances for urea plant designs. PDEng Technical Report, September 2017. (2017/043)

Foreword

Automation is a key driver for improving productivity. Tasks that were performed manually in the past are currently being executed by machines that get the job done faster and better and thus cheaper. This is not only the case in industries that produce tangible artefacts like machines and consumer goods but also in the services sector where engineering companies like Stamicarbon produce design information. Here the essence is to instruct a computer to solve a particular engineering problem, which is to find a design that meets specific requirements within specific design constrains. At Stamicarbon the end-product is a Process Design Package (PDP) for urea plants. It contains the necessary information (minimum requirements) for further detailed design and construction of a urea plant. An essential part of a PDP are Heat and Material Balances (H&MB).

Creating a H&MB is repetitive task executed by an engineer and supported by a computer which requires flexibility with respect to the specification of requirements and design constraints. For that purpose Stamicarbon uses an in-house developed software tool called Tisflo whose origin dates back to the mid 70ties of the last century. This tool's strengths are also its weaknesses on two levels: the tool smith's level and practitioner's level. The tool smith is confronted with a FORTRAN implementation (parser, domain model, and solver) that is compact and fast but undocumented, ill-structured and hardly maintainable which hampers modification and extension of the tool. The practitioner is confronted with an extremely fast flowsheet solver and a very flexible but archaic, hard-to-learn and error-prone low level problem specification language with little help on diagnosing specification problems. Productivity gain is only to be expected when the weaknesses on both levels are addressed: specification on higher levels of abstraction both of the tool itself as well as the problems to be solved by the tool.

Model Driven Software Engineering promises to be the perfect candidate for the redesign job of the software. It should get you from A to B fast and good and improve productivity. This is why Stamicarbon embarked on journey for a step-wise transformation of Tisflo: a first step (in hind sight a side step) was to wrap the essential FORTRAN code in C++ wrappers, rewrite the parser (using ANTLR), the domain model and the solver in C++ and produce a functional kernel. A second more fundamental step was the development of an EMF based meta-model for the flowsheet domain that allows easy integration with a graphical front and allows for M2M and M2T transformations serving and increasing both the productivity of the tool smith and the practitioners. The thesis you are about to read reflects the work done by Konstantinos Raptis on developing the meta-model and the graphical front-end for Tisflo 2.0 whose result shows that MDSE is truly bringing value to development and deployment of real-world engineering tools. We are not there yet but we have taken a first step in the right direction. On behalf of the colleagues in Stamicarbon I would like to thank Kostas and his TU/e mentor prof. dr. Mark van den Brand for the efforts they put into the project. I hope you enjoy reading Kostas' thesis.

ir. Rob Faessen
August 2017

Preface

This report summarizes the "Visual environment for editing and solving flow-sheets" project. The project was carried out by Konstantinos Raptis as a final assignment for the Professional Doctorate in Engineering (PDEng) program in Software Technology (ST). The program is provided by the Stan Ackermans Institute of the Eindhoven University of Technology. The project was executed over a period of a nine-months at the end of the two-year program, under supervision of Stamicarbon B.V. in Sittard.

This report is primarily intended for a reader with a technical background in different disciplines, such as model-based engineering, visual editing, and general software engineering.

Chapters 1 to 4 are more suitable for readers with a non-technical background who are interested in getting an introduction about the project, the problem, and learning details about process flow diagrams from urea plant designs.

Chapters 6 to 10 are more interesting for readers with a technical background. These chapters cover the system requirements, the system architecture, the system implementation, the verification and validation, and the deployment of the project.

Finally, Chapters 2, 5, 11, 12, and 13 cover the project management, conclusions, and the project retrospective.

Konstantinos Raptis
September 2017

Acknowledgements

I would like to express my sincere gratitude to all the people who helped me, guided me, and supported me during this nine-month project. This project was a great experience for me and the success would not be possible without them.

First of all, I would like to thank all the people working at Stamicarbon for their support and the great working atmosphere that they provided me during this project. More specifically, I would like to thank my Stamicarbon supervisor, Rob Faessen, for his guidance, knowledge, and enthusiasm that contributed to the success of this project. I would also like to thank Harry Welten for the support and valuable information that helped me understand the domain. Furthermore, I would like to thank process engineers, Chuanbo Gao, Gijs de Jong, Hoa Bui, Paz Munoz, Rahul Patil, Veronica Rivas, and Yuniyono Kho. Finally, I would like to express my thanks to the Head of the Process Department Harold Borkink.

I also owe the success of this project to my university supervisor, prof. dr. Mark van den Brand who pinpointed improvements of the project and gave me valuable feedback. His expertise in model-driven software engineering encouraged me to explore different angles and views of the project.

Moreover, I would like to thank everyone involved in the PDEng program during the past two years. More specifically I would to thank our program directors, dr. Ad Aerts and dr. Yanja Dajsuren PDEng; our secretary, Desiree van Oorschot; and all the OOTI coaches.

Furthermore, I would like to thank my colleagues from the PDEng program for the experiences was shared during the past two years. It was a great opportunity for me to meet people from different cultures and work with them.

Last but not least, I would like to thank my family, friends, and girlfriend for all the support and trust that they gave me.

Konstantinos Raptis
September 2017

Executive Summary

The world's population is increasing by more than 1% per year. More than 7.4 billion humans live on earth. This number is expected to be more than 9 billion by 2040 [1]. As the number of humans is increasing, the demand for food is also increasing. Since the area of the world's agricultural land is expected to be almost the same in the next 20 years [2] a solution for producing enough food has to come from somewhere else. Urea can be used to increase the global food production. Urea is an organic compound that is used widely as a fertilizer to increase the crop size and the yield. Urea is synthesized in chemical plants from ammonia and carbon dioxide.

Stamicarbon's main activity is licensing urea plants. The licensing requires the collaboration of people from different engineering disciplines, for example, process engineers, process control engineers, and mechanical engineers. An important task of the process engineers at Stamicarbon consists of the design of flowsheet diagrams and the calculation of the heat and material balances.

Process engineers at Stamicarbon design flowsheet diagrams with a text editor. The flowsheet diagrams are specified in text format that has a rigid layout; an extra space could make the text file invalid. A second tool is used for the calculation of the heat and material balances. This tool is called Tisflo.

Improving the productivity of the current process engineers and shortening the learning curve of the new process engineers is of great importance to Stamicarbon. Stamicarbon's vision is to the change the flowsheet design from text-based to graphics-based.

A famous English language proverb says "a picture is worth a thousand words." This project aimed to provide a graphics-based solution that would increase the comprehension of the structure and the state of the flowsheet design. Editable forms aimed to eliminate the number of errors made because of the rigid layout of the text files. This project also aimed to enable the process engineers to visually merge plant parts that could be reused between different designs. Finally, a part of this project involved the integration of the editor and the solver into one tool.

This report presents the architecture, the design, and the implementation of the graphical-based Tisflo. The three major design criteria are usability, navigability, and extensibility. The main tools used for the implementation of this project are the Eclipse Modeling Framework (EMF) and the Eclipse Sirius. The domain model is designed with EMF. The visual representations are created with Eclipse Sirius. The architecture of the system is plug-in based. The final prototype is deployed as an RCP outside the Eclipse IDE.

In conclusion, the prototype is the first version of the graphical-based Tisflo that calculates the heat and material balances of urea plant designs. According to the feedback from the process engineers the prototype achieved the main goals and aims of the project, although extra functionality needs to be added until it can fully replace the old tools. The extra functionality is mentioned as a future work in this report.

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1.Introduction

This chapter introduces Stamicarbon as a company. The project and its context are briefly mentioned. The outline section at the end of this chapter gives a brief overview of what is discussed in the following chapters.

1.1 About Stamicarbon

Stamicarbon was founded in 1947 and currently is a member of Maire Tecnimont SpA. Stamicarbon's main activity is the development and the licensing of urea technology for the fertilizer industry. More than 250 urea plants around the world are based on Stamicarbon's technology to produce urea, which adds nutrients to crops, replenishes arable land, and increases crop yields [3].

Figure 1 Urea plant

Licensing commercializes the know-how that has been developed and patented over the years as a result of Research and Development activities and experience gained of plant operations. Stamicarbon designs have to meet customers' needs with respect to safety, product quality and quantity, reliability, emissions, and energy consumption.

1.2 About urea

Urea is an organic compound with the chemical formula $CO(NH_2)_2$. Since its discovery in 1773, urea has become the most important nitrogen-based fertilizer in the world.

Urea is produced from a mixture of simple inorganic molecules (ammonia and carbon dioxide); the white crystalline organic compound contains about 46% nitrogen.

The vast majority of urea is used in the agricultural sector as a fertilizer to increase crop yield and as an additive for animal feed. Urea is also used as a base product in the manufacture of resins and commercial adhesives. Cosmetics products, for instance, hair conditioners, tooth-whitening, and facial cleaners might contain urea. Cars and trucks use urea in the exhaust gas catalysts in order to reduce the NO_X emissions.
Urea facts [4]:

- Urea is the world's most produced chemical.
- Over 190 million tons of urea is produced each year.
- Over 80% of urea is used to fertilize crops.
- Demand for urea fertilizer is growing at over 3% (faster than the global rise in population).

1.3 *Life cycle of a urea plant*

Stamicarbon’s main activity is licensing new urea plants, maintaining, upgrading and optimizing existing plants. Each license requires the collaboration of many people from different engineering disciplines, for example, process engineers, process control engineers, and mechanical engineers.

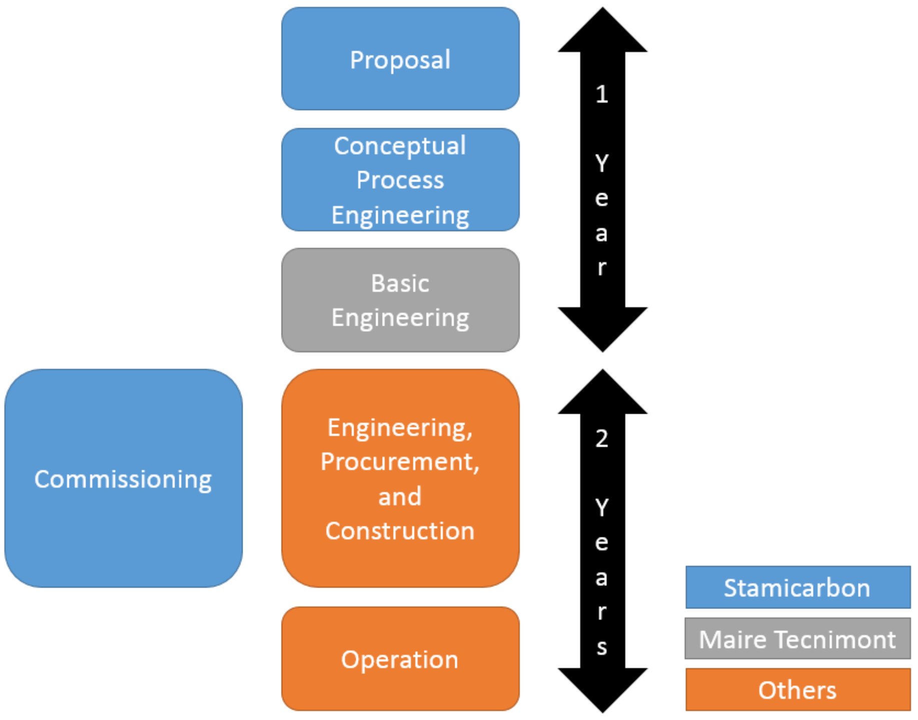


Figure 2 Life cycle of a new urea plant

The life cycle of a project depends on the type of the project and on the customer requirements. An average time of three years from a concept proposed by a customer to an actual new plant that produces urea is required. Projects that involve optimization or upgrade of an existing plant start with a feasibility study; however, this phase is omitted in projects that involve the creation of a new urea plant. For a new urea plant projects Stamicarbon delivers a proposal to the customer about the equipment that can be used, an estimation of the costs of the project, the process flow diagrams, and the heat and material balances of the plant.

The next stage is the conceptual process engineering phase. At the end of this stage the customer receives the Process Design Package (PDP). The PDP contains documents with more detailed information about the plant, for instance, the piping and instrumentation diagrams, and equipment datasheets, in addition to the process flow diagrams, and the heat and material balances with minor changes for tuning purposes.

The next stage is the basic engineering phase. In this phase a company of the Maire Tecnimont group delivers to the customer and to the constructors the Basic Engineering Package (BEP). The BEP contains more detailed information about the construction, for instance, the physical position of the equipment. Finally, Stamicarbon is also involved during the detailed Engineering, Procurement, and Construction (EPC) phase of the plant in order to verify if it functions according to its design objectives and specifications. At the end of a three year period the plant is ready to operate.

1.4 *Process engineers' responsibilities*

In order to meet customers' needs for licensing a urea plant, a part of the process engineers' job is designing process flow diagrams and calculating the heat and material balances based on the process flow diagram. A process flow diagram is the conceptual layout of a plant. A process flow diagram indicate the equipment and the main process streams between the equipment. A process engineer spends a week on the design of a process flow diagram.

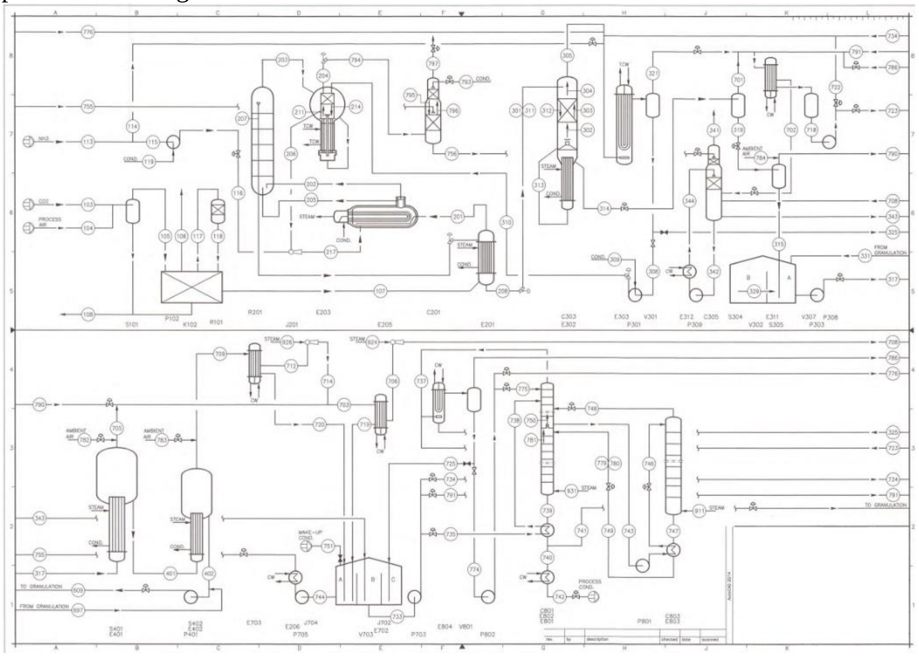


Figure 3 Process flow diagram

A heat and material balance is a document produced by process design engineers. The heat and material balance document includes operating conditions, composition and key physical properties of every major process stream on the process flow diagram. The calculation of the heat and material balances is performed by applying the mass balance equation and the energy balance equation to each piece of equipment. A process engineer spends five weeks on the calculation of the heat and material balances.

1.5 *Project introduction*

The idea behind the project is the utilization of a new tool that the process engineers could use for creating or editing flowsheet diagrams and calculating the heat and material balances.

The process engineers are currently using text files with a rigid layout for storing the definition of urea plant designs and for specifying what heat and material balances are calculated. However, the rigid layout could lead to many errors. In order to create or edit a urea plant design and calculate the heat and material balances, the process engineers have to use two different tools.

The first tool is a text editor to create or modify the structure of a urea plant design. For example, a process engineer can use a text editor for adding a new stream or changing the name of an existing stream. However, the process engineers have to be very careful while editing because of the rigid layout that the files have.

The second tool is a flowsheet solver. The process engineers use the flowsheet solver for calculating the heat and material balances of a urea plant design. However, the process engineers using the flowsheet solver cannot modify the structure of a urea plant design.

It is worth mentioning that the process engineers are mostly working on files that contain information of a complete urea plant and not on files that contain different parts of a urea plant. The main reason for not working on files containing different parts is again the rigid layout that the files have. Combining all the different plant parts into one could lead to many errors.

This project focuses on a graphics-based tool that could increase the comprehension of the structure and the state of the flowsheet design. This project also focuses on a tool that the process engineers could use for combining different plant sections into one. The elements contained in the different sections have to be editable and the tool has to allow the process engineers to simulate the plant sections or the complete plant. In addition, the new tool has to provide ways to eliminate syntax errors made with the text editors. Finally, the new tool has to integrate the graphics-based editor and the flowsheet solver into one tool.

1.6 Outline

The next chapter introduces the stakeholders involved in this project as well as their goals and interests. After the presentation of the stakeholders, the problem analysis is presented (Chapter 3), which describes the aspects and the expectations of the project. Next, the domain analysis is presented (Chapter 4), namely urea plant designs.

Chapter 5 presents the feasibility analysis of the problem. Potential issues, challenges, and risks are identified are presented. After the feasibility analysis, the system requirements are presented in Chapter 6. The requirements are presented in two categories the functions and the non-functional.

Chapter 7 presents the system architecture. Chapter 8 presents the system design and implementation. Design decisions are also covered on this chapter. Next, Chapter 9, elaborates on the verification and validation. Chapter 10 depicts the deployment of the system.

Chapter 11 discusses the results and future work for the project. Chapter 12 reflects on the project management. Finally, Chapter 13 presents the retrospective of the project from the author’s point of view.

2.Stakeholder Analysis

In the previous chapter an introduction about Stamicarbon is given.
This chapter analyzes the stakeholders involved in the project, their interests, and their goals. The two main parties involved in the project are Stamicarbon and Eindhoven University of Technology.

2.1 Stamicarbon

Stamicarbon is the project owner. Stamicarbon has two interests as their key drivers for the project. The first interest is to shorten the learning curve for new engineers. New process engineers receive six month training courses to learn the domain and the company's software tools. Stamicarbon is also interested in improving the productivity of process engineers. Process engineers use two separate text-based environments for designing urea plants. In order to achieve the aforementioned interests Stamicarbon envisions a new graphic-based environment for designing urea plants.

The Stamicarbon stakeholders can be grouped in two categories:

1) Process Control and Modelling Department:

Process Control and Modelling Department	
Name	Role
Rob Faessen Head of Department	Project supervisor and owner. Member of the Progress Steering Group. Manages project progress and defines priorities and requirements. Provides knowledge about the existing software tools and extends the back-end code.
Harry Welten Technical Software Engineer	Provides knowledge about the existing software tools and is responsible for extending the back-end code.

2) Process Engineering Department:

Process Engineer Department	
Name	Role
Chuanbo Gao Gijs de Jong Hoa Bui Harold Borkink Paz Munoz Rahul Patil Veronica Rivas Yuniyono Kho	The actual users of the deliverable of the project. Provide feedback and request new features.

2.2 Eindhoven University of Technology (TU/e)

The Eindhoven University of Technology is responsible for the educational aspect of the project. The educational aspects of the project are related to the software design process, project implementation, project management, and risk management. That means certain standards have to be met.

TU/e Stakeholders	
Name	Role
Ad Aerts	Ensures the quality and the deliverables of the project that are in line with the program standards.

Program Director of PDEng in Software Technology	
Mark van den Brand TU/e Supervisor	Ensures quality of the design and the scientific aspect of the report.
Yanja Dajsuren Program Director of PDEng in Software Technology	Ensures the quality and the deliverables of the project that are in line with the program standards.
Konstantinos Raptis PDEng Candidate	Responsible for the design and the implementation of the project. In parallel, responsible for matching project results with company and university standards.

3.Problem Analysis

In the previous chapter the stakeholders and their interests are mentioned.
This chapter focuses on the problem that this project is trying to solve. First, there is an introduction about the project and the problem. Next, there is an introduction and brief explanation about how the process engineers interact with the text files, the text editor, and the flowsheet solver. Finally, reasons why a new tool for the process engineers is needed, are given.

3.1 Introduction

The flowsheet design of a urea plant is an important step for the calculation of the heat and material balances that are needed for granting a license. New process engineers receive six month training courses in order to learn the domain and the company's software tools. A process engineer on average can calculate the heat and material balances in five weeks. Stamicarbon is interested in ways that can shorten the learning curve of new engineers and improve the productivity of the process engineers.

The information needed for the heat and material balances of a plant is stored in text files, for instance, in a text file the process engineers specify what heat and material balances will be calculated. The text files have two big downsides. The first is a rigid layout. The second is the limited overview that they provide to the process engineers, for example, the best way for a process engineer to find where a specific artifact is used is to search for the name of the artifact within the text.

In order to create or edit a urea plant design and calculate the heat and material balances, the process engineers use two different tools. A text editor is a tool that the process engineers use for creating or modifying the structure and the state of a urea plant design. The flowsheet solver is the tool that the process engineers use for calculating the heat and material balances of a urea plant design. Tisflo is the name of the flowsheet solver that the process engineers use.

This project aims at designing and implementing a tool that could be used both as an editor and as a flowsheet solver and it would provide visual representations of the different artifacts. Another aim of the tool is to allow the process engineers to work on small parts that could be reused between different designs. The tool aims to allow process engineers to merge the different parts for the definition of a urea plant design. By providing a merge functionality, it would possible to allow the process engineers to work simultaneously on different parts of the same plant. In general, the new tool aims to improve the productivity and the overview that the process engineers have about the urea plant designs.

3.2 Text files

The text files contain the information needed for the calculation of heat and material balances. The information required is:

- Process definition
- Process determination

The definition should include the following specifications:

- Chemical components occurring in the process
- Nodes involved and how they are linked

The determination consists of:

- Specification of known data

- Requirements

The file extension of the text files is DAT. The text in the file has to follow a strict syntax and each character should be placed in a specific position. A text editor is a tool that the process engineers use for creating or editing text files. A process engineer can load a text file to Tisflo for calculating the heat and material balances.

3.2.1. Text files example

For example, if a process engineer would like to calculate the heat and material balances of the flowsheet diagram as shown in *Figure 4*, then a text file with text similar to *Figure 5* should be created. The text file can contain extra information, for instance, in *Figure 5* two chemical components with names A and B are added. The two chemical components are not visible from *Figure 4.*

The biggest downside, as already mentioned, with the text files is the strict syntax the specific position that each character should have. A character in a wrong position always leads to an invalid file. *Figure 6* shows an invalid file because the X of component A from stream STR2 is not aligned in correct position. In addition, the names have a maximum size, for example, the stream names cannot have more than six characters.

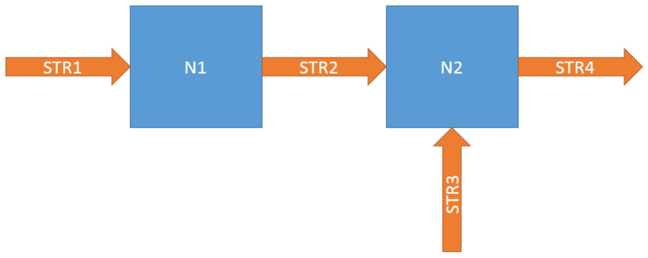
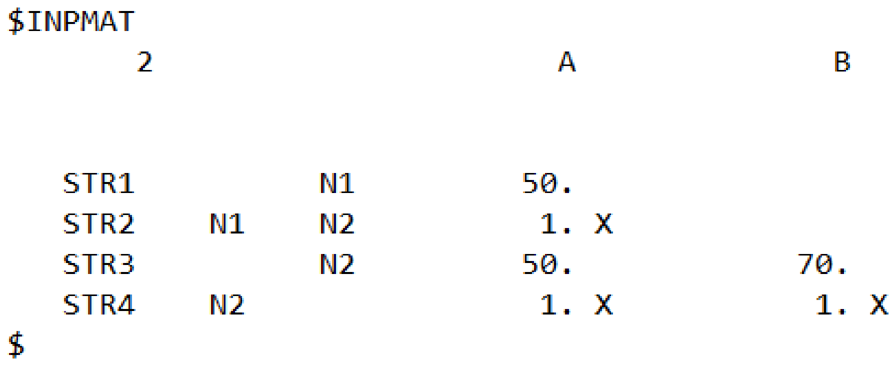


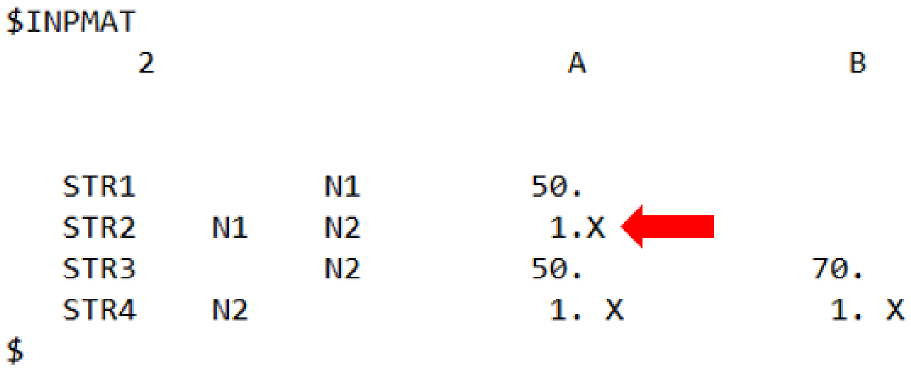
Figure 4 Flowsheet diagram with 2 nodes and 4 streams



```
$INPMAT
       2                      A              B


   STR1         N1         50.
   STR2   N1    N2          1. X
   STR3         N2         50.            70.
   STR4   N2                1. X           1. X
$
```

Figure 5 Textual representation of Figure 4



```
$INPMAT
       2                      A              B


   STR1         N1         50.
   STR2   N1    N2          1.X
   STR3         N2         50.            70.
   STR4   N2                1. X           1. X
$
```

Figure 6 Invalid textual representation of Figure 4

3.3 *Text editor*

A text editor is a tool that process engineers use for creating or modifying the structure and the state of urea plant designs. The choice of the text editor is up to the process engineers. The text editor choice could vary from Notepad to more sophisticated text editors such as Notepad++ or UltraEdit.

3.3.1. Text editing example

For example, if a process engineer would like to add a new incoming stream with name STR5 and 25 units of component B to the node N2, then the process engineer has to open with a text editor a text file that contains text similar to *Figure 5* and modify it. Otherwise the process engineer could create a new text file from scratch.

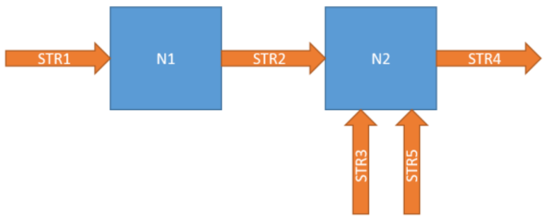


Figure 7 Flowsheet diagram with the addition of stream STR5

```
$INPMAT
       2                      A              B


   STR1          N1         50.
   STR2    N1    N2          1. X
   STR3          N2         50.            70.
   STR4    N2                1. X           1. X
   STR5          N2                        25.
$
```

Figure 8 Textual representation with the addition of stream STR5

3.4 *Tisflo*

Tisflo is the software tool used as a flowsheet solver. Tisflo is intended for use by process engineers for calculating the heat and material balances. The process engineers have to provide the information needed for Tisflo in a text file.

Tisflo can be used for simulation, balancing of redundant data, and optimization [5].

- Simulation: calculation of a system without degrees of freedom. The system is determined by the combination of given information and requirements. The number of unknowns is equal to the number of equations.
- Balancing: calculation of a system with redundant data (measured data); there is more information available than is necessary for solving all the equations.
- Optimization: calculation of a system with degrees of freedom to which an object function has been added. In addition, constraints are also incorporated.

The program solves the problem in such a way that the conditions of all equations are satisfied, the constrained variables lie in their allowable range, and the object function is maximum.

3.4.1. Tisflo example

In this section an example of how Tisflo works is presented. As mentioned, Tisflo can calculate the heat and material balances according the text files. In the example below stream matrixes present the information contained in the text files because they are easier to read. The stream matrix of the flowsheet diagram in *Figure 4* is as *Table 1* shows.

Table 1 Stream matrix

Stream	From Node	To Node
STR1		N1
STR2	N1	N2
STR3		N2
STR4	N2	

Figure 5 shows that the flowsheet diagram has two chemical components with names A and B. The amount can represent a quantity in a specific unit, for instance, kg/h; however, it is omitted. If the amount is unknown an X is added. In the textual representation a number before the X is required, although in the stream matrix we could skip this unnecessary information.

Table 2 Stream matrix with chemical components A and B

Stream	From Node	To Node	Chemical Component A	Chemical Component B
STR1		N1	50	
STR2	N1	N2	X	
STR3		N2	50	70
STR4	N2		X	X

In order to calculate the heat and material balances of *Table 2* a process engineer has to load a text file into Tisflo and run the flowsheet problem.

Table 3 Result of the stream matrix with chemical components A and B

Stream	From Node	To Node	Chemical Component A	Chemical Component B
STR1		N1	50	
STR2	N1	N2	50	
STR3		N2	50	70
STR4	N2		100	70

Results explanation: Every chemical component that goes into a node has to go out. In our case the 50 units of A that go into the node N1 from stream STR1 should go out via the stream STR2. The incoming units to node N2 are 50 units of A from stream STR2, 50 units of A and 70 units of B from stream STR3. The units that pass through stream STR4 should be 100 of A and 70 of B.

3.5 New tool

When a process engineer is working on different plant parts it means that he or she is working on different text files. A complete plant can be a combination of text files defining different plant parts. However, different text files might have the same information written in a different order. Text files could have a different order for the chemical components. In case of a merge a process engineer decides which order to follow and modifies the text accordingly. In a merged file the naming of the different elements should be taken into consideration. A name that appears the same in two files means that either the name from one file must change or the name must be added only once in the merged file. The process engineer should also consider the predefined position of the characters. Errors can appear even with an extra space. Taking into consideration everything that is mentioned in this paragraph means that merging two text files is not an easy task, and that is the reason that usually only one process engineer works on a project.

The text files also limit the overview that the process engineers have about the design. Having more complex flowsheet diagrams than the diagram shown in *Figure 4,* for instance, a diagram with 20 nodes and 100 streams, would require a considerable amount of time for the process engineers to understand which streams are connected to which nodes.

Another downside of the current infrastructure is that the process engineers use two tools, one tool for editing the structure and another tool as a problem solver. If the same text file is opened with both tools then for every structure change made in text editor the changes would be reflected in the problem solver only if the file is reloaded.

The original proposal for the new tool was the following:
The new tool should be graphics-based and therefore should increase of the overview that the process engineers have about design. In order to eliminate the syntax errors and the errors caused from the predefined position of the characters in the text file the new tool should have forms that the process engineers could fill. The new tool should simplify how different plant parts can be merged. There are different designs that could be reused, for instance, there are four different reactors that the process engineers could choose for their design. The process engineers could reuse designs or work in parallel on different parts and decrease their scope if they could easily merge the different plant parts. Last but not least, the new tool should combine the editing and problem solving into one tool.

The high level goals were:

- Shorten the learning curve of the new engineers
- Improve the productivity of engineers

The project aimed to:

- Increase the comprehension of the structure and the state of the flowsheet design
- Decrease the number of errors made by the engineers
- Allow the process engineers to use predefined reusable sections that can be merged
- Allow the process engineers to work simultaneously on different plant parts
- Integrate the editor and the solver into one tool

3.6 Design Criteria

In this section we introduce the design criteria that surround the software design of the project. The criteria are from a high level point of view and based on the problem that project is trying to solve. The three major criteria for the design are:

Usability
The issues discussed in this chapter suggest a need for a tool that can improve process engineers' productivity and shorten their learning curve. Usability should be addressed by means of making the product easy to understand and use.

Navigability
Navigability could improve the overview that the process engineers have about their design. The way that the process engineers interact with the diagrams and navigate between the different elements of the diagrams should be taken into consideration.

Extensibility
The design is a unified solution for editing and solving flowsheets. The new tool should be easily extendable with functionality that the process engineers might require in the future.

Based on the design, the design criterion that is less applicable is:

Simplicity
Version management of visual representations is also more complex than version management of text because extra information is stored, such as the position, the size, and the color of the different elements. An experienced process engineer might require more time to edit visual representations compared to text. Last but not least, in the software design extra associations between the elements could be used in order to improve the usability and navigability.

4.Domain Analysis

In the previous chapter the problem analysis is discussed, which revealed the domain of the project, namely urea plant designs.
This chapter gives a more detailed explanation about the domain and focuses on the relevant part of the solution of the problem. The following sections give a detailed view of the urea plant design from the point of view of a process engineer.

4.1 Introduction

This chapter describes what a process flow diagram is, what a process flow diagram contains, and how the process engineers calculate the heat and material balances.

4.2 Process flow diagrams

A process flow diagram is the conceptual layout of a plant. A process flow diagram displays equipment and relationships between the equipment of a plant. It also indicates the general flow of chemical components between equipment in a urea plant design.

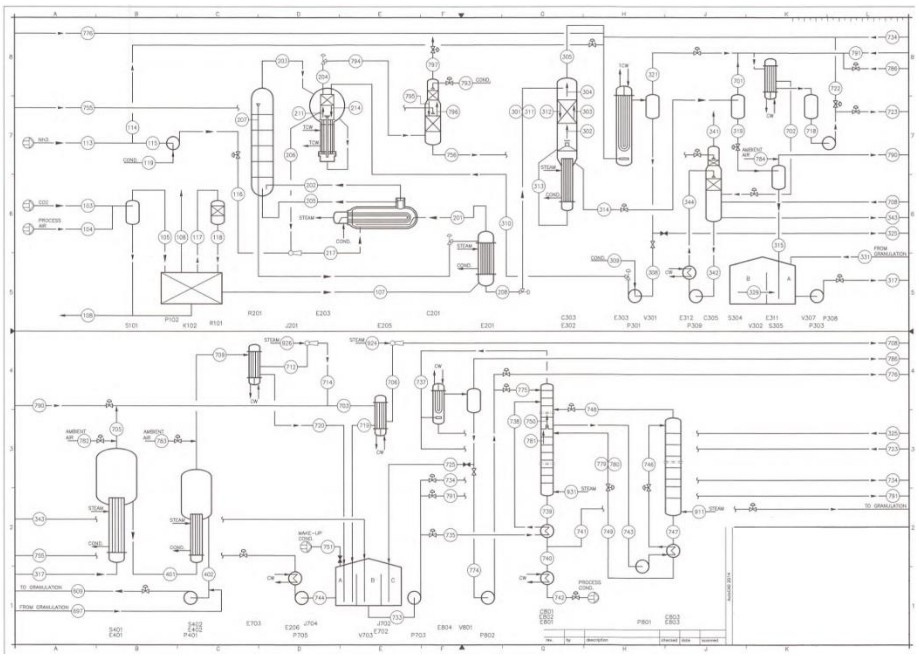


Figure 9 Process flow diagram

A process flow diagram that represents a complete urea plant can be decomposed into smaller parts that are called *sections*. Sections are responsible for a specific function in a urea plant. Some of the most common sections are

- Synthesis
- Low pressure recycle
- Evaporation
- Water treatment
- Finishing

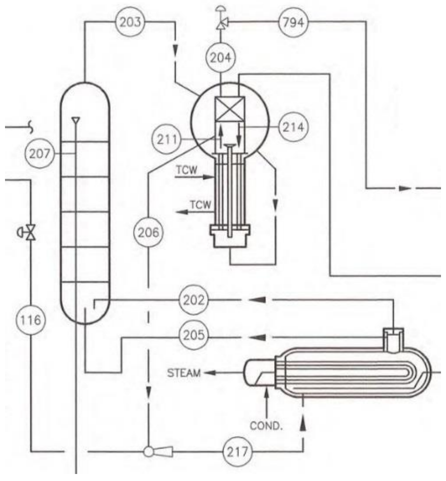


Figure 10 Synthesis section

Each section consists of different equipment. Some of the most common pieces of equipment are

- Reactor
- Stripper
- Carbamate Condenser
- Scrubber

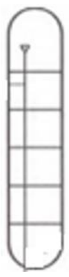


Figure 11 Reactor in a urea process flow diagram

The process flow diagram also displays the relationship between pieces of equipment of a plant. The relationship is described as stream. A stream contains a mixture of chemical components flowing from one piece equipment to the other. Stream is an abstraction of a pipe. Streams are used for structuring and decomposing the problem; therefore, a pipe in a plant may consist of more than one stream.

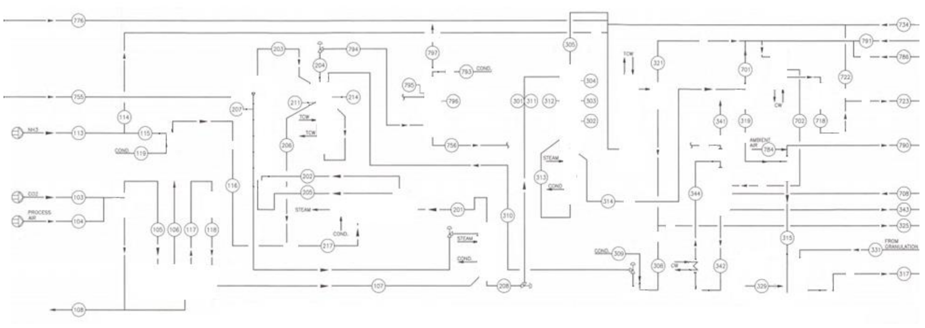


Figure 12 Streams in a process flow diagram

4.3 Heat and material balances calculation

As described the information needed for the calculation of heat and balances is stored in text files. A text file may contain the information of a complete plant or a section or a piece of equipment. Streams are responsible for physical property and chemical component flow. A stream can be attached to up to two nodes (from node and to node). A node is a joint point with zero to many input and output streams. A piece of equipment can be represented as a set of nodes.

The streams are responsible for physical property and chemical component flow. Examples of chemical components in a urea plant design are:

- Urea (CH_4N_2O)
- Ammonia (NH_3)
- Water (H_2O)
- Carbon dioxide (CO_2)

Examples of physical properties in a urea plant design are:

- Temperature
- Pressure
- Enthalpy

Each stream has variables equal to the number of chemical components and physical properties. The total number of variables is equal to the number of all the stream variables. The name of the variable is the stream name plus the chemical component or the physical property. A variable can be free or fixed. Fixed means that the value of the variables is given by the process engineers. Free means that the value is not known and it should be calculated for the problem solution from the flowsheet solver.

A necessary rule for a flowsheet problem to be considered as determined is that the total number of equations must be equal to the free variables. If the number of variables is more or less than the number of equations, then the problem is considered as over-determined or under-determined respectively. In a flowsheet all the chemical components that go into a node must go out.

4.3.1. Heat and material balances calculation example

The calculation of the heat and material balances is based on mathematical equations. The steam matrix of *Table 4* has six variables; three are fixed and the other three free. The problem has three equations:

$$\mathrm{STR1.H2O} = STR2.H2O$$
$$STR2.H2O + STR3.H2O = STR4.H2O$$
$$\mathrm{STR3.CO2} = STR4.CO2$$

The number of equations is equal to the number of free variables and the problem is determined.

Table 4 Stream matrix with a determined problem

Stream	From Node	To Node	H2O	CO2
STR1		N1	50	
STR2	N1	N2	X	
STR3		N2	50	70
STR4	N2		X	X

By changing the state of one variable from free to fixed or vice-versa, the problem would be over-determined or under-determined respectively.

Table 5 Stream matrix with an over-determined problem

Stream	From Node	To Node	H_2O	CO_2
STR1		N1	50	
STR2	N1	N2	X	
STR3		N2	50	70
STR4	N2		X	80

Table 6 Stream matrix with an under-determined problem

Stream	From Node	To Node	H_2O	CO_2
STR1		N1	X	
STR2	N1	N2	X	
STR3		N2	50	70
STR4	N2		X	X

For the calculation of the heat and material balances the process engineers can specify the ratio between chemical components or between physical properties by using labels. For instance, *Table 7* is equivalent to *Table 4*.

Table 7 Stream matrix with labels

Stream	From Node	To Node	Labels	H_2O	Labels	CO_2
STR1		N1		50		
STR2	N1	N2		X		
STR3		N2	LB1	1	LB1	1.4
STR4	N2			X		X
Label	Value					
LB1	50					

In the previous examples the equations are linear; however, in real plants non-linear equations are being used. The process engineers can create their own models or use existing thermodynamic-models that are available in the flowsheet solver. Each model contains one or more non-linear equations and a convergence criterion. If the equation residual value is greater than the value in the convergence criterion then the equation is not converged. In case the equation is not converged the process engineers may need to conduct more than one iteration in a simulation until all the non-linear equations are converged.

Example of a non-linear equation with four variables is

$$F(A, B, C, D) = (C * D) - (2.2 * A * B)$$

An example of a converge criterion is

$$0.001 * |C| * |D|$$

It is possible that an equation will never converge. In this case the process engineers have to change the initial values of the variables or add extra information to the parameters. For instance, the process engineers could add a maximum or a minimum value of the variable in order facilitate convergence.

Apart from the variables that are related to actual streams and to chemical components or to physical properties, there are other types of variables that the process engineers can use. Those variables are named as auxiliary variables and are used in the thermo-dynamic-models for simulation and optimization of the urea plant designs.

5.Feasibility Analysis

After explaining the problem and domain analysis, a feasibility analysis is performed in order to identify potential issues and challenges as well as potential risks that may arise or exist. This chapter describes issues and risks identified and presents their mitigation strategies.

5.1 Potential issues and challenges

Working on a project that combines more than one domain is challenging. In this project, an understanding of the terminology used by process engineers and a basic understanding of how a urea plant is designed is required. Domain knowledge can be gained by reading documents; however, there are cases that the existing documentation is poor or uses outdated terminology. Another way of gaining the knowledge needed is by discussing with process engineers, although proper language is required in order to prevent miscommunication. People from different domains might use the same terminologies for completely different purposes. For example, the word model for a software engineer could mean the software model, although for a process engineer could mean the thermodynamic model.

5.2 Potential risks

Several risks are identified within this project. The risk management is applied from the first months of the project. There are two different types of risk: the process related risks and the technical related risks. The description of the risks is written together with their impact on the end result and probability of appearance in the project.

The meaning of the values of the impact on the end result and the probability of appearance based on relative importance is:

1. Limited
2. Low
3. Moderate
4. High
5. Extreme

The last column of the table is corresponding to the mitigation strategy.

Table 8 Process risks

ID	Description	Impact (1-5)	Probability (1-5)	Mitigation Strategy
RP1	Conflicting opinion between the stake-holders about the end product.	3	4	A demonstration with the progress of end product with all the stakeholder present shall be made. At the end of the presentation a decision shall be made according to the time given.
RP2	Not all the requirements can be met given the time constraints.	4	5	Prioritize the requirement with the stakeholders. Requirements with medium or low prior-ity might be carried on as a future work.
RP3	Stakeholder unavailability	5	3	Organize meetings in advance. Communicate regularly and upfront about the new func-tionality needed for the project.
RP4	Extension of the back-end API by stake-holder is slower than expected	5	2	Inform the stakeholder on-time about the new functionality needed. Work on other tasks from the backlog.
RP5	A file containing a complete urea plant design suitable for performance test appli-cation is not given on time	4	3	Performance test of the application with smaller sections shall be made every time a new functionality is added. Inform the stakeholder on time about the concern.

Table 9 Technical risks

ID	Description	Impact (1-5)	Probability (1-5)	Mitigation Strategy
RT1	Process engineers might prefer textual based editing instead of graphical-based editing	3	3	The meta-model shall be easily extendable with textual based editors
RT2	Back-end API does not return expected values	5	3	Test cases could automate the verification procedure. Inform the stakeholders about the issues identified.
RT3	New releases of the development environ-ment	2	5	Read documentation about new features and check whether the new features are could ad-vocate the development of the project. Check for backwards compatibility before migrat-ing.

RT4	The performance of the new tool on specific tasks is significant slower than the previous tools	5	3	Identify the root of the problem. Try to optimize the code of the tool. If the problem exists because of the technology used inform the community about the issue. Finally try implement workarounds.

6.System Requirements

In the previous chapters the problem and the domain are defined.
This chapter describes the functional and non-functional requirements that have to be satisfied by the project.

6.1 Requirements gathering process

The problem and domain analysis revealed core parts that this project aims to implement. However, in order to narrow the project scope requirements should be defined. Well defined requirements aim to further decompose the problem into small and traceable sub-problems. The requirements phase occurred in parallel with the software development activities. There were two main phases in the process:

- **High-level requirements and use cases**: This phase started at the beginning of the project and lasted for two months. The main focus of this stage was to define the technology constraints and necessary system use cases.
- **Detailed requirements**: This phase focused on more concrete requirements according to the previous high-level requirements. The requirements were defined on biweekly iterations during the sprint planning. The agile way of working aimed at a prototype at the end of each iteration.

The requirements were discussed with the involved stakeholders. The following four categories are defined as the priority according to the MoSCoW method [6]:

1. **Must** – A requirement that the project must fulfill
2. **Should** – A requirement that is important, but the project success does not rely on it
3. **Could** – A requirement that is desirable but not necessary
4. **Would** – A requirement that is the least-critical

6.2 High-level requirements and use cases

The high-level requirements and use cases are based on the project aims and goals as mentioned in Section 3.5 Stamicarbon wants to change the way that the process engineers work from text-based to graphics-based. The new tool should allow process engineers to load and combine sections in order to gradually construct a complete urea plant. The new tool should also integrate the editor and the flowsheet solver functionality. Finally, the new tool should be a standalone application.

6.2.1. Use cases

Six main use cases are identified from the high-level requirements, namely create flowsheet canvas, load section, view section variables, modify section variables, merge sections, and simulate flowsheet.

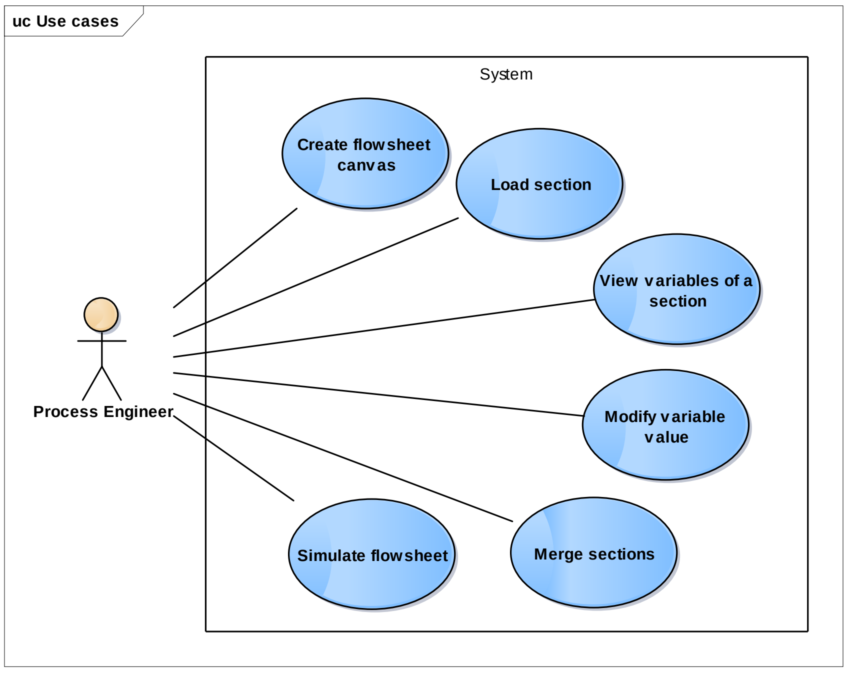


Figure 13 Main use cases

Table 10 Create flowsheet canvas use case specification

Create flowsheet canvas use case specification	
Use Case Name	Create flowsheet canvas.
ID	UC1
Description	A process engineer wants to create a new flowsheet canvas.
Actors	Process engineer
Pre-conditions	• Application is open.
Basic Flow	1. User selects new Tisflo project. 2. User inserts the project name and presses finish.
Post-conditions	• An empty flowsheet canvas is created and displayed to the user.
Alternate Flows	2a. Project name exists. 2a1. User has to type another name.

Table 11 Load section use case specification

Load section use case specification	
Use Case Name	Load section.
ID	UC2
Description	A process engineer wants to load a section in the flowsheet canvas.
Actors	Process engineer
Pre-conditions	• A flowsheet canvas is displayed to the user.
Basic Flow	1. User selects load section. 2. User selects a DAT file.
Post-conditions	• A section with all the available diagrams is created on flowsheet canvas. • All section elements and their diagrams are created.

Alternate Flows	1a. User selects load predefined section. 2a. User selects a DAT file.

Table 12 View variables of a section use case specification

View variables of a section use case specification	
Use Case Name	View variables of a section.
ID	UC3
Description	A process engineer wants to view the variables of a section.
Actors	Process engineer
Pre-conditions	• A flowsheet canvas with one or more sections is displayed to the user.
Basic Flow	1. User selects a section. 2. User selects the section variables diagram.
Post-conditions	• A table diagram with all the section variables is displayed.
Alternate Flows	1a. User selects the flowsheet canvas. 2a. User selects the flowsheet variables diagram. 2a. User navigates to the section.

Table 13 Modify variable value use case specification

Modify variable value use case specification	
Use Case Name	Modify variable value.
ID	UC4
Description	A process engineer wants to modify the value of a variable.
Actors	Process engineer
Pre-conditions	• A diagram with variable is displayed to the user.
Basic Flow	1. User selects the value of a variable from the table diagram. 2. User inserts a new value.
Post-conditions	• The value of a variable has changed.
Alternate Flows	

Table 14 Merge sections use case specification

Merge sections use case specification	
Use Case Name	Merge sections.
ID	UC5
Description	A process engineer wants to merge two sections.
Actors	Process engineer
Pre-conditions	• A flowsheet canvas with two or more sections is displayed to the user.
Basic Flow	1. User selects the stream connector. 2. User selects an output stream of a section.

	3. User selects an input stream of another section. 4. User selects merge sections. 5. User selects the folder that the merged section will be saved. 6. User inserts a name for the new section.
Post-conditions	• Sections are merged and sorted in a new DAT file.
Alternate Flows	

Table 15 Simulate flowsheet use case specification

Simulate flowsheet use case specification	
Use Case Name	Simulate flowsheet.
ID	UC6
Description	A process engineer wants to simulate the flowsheet.
Actors	Process engineer
Pre-conditions	• A flowsheet canvas with one or more sections is displayed to the user.
Basic Flow	1. User selects simulate. 2. User inserts number of iterations.
Post-conditions	• A message if the flowsheet is converged or not is displayed. • The variable values have changed.
Alternate Flows	

6.2.2. Technology constraints

The technology stack was defined at the beginning of the project by the stakeholders. Eclipse is the development tool picked by the stakeholders. The usage of two Eclipse tools was also defined at the beginning of the project. The Eclipse Modeling Framework (EMF) is the first tool that the stakeholders picked for defining the vocabulary (concept, relations, and properties) of the application. Eclipse Sirius is the second tool that the stakeholders picked for visual representations of the application. The stakeholders also envisioned that the product should run as a standalone application outside Eclipse.

The programming language that the stakeholders picked for the application is Java. Finally, the Java Native Interface (JNI) picked by the stakeholders in order to enable Java code to call C++ functions of the kernel.

Stamicarbon implemented a proof of concept of the application before the beginning of this project using the aforementioned technology stack.

6.3 Detailed requirements

This section presents more concrete requirements that were decided during the sprint planning. The detailed requirements are split in two categories, namely the user functional requirements and the system functional requirements. The user functional requirements are from the process engineer perspective and apply to parts visible to the end users of the application. The system functional requirements describe the behavior that the application should satisfy.

6.3.1. User functional requirements

Each user functional requirement has and ID, a short description, and an assigned priority according to the MoSCoW method.

Table 16 User functional requirements

ID	Description	Priority
UFR1	A user shall be able to create a flowsheet canvas	M
UFR2	A user shall be able to load DAT files in a flowsheet canvas	M
UFR3	A user shall be able to load predefined sections in the flowsheet canvas	S
UFR4	A user shall be able to view in diagrams all the information retrieved from a DAT file	M
UFR5	A user shall be able to modify the variables of a section	M
UFR6	A user shall be able to modify the labels of a section	M
UFR7	A user shall be able to simulate the flowsheet	M
UFR8	A user shall be able to view the simulated results	M
UFR9	A user shall be able to specify the number of iterations	S
UFR10	A user shall be able to modify section variables while the simulation is running	S
UFR11	A user shall be able to merge sections by connecting streams	M
UFR12	A user shall be able to navigate inside a section	M
UFR13	A user shall be able to auto arrange the size and the position of the elements	W
UFR14	A user shall be able to use hotkeys for merging and simulating	C

6.3.2. System Functional requirements

Each system functional requirement has an ID, a short description, and an assigned priority according to the MoSCoW method.

Table 17 System Functional Requirements

ID	Description	Priority
SFR1	The DAT files shall be identified as sections by the system	M
SFR2	The system shall generate unique names for each section	M
SFR3	The system shall be able to store information, which is used by process engineers, in a DAT file	M
SFR4	The system shall generate automatically all the visual representations	M
SFR5	The system shall present the sections with a predefined image according to their type	M
SFR6	The system shall map the kernel instances to the model instances	M
SFR7	The system shall be able to simulate the flowsheet	M
SFR8	The system shall display the streams with different color according to their flow	S
SFR9	Test cases that verify the returning values of the kernel shall be created	C
SFR10	The system shall be able to run as a standalone application	M

SFR11	The system shall synchronize the model instances with the kernel instances	S
SFR12	The system shall track when a variable changes from free to fixed or the opposite	S
SFR13	The system shall display error and warning messages to the users	S

6.4 Non-functional requirements

In this section, the non-functional requirements of the project are listed. The non-functional requirements derived from the two main goals of the project, namely shorten the learning curve of the new engineers and improve the productivity of engineers.

6.4.1. Ease of use

In order to shorten the learning curve of the new engineers and improve the productivity of engineers, the system shall be easy to use. The tool shall be easier to use than the tools that the process engineers were using before the start of this project. Metrics that could be used to quantify the ease of use of the tool are:

- Time required to learn how to use the tool
- Time required to learn all the tool features
- Time required to create a new urea plant design

6.4.2. Performance

The system shall respond reasonably fast to the process engineer requests. The performance shall be comparable to the tools that the process engineers were using before the start of this project. Metrics that could be used to quantify the performance of the tool are:

- Time required to create the model instances
- Time required to open the diagrams
- Time required to edit the model element instances
- Time required to simulate a flowsheet

6.4.3. Extensibility

The system shall be open to addition or modification of functionality and features. Metrics that could be used to quantify the extensibility of the tool are:

- Effort required to create or modify visual representations
- Effort required to integrate new components or plug-ins

7.System Architecture

In the previous chapters the problem and the requirements are defined.
This chapter elaborates on the architectural reasoning and relevant decisions based on the requirements. This chapter also presents a comparison between the envisioned system architecture and the old architecture.

7.1 Architecture before this project

This section describes how the different components were organized before the start of this project. As already described in the problem analysis in Chapter 3, before the beginning of this project, the process engineers were using two applications, a flowsheet solver and a text editor.

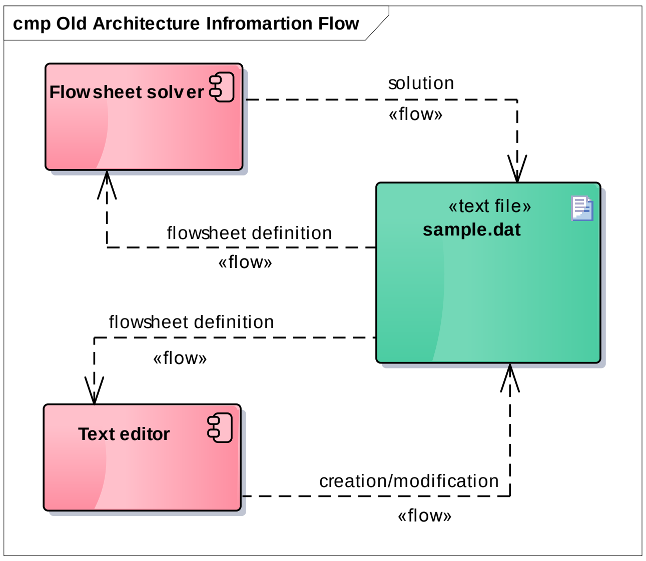


Figure 14 Information flow before this project

With a text editor it is possible to open a flowsheet definition contained in a DAT file. A text editor can be used to modify the structure of a flowsheet. A text editor can also be used to create a flowsheet from scratch.

On the other hand, with the flowsheet solver it is possible to open a flowsheet definition contained in a DAT file. A flowsheet solver cannot modify the structure of a flowsheet; however, it can calculate the heat and material balances of a flowsheet.

On the front-end layer of the flowsheet solver, there is a user interface, which is written in Visual Basic. On the back-end and hidden from the process engineers there are a kernel and thermodynamic libraries, both written in FORTRAN. The kernel and the thermodynamic libraries are the components that handle the calculation of the heat and material balances.

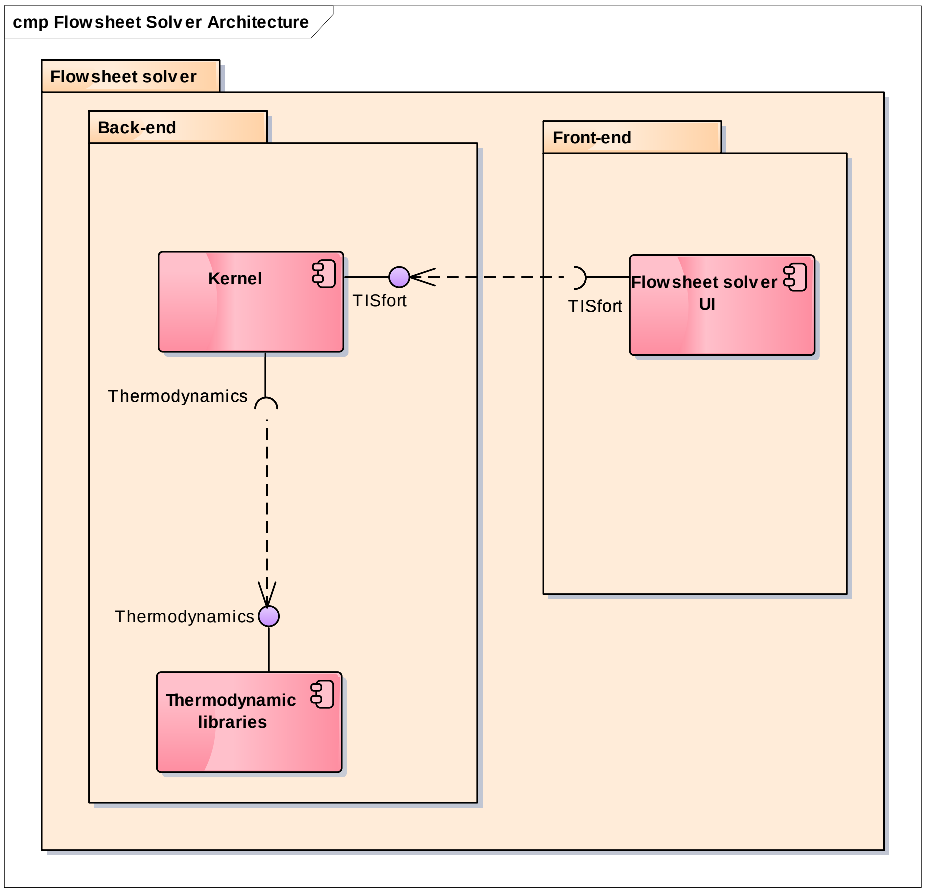


Figure 15 Flowsheet solver architecture before this project

7.2 Architecture decision

The starting point for the design of the system architecture is the choice for a suitable architectural pattern. An architectural pattern is a general and reusable abstract framework that could be used for solving a commonly occurring problem. The decision for the ideal architectural pattern is typically based on the high-level requirements, technology constraints, and on the non-functional requirements.

The two main requirements of the product are stated in Section 6.2 The first is to change the way of working from text-based to graphics-based. The second is to combine the editor and the solver into one tool. The technology for the implementation of the project, as stated in Section 6.2.2. was defined at the beginning of the project by the stakeholders.

7.3 Plug-in architecture

According to the technology chosen by the stakeholders, namely Eclipse, the plug-in architecture is the most suitable for the project. The main reason is that everything in Eclipse is a plug-in, with the exception of a small runtime kernel [7]. A plug-in requires an extension point to plug into in order to function. The most important plug-in that provides extension points that allow a user to create plug-ins is the Eclipse platform plug-in.

7.3.1. Eclipse platform plug-in

The Eclipse platform defines the set of frameworks and common services that collectively make up the infrastructure required to support the use of Eclipse as a component model, as a Rich Client Platform (RCP) and as a comprehensive tool integration platform. These services and frameworks include a standard workbench user interface model and portable native widget toolkit [8].

The Workbench component contains extension points that allow the user plug-ins to extend the Eclipse user interface with menu selections and toolbar buttons, to request notification of different types of events, and to create new views. The Workspace component contains extension points that allow users interact with resources, including projects and files [7].

The Help component allow users to provide documentation and context-sensitive help in their application. The help documentation could help the end users of the application; however, it does not have essential functionality. The Debug component allow the user plug-ins to launch a program, interact with the running program, and handle errors. Finally, the Team component allows Eclipse resources to interact with version control systems [7].

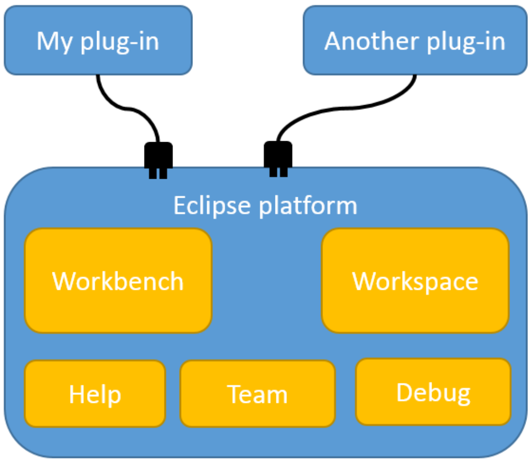


Figure 16 Eclipse architecture

7.3.2. Plug-in architecture advantages

Plug-in based architectures are ideal for the development of applications that are modular, customizable, and easily extensible. The different plug-ins in the system provide a higher level of abstraction and divide the problem into sub-problems. For example, a plug-in is a separate module that can isolate and solve a specific problem. With a plug-in based architecture, it is possible to create a different version of an application without source code modifications. Another advantage of the plug-in based architecture is the development of additional features. New features can be created without any change on the original application.

7.4 Architecture of the project

This section describes the different plug-ins and components of the project. It also presents the information flow between the application and the data files.

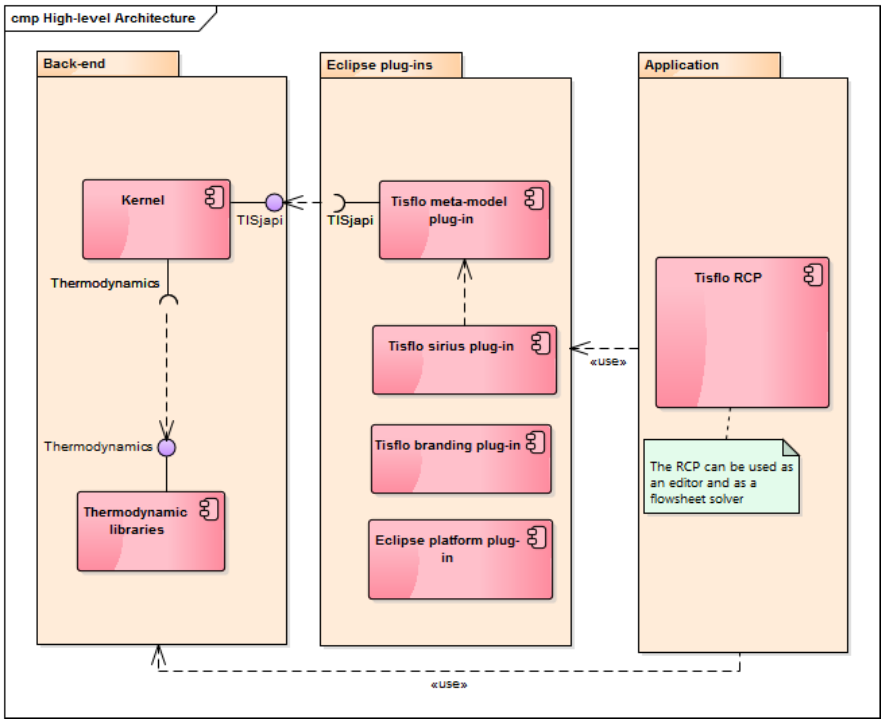


Figure 17 High-level architecture of this project

7.4.1. Meta-model plug-in

Eclipse modeling framework (EMF) is the tool picked for the definition of the domain model. In the case of the project, the flowsheet solving. The domain model contains the business vocabulary (concept, relations, properties) needed for the application. EMF is a modeling framework and code generation facility for building tools and applications based on a structured data model. EMF provides tools and runtime support to produce a set of Java classes for the model, along with a set of adapter classes that enable viewing and command-based editing of the model, and a basic editor [9]. The Tisflo meta-model plug-in is a set of three plug-ins, the Tisflo plug-in, the Tisflo edit plug-in, and the Tisflo editor plug-in. The Tisflo plug-in contains the meta-model description. The Tisflo edit plug-in and the Tisflo editor plug-in are automatically generated according to the meta-model description. Therefore, for simplicity reasons, the combination of all three plug-ins is identified as the Tisflo meta-model plug-in.

7.4.2. Sirius plug-in

Eclipse Sirius is that tool that the stakeholders picked for visual representations of the application. Sirius is an Eclipse project, which allows the creation of graphical modeling workbenches by leveraging the Eclipse Modeling technologies. A modeling workbench created using Sirius is composed of a set of Eclipse editors (diagrams, tables, and trees), which allow the users to create, edit, and visualize EMF instance models. The editors are defined by a model, which defines the complete structure of the modeling workbench, its behavior, and all the edition and navigation tools. This description of a Sirius modeling workbench is dynamically interpreted by a runtime within the Eclipse IDE [10].

7.4.3. RCP

The stakeholders envisioned that the product should run as a standalone application. The standalone application must combine the editor and the flowsheet solver functionality. In Eclipse in order to fulfill that requirement, a Rich Client Platform (RCP) should be created. As explained, the Eclipse platform is designed to serve as an open tool platform. It is architected so that its components could be used to build client application. The minimal set of plug-ins needed to build a standalone application is collectively known as the Rich Client Platform [11].

7.4.4. Branding plug-in

A RCP based application without branding looks similar to a default Eclipse application. By creating a branding plug-in it is possible to change the appearance of the application. For example, with a branding plug-in it is possible to change the application icon and splash screen from the default provided by Eclipse to one that is more relevant for the application. The branding of the application could also be used for hiding buttons or menu options, provided by default from the Eclipse platform, which is more relevant to software engineers rather than process engineers [12].

7.4.5. Back-end components

The communication interface between the Eclipse plug-ins and the back-end is called *TISjapi*. The kernel in the graphical-based Tisflo did not remain the same; the implementation of the kernel changed from FORTRAN code to C++ code. The functionality of the kernel remained the same; however, new API calls to extend the kernel were defined. The design and implementation of the kernel and the thermodynamic libraries are not part of this project.

7.4.6. Data files

In order to satisfy the requirements the application remained compatible with the DAT files that are being used on the applications of the previous architecture. In addition to the DAT files, it is visible in *Figure 18* that a new file format, XMI, is also supported. XMI (XML Metadata Interchange) is a standard for exchanging metadata information via Extensible Markup Language (XML). The XMI files of the application are automatically generated from the serialization that takes part in the Tisflo meta-model plug-in and in the Tisflo Sirius plug-in. The information that is stored in the XMI files is a superset of the information stored in the DAT files. Additional information of the XMI files is extra associations between elements for easier navigability, information of how an element is visually represented, and where the element is located on a particular diagram.

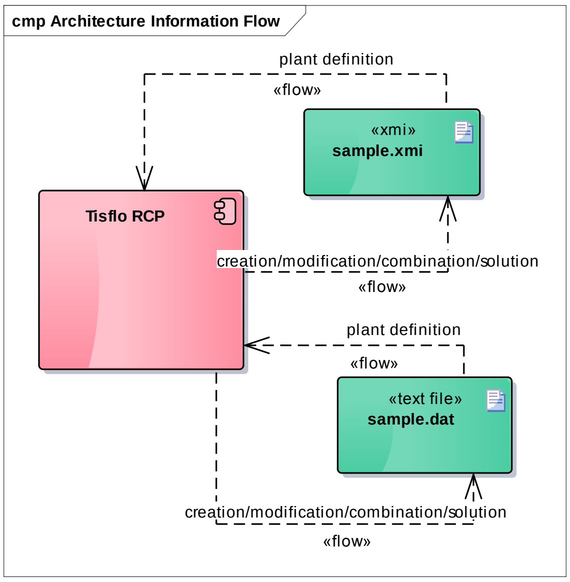

cmp Architecture Information Flow
plant definition
«flow»
«xmi»
sample.xmi
Tisflo RCP
creation/modification/combination/solution
«flow»
plant definition
«flow»
«text file»
sample.dat
creation/modification/combination/solution
«flow»

Figure 18 Information flow of the project

8.System Design and Implementation

In the previous chapter the high-level architecture of the system is defined.
This chapter decomposes the high-level architecture into a detailed design. This chapter elaborates on the system design and the implementation.

8.1 Introduction

The system design is explained by utilizing the 4+1 view model. The 4+1 view model is designed by Philippe Kruchten [13] and it is being used for describing software-intensive systems, based on the use of multiple, concurrent views. The views are used to describe the system from the viewpoint of different stakeholders, such as end-users and developers. The four views of the model are:

- Logical view – Describes the structure (object model) of the design. UML diagrams to represent the logical view include class diagrams and object diagrams. The logical view is mandatory when using the 4+1 views.
- Process view – Describes the run-time behavior of the system. UML diagrams to represent to the process view include activity diagrams and sequence diagrams. The process view is optional when using the 4+1 views.
- Development view – Describes the static organization of the system. UML diagrams to represent the development view include component diagrams and package diagrams. The development view is optional when using the 4+1 views.
- Physical view – Describes how the software is mapped to the hardware. The deployment view is optional when using the 4+1 views.

The fifth view is the use-case or scenario view. The use-case view describes the functionality of the system and its users. The main use-cases of the system were defined in Section 6.2.1. The use-case view is mandatory when using the 4+1 views.

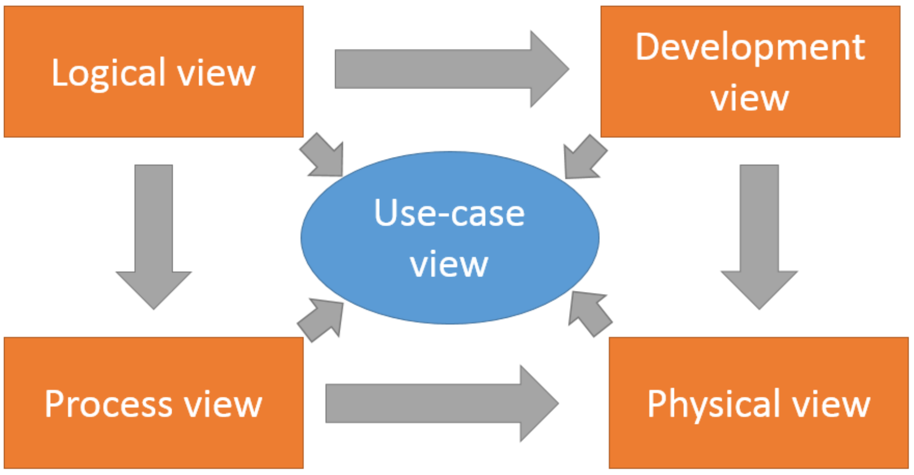


Figure 19 4+1 view model

8.2 Logical view

The logical view describes the structure of the design. The logical architecture primarily supports the functional requirements – what the system should provide in terms of services to its users.

8.2.1. Meta-model

As introduced in the previous chapter, the EMF is a modeling framework and code generation facility for building tools and applications based on a structured data model. The meta-model of the EMF is aligned with the Meta-Object Facility. The Meta-Object Facility (MOF) is an Object Management Group (OMG) standard for Model-driven engineering (MDE) [14].

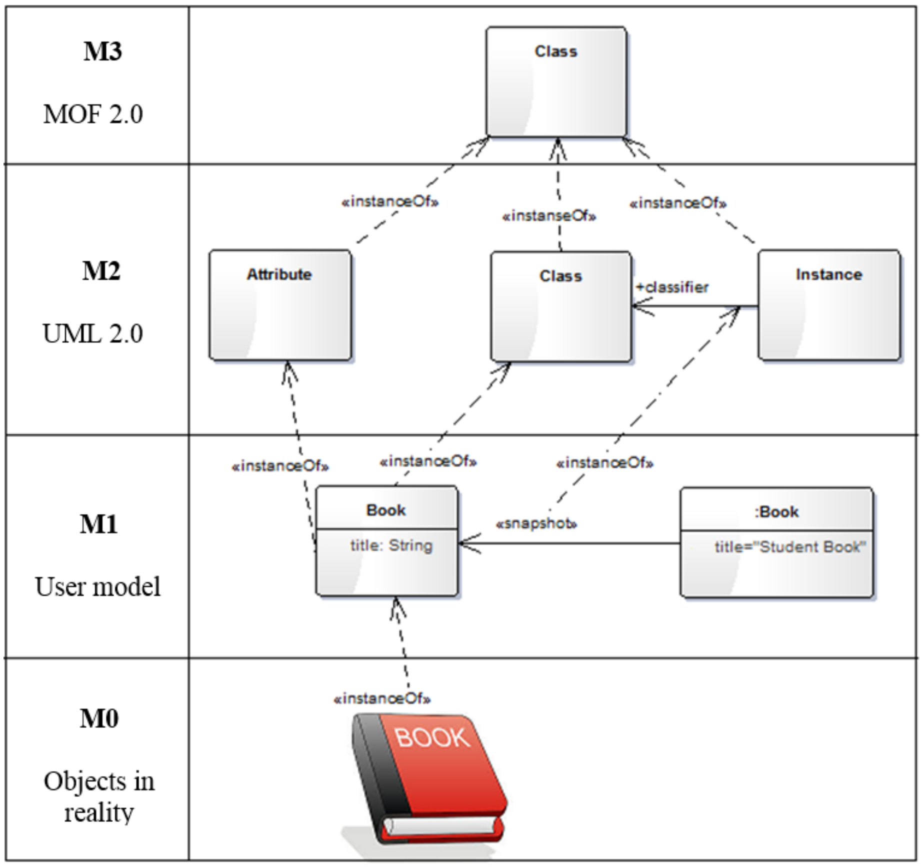


Figure 20 Meta-Object Facility layers example

MOF is designed as a four-layered architecture. It provides a meta-meta model at the top layer, called the M3 layer. This M3-model is the language used by MOF to build meta-models, called the M2-models. The M2-models describe the elements of the M1-layer, and therefore M1-models. The last layer is the M0-layer or data layer. It is used to describe real-world objects.

The meta-model of the system is designed based on the domain analysis in Chapter 4. The meta-model of the system captures all the elements needed for flowsheet solving. A model is a concrete instance of the meta-model. The model instances are created according to the kernel. The kernel is the component that is responsible for the parsing of the DAT files. The kernel is also responsible for the calculation of the heat and material balances. A part of the meta-model is presented in *Figure 21*. The complete meta-model is presented in Appendix A: The complete meta-model.

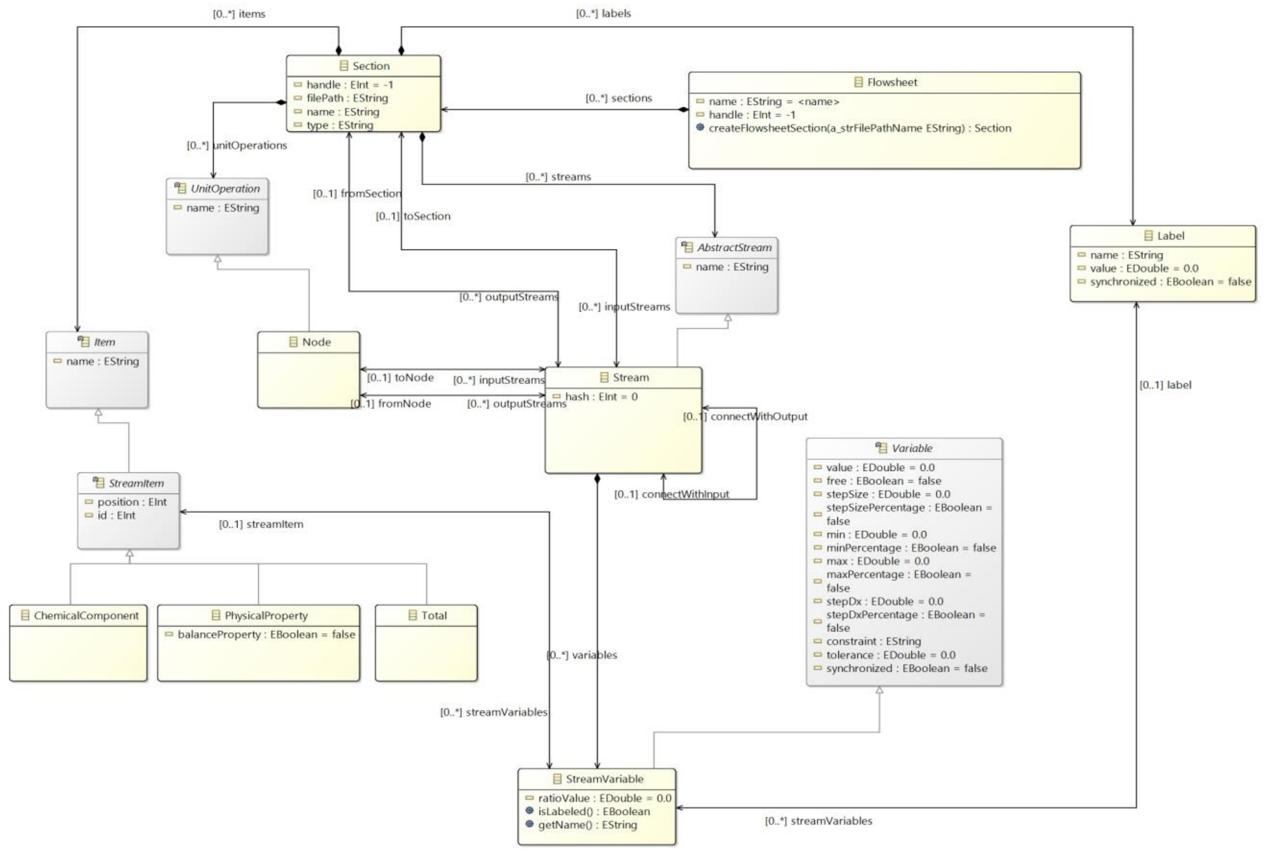


Figure 21 Part of the meta-model

The root class of the meta-model is called a *flowsheet*. The flowsheet has a name and a handle. The handle is a transient attribute that stores the memory location of the flowsheet that is created by the kernel. A transient attribute is not serialized. The operation createFlowsheetSection has one input parameter. The input parameter is the file path of the DAT file. The operation createFlowsheetSection calls a JNI function. The JNI function calls a kernel function that parses a DAT file and creates instances of all the DAT file elements in the kernel. Next, inside the createFlowsheetSection operation there are other JNI functions that query the kernel and create the model instances (see Section 8.3.1.). This approach was used for the instantiation of the model because:

- The application needed to support the DAT files and the kernel already had a DAT file parsing mechanism.
- The kernel handles the calculation of the heat and material balances and therefore the kernel should also have instances of the elements of a DAT file.
- The kernel does not support functions to create all the elements that are needed for the calculation of the heat and material balances. Therefore a parsing DAT file mechanism on the Tisflo meta-model plug-in would not work.

The flowsheet instance can contain zero or more sections. For every DAT file that is loaded in the flowsheet a section is created. Every DAT file is considered as a section. A section can be a small segment of a plant or even the complete plant. A section has a name and a type. According to the type a section has different visual representations. Each section also has a handle. Similarly to the flowsheet class, the handle is a transient attribute. The handle stores the memory location of the section that is created by the kernel. The handle is used as an input parameter in the JNI functions in order to query or set values to the kernel for a section or for elements contained by a section.

On the top part of every DAT file the stream items (the chemical components, the physical properties, and the total) are defined. The stream items are almost the same in every DAT file. For reusability reasons the stream items could be contained by the flowsheet; however, the order (the position) that the stream items are specified in the DAT file is important. The position of the stream items might differ from DAT file to DAT file. The kernel cannot merge sections that have the stream items in a different order, although in the future it is expected that it would. In order to serialize the position of the stream items; the stream items are contained by the section class.

Next, in the DAT file, the nodes, the streams, the stream variables, and the labels are specified. As explained in Chapter 4, a node is a joint point with zero to many input and output streams. A stream can be connected with one or two nodes. Streams that are connected with one node are either an input or an output stream of a section. Output streams of a section can be connected with input streams of another section. In order to prevent connections between output streams with input streams that do not have identical stream items, a hash attribute is used. The value of the hash is based on the items defined in a stream. An output stream can be connected with an input stream with the same hash. The attribute synchronized on the label class is a transient attribute and it is used for the synchronization of the model instances with the kernel instances. More details about the synchronization will be provided later on this chapter.

All the variables have a value and it is specified if it is free or fixed. However, a variable could have additional information, for instance, a step size value, a step size percentage, a minimum value, and a minimum percentage. The additional information of a variable is rarely used. According to the DAT files used while the application was developed fewer than 5% of the total number of variables have additional information. Since the majority of the variables do not have additional information in the initial design there was another class called an *additional information* and it was contained by the variable class. With that approach fewer queries to the kernel had to be made and less information had to be serialized. However, the kernel stores additional information for all the variables, for example, if the minimum value of a variable is not specified in a DAT file, then the kernel stores the lowest value of type double as the minimum value of that variable. In order to reflect the kernel instances in the model instances all the additional information of a variable is added as attributes of a variable. Finally, an extra attribute called a *synchronized* is added in the meta-model. Synchronized is a transient attribute and it is used for the synchronization of the model instances with the kernel instances (see Section 8.2.2.

To sum up, the meta-model represents the different elements of the DAT files. The model instances are created in a way that they can represent the kernel instances. The same principles are applied for the rest of the meta-model that is presented in Appendix A: The complete meta-model.

8.2.2. Synchronization of the model instances with the kernel instances

As already explained the instances in the kernel are created by parsing DAT files. The first time that a section is loaded on the flowsheet the model instance elements are created by querying the kernel. The model instance and its non-transient attributes are serialized in XMI files when saving the model instance. Every time that a flowsheet is reloaded the model instances are created according the information that is available in the XMI files (without querying the kernel) and the kernel instances are created according the information that is serialized in the DAT files.

While the application is running any change made in the model instance is reflected in the XMI files and in the kernel; however, the DAT files remain the same. A DAT file is modified when the user of an application decides to save the changes made in a DAT file. In case that there is a crash on the computer or on the application, or if the user decide to exit the application without saving the changes in the DAT file, there will be inconsistency between the DAT file and the XMI file. It is worth to mention that even if there was a mechanism that auto-updates the DAT files it would not work as a solution to the problem. The reason is that the kernel cannot serialize all the information needed in the DAT files.

In order to synchronize the model instances and the kernel instances a monitoring service is created. The monitoring service extends the org.eclipse.emf.common.notify.impl.AdapterImpl class. Every time that a flowsheet is reloaded the monitoring service modifies the kernel instances according to the model instances and sets the transient attribute synchronized as true. This approach allows the synchronization of the model instances with the kernel instances; however, it is not possible to change the naming of the elements or the structure of the flowsheet design. For instance, if the labels in an XMI file have different names from the labels in a DAT file then the synchronization would not work. It is possible to overcome such a constraint if the kernel instances are created by parsing the XMI files or if new JNI functions are implemented that would allow the creation of all the kernel instances.

8.2.3. Sirius

Sirius is an Eclipse project which allows the creation of graphical modeling workbenches by leveraging EMF. Sirius allows users to specify representation for their domain models. Representation can be diagrams, tables, matrices (cross-tables) or hierarchies (trees). Representation can be organized in viewpoints. Viewpoints are defined in Viewpoint Specification Models and they are specified as models inside Viewpoint Specification Projects. Viewpoint Specification Projects (VSPs) are Eclipse plug-in projects, which contain one or more *.odesign files (the extension used for Viewpoint Specification Model). By convention, the VSM (or VSMs) defined in a project are stored inside a folder called a *description* [15].

In this project the visual representations created with Sirius involve the UI that the users of the application interact with. In the Tisflo Sirius plug-in one VSP and one VSM are created. Representations for the flowsheet, the sections, the streams, and the auxiliary streams are created. The main diagram where process engineer can load and view sections is called a *flowsheet canvas*.

In order to increase the navigability options and to provide all the necessary information in the diagrams, extra associations are added in the meta-model. For example, in the meta-model there is a bi-directional reference between the stream variable and the label. The flowsheet solving domain could be captured with a simple reference from the stream variable to the label; however, in order to provide more detailed diagrams to the process engineers a bi-directional reference is added. With this approach the process engineers can view a diagram with all the stream variables that are attached to a label. Such a diagram is not required for the flowsheet solving, although it increases the navigability options and the overview about the flowsheet design.

8.3 Process view

The process view describes how the run-time system is structured as a set of elements that have run-time behavior and interactions. The process architecture takes into account some non-functional requirements, such as performance and availability. The process view is typically explained through sequence and activity diagrams.

8.3.1. Creation of the model instances

In the application all the model instances, apart from the root instance, are created automatically when a user initiate an action and loads a DAT file on the flowsheet canvas. The initial name of a section is equal to the name of the DAT file. The kernel can simulate a flowsheet only if the section names are unique. Therefore a function that generates unique section names is implemented.

After a unique name for the section is generated the system calls the JNI function createFlowsheet. The function createFlowsheet can create a flowsheet or a section instance in the kernel (in the kernel there is no distinction between a flowsheet and a section). The memory location of the kernel instance is returned. Next, a function with name loadFlowsheetProblem sends the location of the DAT file to the kernel. The kernel parses the file and creates the kernel instances. Afterwards, there are JNI functions that query the kernel and create the model instance elements of a section.

The model instance elements can have associations between each other. For instance, a stream variable is associated with zero or one stream item and with zero or one label. In order to associate the instance elements with each other two approaches can be followed. The first approach implies that each stream variable shall query all the section stream items and all the section labels, until it finds the desired one. The second approach implies that every time that an instance element (that may have association with other instance elements) is created is added in a HashMap. In the second approach the association can be made by getting the desired object from the HashMap according to its name. The first approach uses less memory than the second, the second approach uses less CPU cycles than the first. The second approach is implemented in this system.

The sequence diagram in *Figure 22* represents how the chemical component model instance elements of a section are created. In the class TISjapiCreate there are other functions similar to the addChemicalComponents that create all the other model instance elements contained by a section.

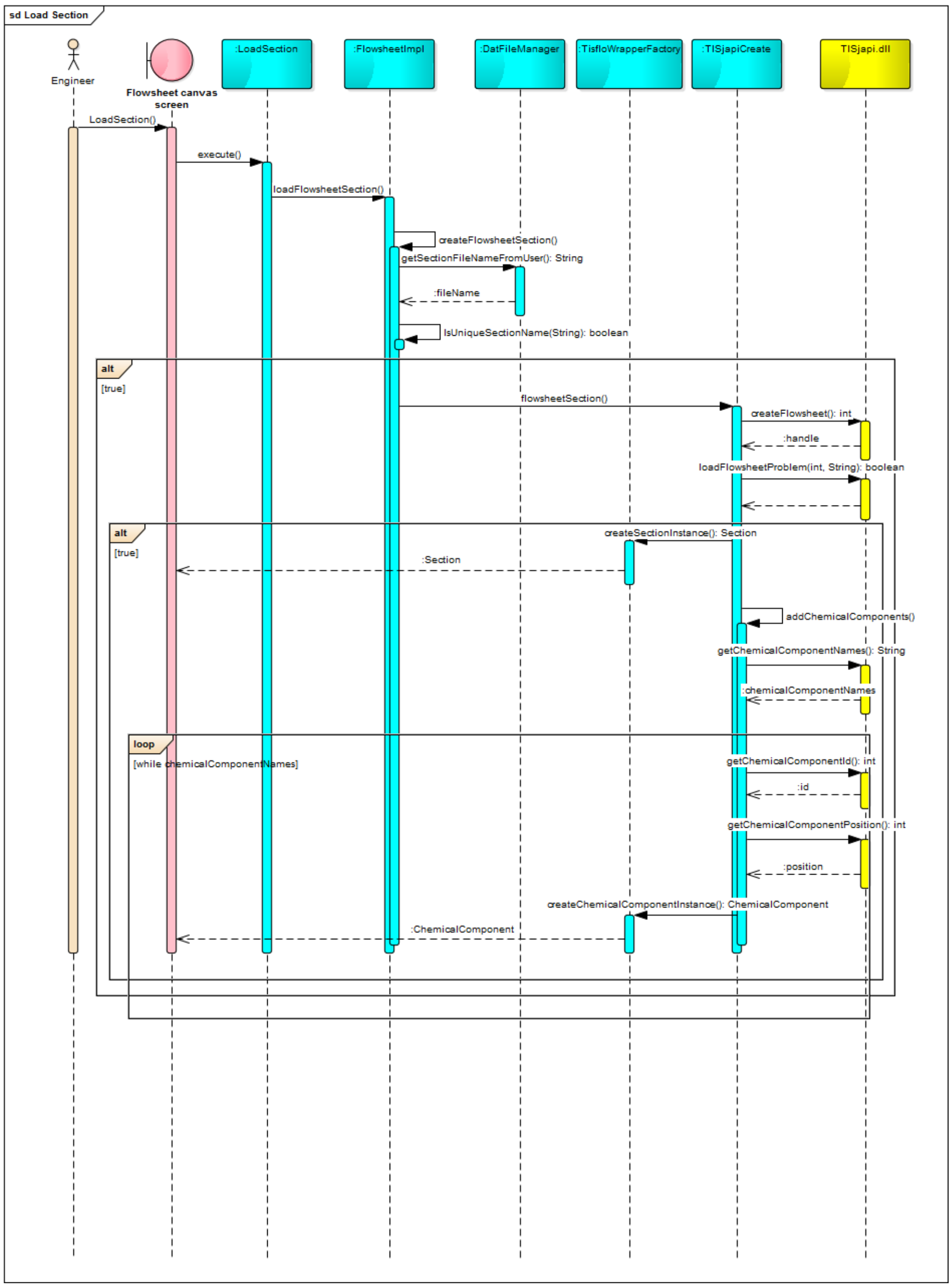


Figure 22 Sequence diagram representing the creation of the chemical component instances

8.3.2. Simulation of a flowsheet

The activity diagrams can present a higher level picture of the behavior of the system compared to the sequence diagrams. The activity diagram in *Figure 23* displays the simulation of a flowsheet. Three tiers are involved in the communication. The process engineer initiates the start of the action by pressing the simulate flowsheet button. An action is triggered in the Tisflo RCP and send a simulation request to the kernel. The simulation is handled in the kernel. After the simulation is finished the Tisflo RCP starts the update of the model instances. For every section the stream variable and the label values are updated by querying the kernel. Next, the Tisflo RCP sends a request to the kernel to verify whether or not the flowsheet is converged. Finally, a message that indicates if the flowsheet is converged or not is displayed to the process engineer.

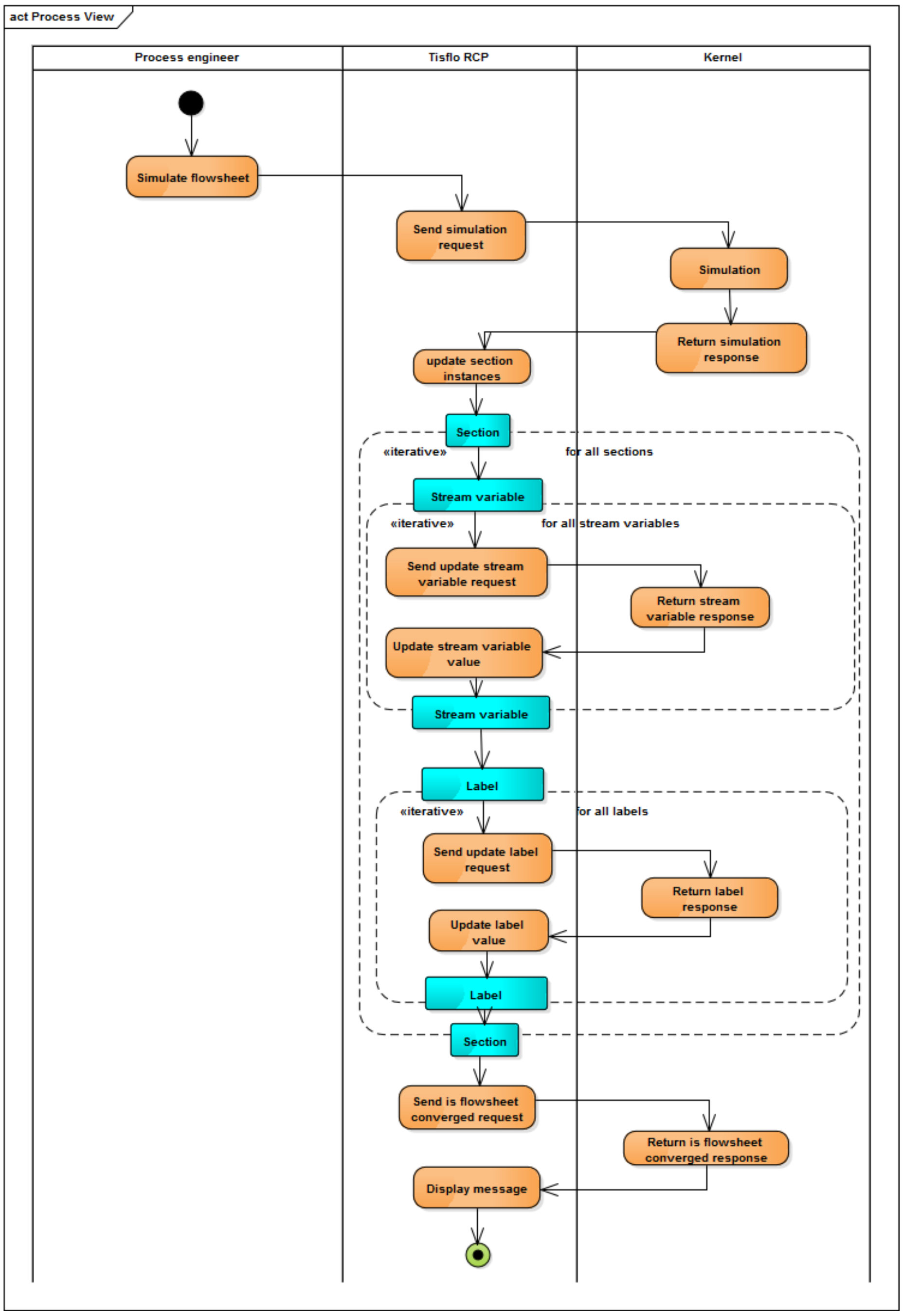


Figure 23 Activity diagram representing the simulation of a flowsheet

From the activity diagram it is visible that there is a delay from the time that a process engineer presses a button that simulates the flowsheet until the time that the final message is displayed. The delay is caused from the processing that needs to be done in the kernel and in the Tisflo RCP.

8.4 Development view

The development view focuses on the static organization of the system. The software is packaged in small chunks – program libraries, or subsystems – that can be developed or extended. This view is primarily intended for developers.

8.4.1. Development view of the Tisflo meta-model plug-in

As described in the previous chapter, the Tisflo meta-model plug-in is a set of three plug-ins, the Tisflo plug-in, the Tisflo edit plug-in, and the Tisflo editor plug-in. The Tisflo plug-in contains the meta-model description. The Tisflo edit plug-in and the Tisflo editor plug-in are automatically generated according to the meta-model description.

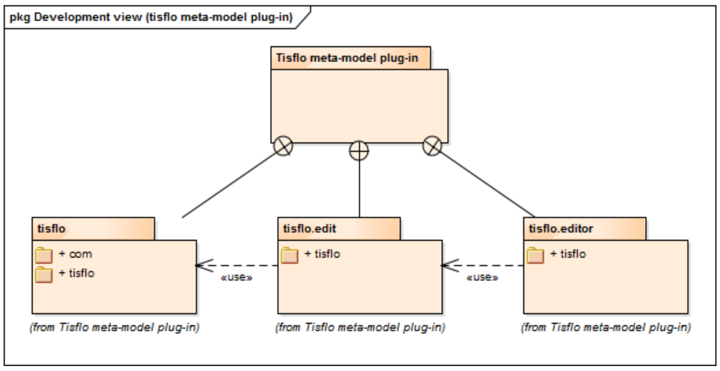

pkg Development view (tisflo meta-model plug-in)
Tisflo meta-model plug-in
tisflo
+ com
+ tisflo
(from Tisflo meta-model plug-in)
«use»
tisflo.edit
+ tisflo
(from Tisflo meta-model plug-in)
«use»
tisflo.editor
+ tisflo
(from Tisflo meta-model plug-in)

Figure 24 Deployment view of the Tisflo meta-model plug-in

The Tisflo plug-in contains two main packages, the *tisflo* and the *com*. The tisflo package contains code generated (with modifications) from the meta-model description. The com package contains extra code that is needed for the application.

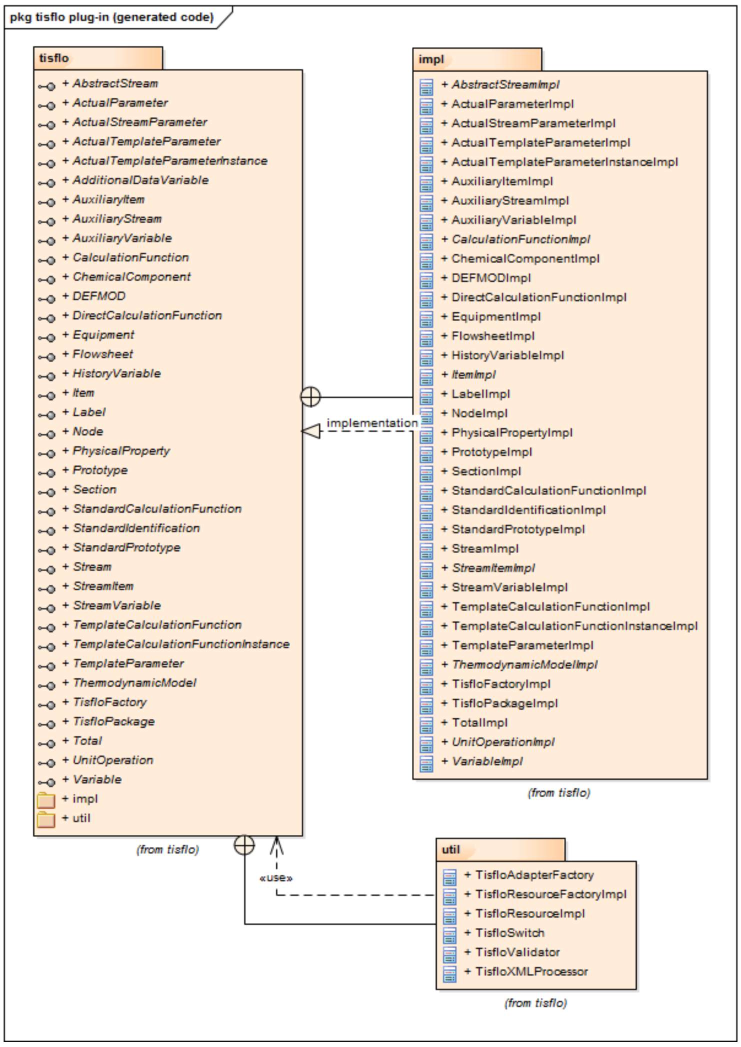


Figure 25 Deployment view of the Tisflo plug-in (generated code)

The tisflo package contains the interfaces of the meta-model classes. An interface of the Factory to create the model instances is also part of the tisflo package. The tisflo.impl package contains the concrete implementation of the interfaces defined in tisflo. Finally, the tisflo.util package contains other implementations, such as the AdapterFactory and the ResourceFactory.

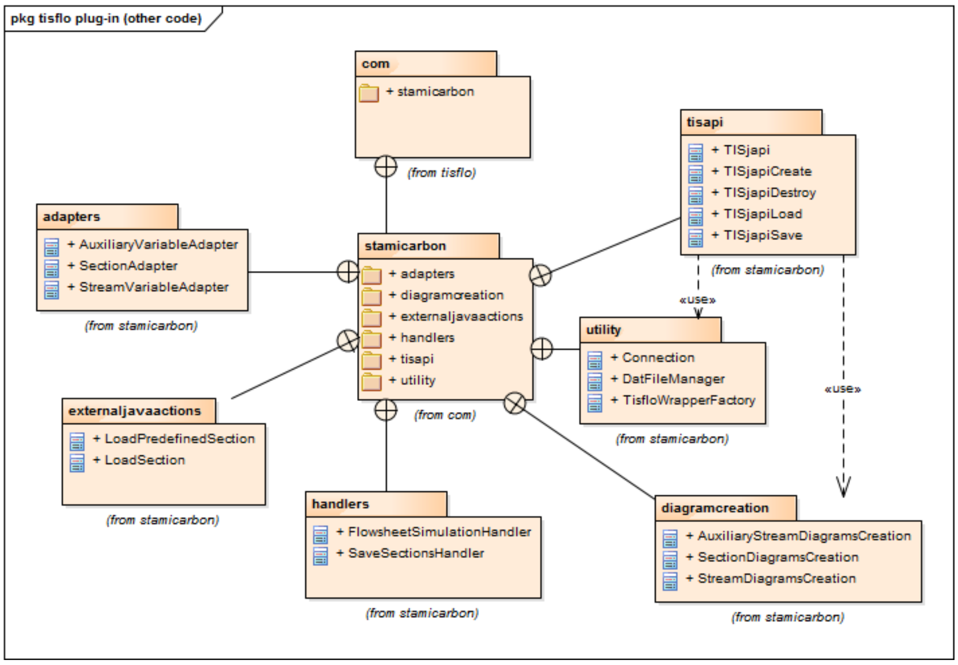


Figure 26 Deployment view of the Tisflo plug-in (other code)

The com.stamicarbon package contains six packages, the adapters, the externalja-vaaactions, the handlers, the tisjapi, this utility, and the diagramcreation. The classes in the adapter package are used for the synchronization of the model instances with the kernel instances (see Section 8.2.2.). The classes in the externaljavaaactions package implement the IExternalJavaAction. They are used in the Tisflo Sirius plug-in to load the information of the DAT files on the flowsheet canvas. The classes in the handlers package extend the AbstractHandler. In the Tisflo meta-model plug-in the extension point org.eclipse.ui.handler uses those two handlers. The tisjapi package contains five classes. The TISjapi class contains all the JNI functions. The other four classes are using those functions. The class TISjapiCreate uses the classes of the diagramcreation package in order to automate the generation of the visual representations. Finally, the package utility contains classes that are used by the classes of the tisjapi package. For example, the TISjapiCreate uses the TisfloWrapperFactory class. The TisfloWrapper-Factory class contain functions that generate model instances. The TisfloWrapperFac-tory wraps functions of the TisfloFactory and setters for the model attributes.

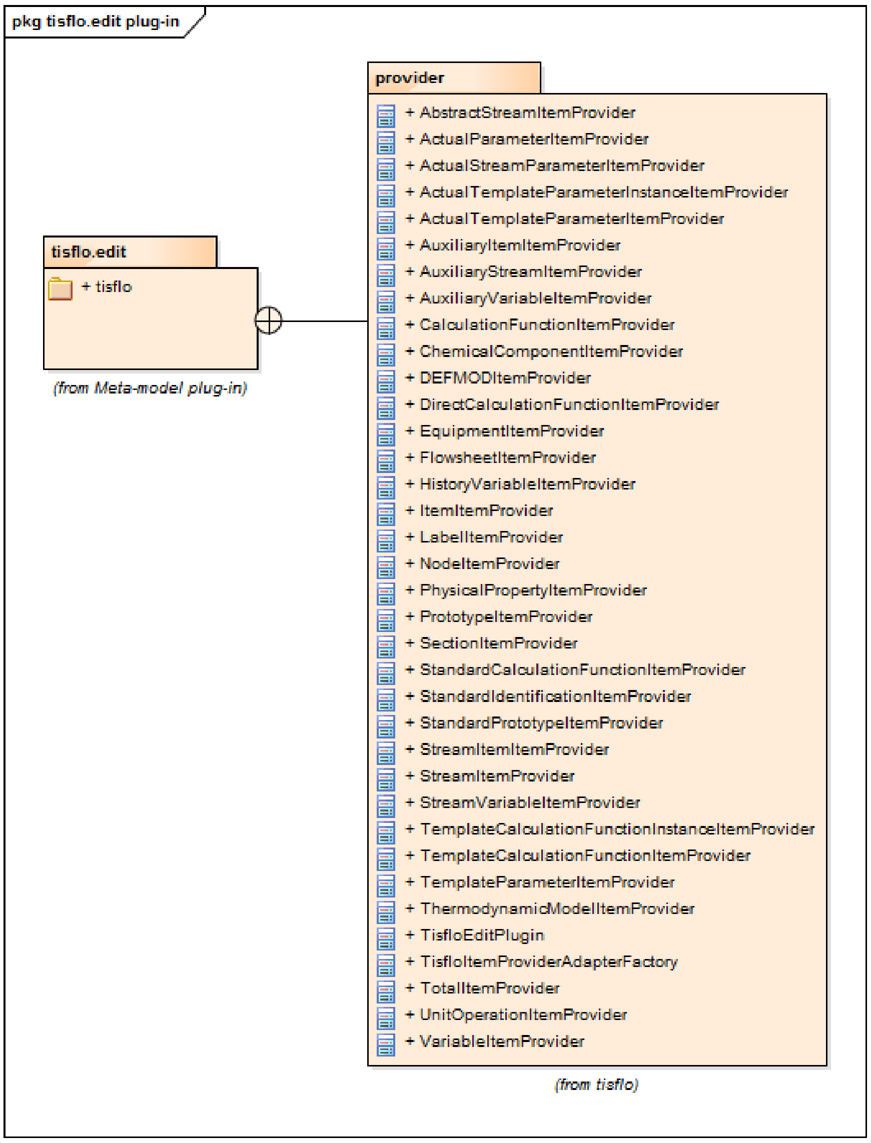

pkg tisflo.edit plug-in
tisflo.edit
+ tisflo
(from Meta-model plug-in)
provider
+ AbstractStreamItemProvider
+ ActualParameterItemProvider
+ ActualStreamParameterItemProvider
+ ActualTemplateParameterInstanceItemProvider
+ ActualTemplateParameterItemProvider
+ AuxiliaryItemItemProvider
+ AuxiliaryStreamItemProvider
+ AuxiliaryVariableItemProvider
+ CalculationFunctionItemProvider
+ ChemicalComponentItemProvider
+ DEFMODItemProvider
+ DirectCalculationFunctionItemProvider
+ EquipmentItemProvider
+ FlowsheetItemProvider
+ HistoryVariableItemProvider
+ ItemItemProvider
+ LabelItemProvider
+ NodeItemProvider
+ PhysicalPropertyItemProvider
+ PrototypeItemProvider
+ SectionItemProvider
+ StandardCalculationFunctionItemProvider
+ StandardIdentificationItemProvider
+ StandardPrototypeItemProvider
+ StreamItemItemProvider
+ StreamItemProvider
+ StreamVariableItemProvider
+ TemplateCalculationFunctionInstanceItemProvider
+ TemplateCalculationFunctionItemProvider
+ TemplateParameterItemProvider
+ ThermodynamicModelItemProvider
+ TisfloEditPlugin
+ TisfloItemProviderAdapterFactory
+ TotalItemProvider
+ UnitOperationItemProvider
+ VariableItemProvider
(from tisflo)

Figure 27 Deployment view of the Tisflo edit plug-in

The Tisflo edit plug-in is atomically generated. It contains providers to display Tisflo in a UI. There are providers for every class of the meta-model. Each provider can be used to display a model instance showing an icon and a name.

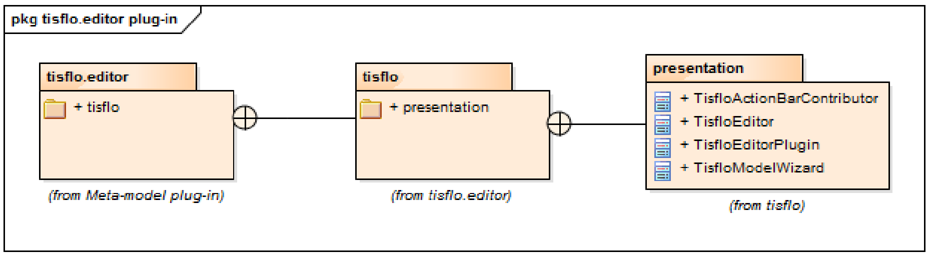


Figure 28 Deployment view of the Tisflo editor plug-in

The Tisflo editor plug-in is also automatically generated. The Tisflo editor plug-in provide wizards for creating new model instances and a UI for the editor that allows users to enter information in the model instances. The Tisflo editor plug-in is included in the RCP; however, it is not intended to be used by the process engineer. The Tisflo Sirius plug-in is the replacement for the Tisflo editor plug-in.

8.4.2. Development view of the Tisflo Sirius plug-in

In *Figure 29* the development view of the Tisflo Sirius plug-in is presented.

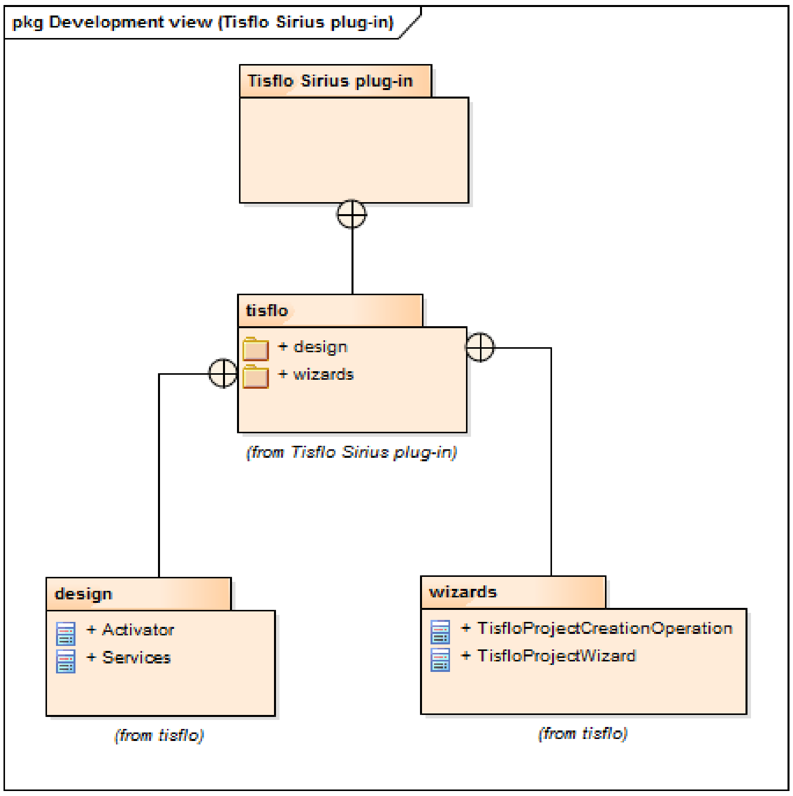


Figure 29 Deployment view of the Tisflo Sirius plug-in

The Tisflo Sirius plug-in contains two packages, the tisflo.design package and the tisflo.wizards package. Inside the tisflo.design package there are two classes, the Activator and the Services. The Activator class controls the plug-in life cycle. The class Services contains Java methods that can be transparently invoked from interpreted expressions in Sirius. Inside the tisflo.wizards package there is a wizard that simplifies the creation of a new Tisflo project for the process engineers. Every time that a new project is created an instance of a Flowsheet (the root element) is created, Sirius diagrams corresponding the Flowsheet instance are created on the background, and a flowsheet canvas is displayed to the process engineers.

8.5 Physical view

The physical or deployment view describes how the software is mapped to the hardware. An extended description about the deployment view is presented in Chapter 10.

9.Validation and Verification

In the previous chapter the design and implementation of the product is defined. This chapter presents the validation and verification techniques used in order to confirm that the right system is being build.

9.1 Validation

The software validation gives an answer to the question: Are we building the right product? Building the right product implies the creation of the requirement specification that contains the needs and the goals of the stakeholders. As presented in Chapter 6, the high-level requirements and goals of the system were known since the first two months of the project. Additional and more concrete requirements were derived from the high-level requirements and were defined on the sprint meetings.

The sprint meetings and the project steering group meetings resulted in a continuously and iterative validation process by the stakeholders. The feedback that the stakeholders provided during those meetings facilitated on the completeness and correctness of the product.

As a part of the validation, a survey was created. The survey was given to the process engineers at a late stage of the project. The survey aimed on an evaluation of the product by the actual users.

9.1.1. Survey

At a late stage of the project one-hour meetings with four process engineers individually were conducted. During those meetings a live demonstration of prototype was given to the process engineers. In addition, the process engineers were able to create their own use cases and interact with the application on their laptops. Moreover, during those meetings the process engineers gave feedback related to missing functionality of the application. Their feedback is included as a future work and it is presented in Section 11.2 Finally, at the end of each meeting a survey was given to the process engineers. The survey is split in two parts: the questions and the statements. The questions are shown in *Table 18* and they are based on the non-functional requirements. The statements are shown in *Table 19* and they are based on the project goals and aims. The answers represent the average grade from all the answers collected from the survey.

Table 18 grading system:

1. N/A (not applicable, not available, or no answer)
2. Bad
3. Not good
4. Good
5. Very good
6. Excellent

Table 18 Survey questions

Question	1	2	3	4	5	6
How do you grade the time required to learn how to use the tool?					X	
How do you grade the time required to create a flowsheet?				X		
How do you grade the appearance of the diagrams?			X			
How do you grade the piece of information that displayed in the diagrams?				X		
How do you grade the loading time of a plant part definition?					X	
How do you grade the loading time of a complete plant definition?					X	
How do you grade the time required for a simulation?	X					
How do you grade overall the application?					X	

Table 19 grading system:

1. N/A (not applicable, not available, or no answer)
2. Strongly disagree
3. Disagree
4. Neither agree nor disagree
5. Agree
6. Strongly Agree

Table 19 Survey statements

Statement	1	2	3	4	5	6
The new application will shorten the learning curve of the new engineers.				X		
The new application will improve the productivity of new engineers.					X	
The new application will improve the productivity of experienced engineers.				X		
The diagrams in the new application increase the overview of the flowsheet design.					X	
The new application simplifies the editing of the flowsheet design.					X	
The predefined sections that can be merged will simplify the flowsheet design.						X
The merging functionality will enable the parallel work of the process engineers on the same project.					X	
The new application will reduce the time required for a design.					X	

The answers in the survey feature a general satisfactory of the process engineers about the application. The process engineers showed great enthusiasm about the predefined sections that can be merged. On the other hand, the appearance of the diagrams is one of the weakest points of the application. Improvement points are presented as a future work in Section 11.2

9.2 *Verification*

The software verification gives an answer to the question: Are we building the product right? The verification process involves the evaluation on whether the software conforms to the requirement specification or not. The software verification aims on the design and implementation of the product. The verification of the application is performed by software testing. The testing conducted with two different approaches: the manual testing and the unit testing.

9.2.1. Manual testing

The manual testing was conducted on the model and on the user interface.
The manual testing of the model covered

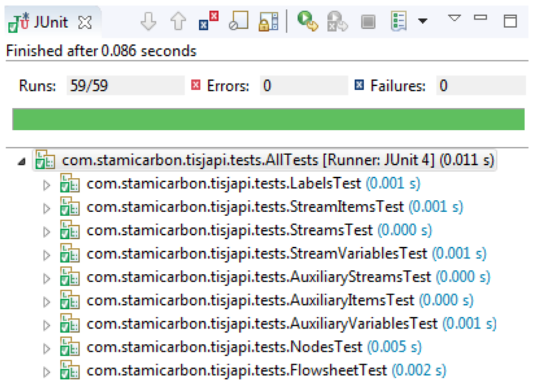
- The creation of the model instances
- The initialization and modification of the attributes of the model instances
- The serialization
- The synchronization

The manual testing of the user interface covered

- The creation of a new urea plant design project
- The functionality of each button
- The appearance of the icons
- The appearance of the diagrams

9.2.2. Unit testing

The unit testing is a software testing method in which individual parts of the source code, called units, are tested. The unit testing was performed on the JNI functions. The unit tests covered 70% of the total JNI functions. 59 test cases were implemented.



```
Finished after 0.086 seconds

Runs: 59/59    Errors: 0    Failures: 0

com.stamicarbon.tisjapi.tests.AllTests [Runner: JUnit 4] (0.011 s)
  com.stamicarbon.tisjapi.tests.LabelsTest (0.001 s)
  com.stamicarbon.tisjapi.tests.StreamItemsTest (0.001 s)
  com.stamicarbon.tisjapi.tests.StreamsTest (0.000 s)
  com.stamicarbon.tisjapi.tests.StreamVariablesTest (0.001 s)
  com.stamicarbon.tisjapi.tests.AuxiliaryStreamsTest (0.000 s)
  com.stamicarbon.tisjapi.tests.AuxiliaryItemsTest (0.000 s)
  com.stamicarbon.tisjapi.tests.AuxiliaryVariablesTest (0.001 s)
  com.stamicarbon.tisjapi.tests.NodesTest (0.005 s)
  com.stamicarbon.tisjapi.tests.FlowsheetTest (0.002 s)
```

Figure 30 Unit tests for the JNI functions

9.3 *Dynamic program analysis*

The dynamic program analysis is the analysis that is performed while the application is being executed. In order to measure the space (memory) and the time complexity and identify possible bottlenecks of an application, software profiling can be conducted. In this project two different profilers were used. The first profiler was the Sirius profiler. The Sirius profiler is a profiler that measures the time complexity of specific parts of Sirius. The second profiler was the VisualVM, which is a Java profiler that is able to provide more in depth information about the time and space usage of the application. In addition to the profilers, the Eclipse debugger was also used in order to optimize the source code. A result of the dynamic program analysis is that the model instance elements are created and presented to the end-users in one eighth of the initial time. The performance improvement is achieved by not serializing automatically the sections when they are created.

10. Deployment

This chapter elaborates on the deployment view of the application, the technologies used for the build of the application, and how to build and deploy newer versions of the application.

10.1 Deployment view

The application can run on any Windows machine that supports the x86 architecture. The Windows machine must have a Java Virtual Machine (JVM) installed. A JVM version 8 update 121 or newer is advised, because the Java Development Kit (JDK) version 8 update 121 is used for the development of the application. The application consists of an RCP that runs outside the Eclipse IDE. The RCP depends on the kernel and the thermodynamic libraries that are contained in the TISjapi.dll. The application is portable and it can be used without any installation.

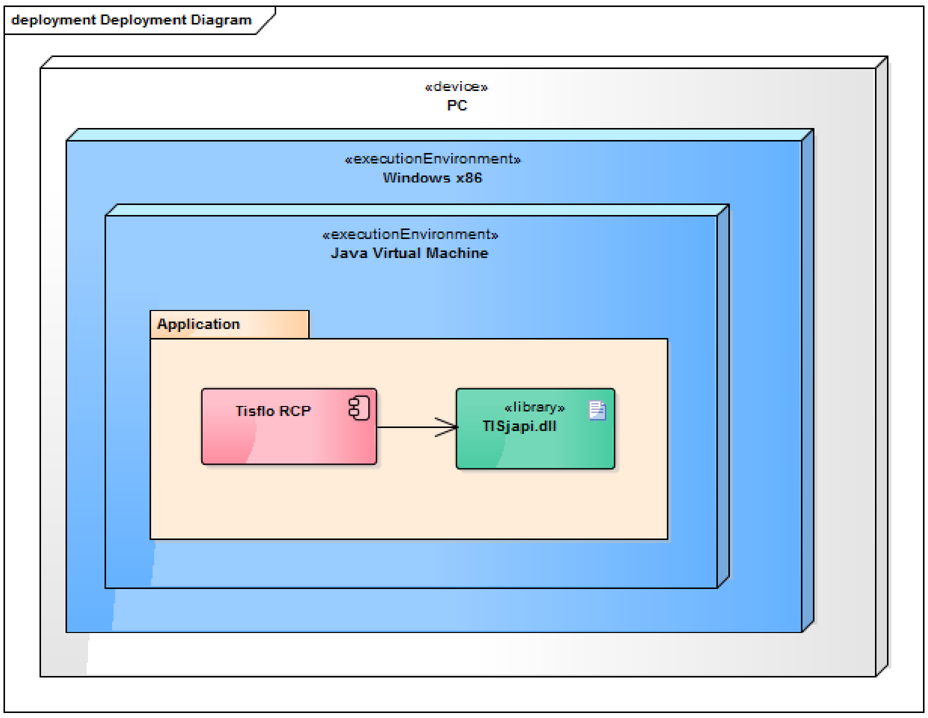


Figure 31 Deployment view of the application

10.2 How to build and deploy the application

In this section there is an introduction about the technologies used for the build of the project. Next, there is information about how the application can be built and deployed.

10.2.1. Maven

Maven is a build automation tool used primarily for Java projects. In Yiddish, the word maven means "accumulator of knowledge" [16]. Maven projects are configured using a Project Object Model (POM), which is stored in a pom.xml file [17]. The XML file describes the software project being built, its dependencies on other external modules and components, the build order, directories, and required plug-ins. It comes with predefined targets for performing certain well-defined tasks such as compilation of code and its packaging.

Maven dynamically downloads Java libraries and Maven plug-ins from one or more repositories, such as the Maven 2 Central Repository, and stores them in a local cache. This local cache of downloaded artifacts can also be updated with artifacts created by local projects.

10.2.2. OSGi

OSGi (Open Service Gateway Initiative) is a Java framework for developing and deploying modular software programs and libraries. Each bundle is a tightly coupled, dynamically loadable collection of classes, jars, and configuration files that explicitly declare their external dependencies [18].

10.2.3. Tycho

Tycho is focused on a Maven-centric, manifest-first approach to building Eclipse plug-ins, features, update sites, RCP applications and OSGi bundles. Tycho is a set of Maven plug-ins and extensions for building Eclipse plug-ins and OSGi bundles with Maven. Tycho uses native metadata for Eclipse plug-ins and OSGi bundles and uses the POM to configure and drive the build. Tycho supports bundles, fragments, features, update site projects and RCP applications. Tycho also knows how to run JUnit test plug-ins using OSGi run-time.

Tycho use OSGi metadata and OSGi rules to calculate project dependencies dynamically and injects them into the Maven project model at build time. Tycho supports all attributes supported by the Eclipse OSGi resolver. Tycho uses proper classpath access rules during compilation. One important design goal in Tycho is to make sure there is no duplication of metadata between POM and OSGi metadata [19]. Tycho also enables Maven to understand package types such as eclipse-plugin, eclipse-feature, and eclipse-repository [20].

10.2.4. Tisflo plug-in projects

The Tisflo plug-in projects are the Tisflo meta-model plug-in, the Tisflo Sirius plug-in, and the Tisflo branding plug-in. The package type of the Tisflo plug-ins is eclipse-plugin. Each plug-in has a Maven based configuration file, the pom.xml, which is used for the Tycho build.

10.2.5. Tisflo feature project

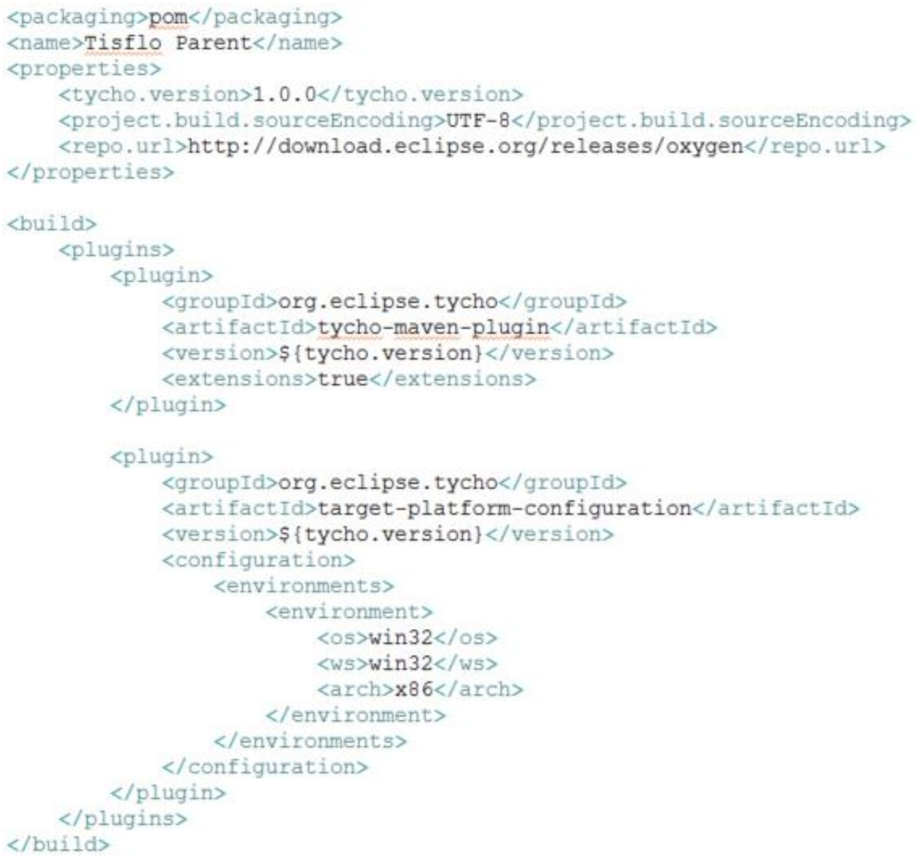
An Eclipse feature project contains features. A feature describes a list of plug-ins and other features which can be seen as a logical unit. A feature has a name, a version number, and in most cases license information assigned to it. Instead of having many individual plug-ins it is possible to group the plug-ins using features. Grouping the plug-ins into logical units improves the system structure. The Tisflo feature contains all the Tisflo plug-ins. The feature project has package type eclipse-feature and it has Maven based configuration file, the pom.xml, which is used for the Tycho build.

10.2.6. Tisflo product project

The Tisflo product contains a product configuration file and a Maven based configuration file, the pom.xml. The product configuration file defines the configuration of an Eclipse application. The configuration of an Eclipse application includes icons, splash screen, and the plug-ins or features. The Tisflo product contains the Tisflo feature project and the Eclipse platform. The Tisflo product has a package type eclipse-repository.

10.2.7. Tisflo parent project

The Tisflo parent project contains only a Maven-based configuration file, the pom.xml. The packaging type of the Tisflo parent is pom. The pom.xml of the Tisflo parent contains general configurations that are inherited by all the other projects. The general configurations include the Tycho version, the build environment, and a repository where Tycho can find and download the dependencies of the projects.



```xml
<packaging>pom</packaging>
<name>Tisflo Parent</name>
<properties>
    <tycho.version>1.0.0</tycho.version>
    <project.build.sourceEncoding>UTF-8</project.build.sourceEncoding>
    <repo.url>http://download.eclipse.org/releases/oxygen</repo.url>
</properties>

<build>
    <plugins>
        <plugin>
            <groupId>org.eclipse.tycho</groupId>
            <artifactId>tycho-maven-plugin</artifactId>
            <version>${tycho.version}</version>
            <extensions>true</extensions>
        </plugin>

        <plugin>
            <groupId>org.eclipse.tycho</groupId>
            <artifactId>target-platform-configuration</artifactId>
            <version>${tycho.version}</version>
            <configuration>
                <environments>
                    <environment>
                        <os>win32</os>
                        <ws>win32</ws>
                        <arch>x86</arch>
                    </environment>
                </environments>
            </configuration>
        </plugin>
    </plugins>
</build>
```

Figure 32 Part of the Tisflo parent pom.xml

The build environments that are specified on the parent pom.xml are independent of the development environment. For instance, Eclipse Neon and a 64-bit version of Windows can be used for the development; however, the build could be based on the Eclipse Oxygen and the application could run on a 32-bit Linux machine or on a 32-bit Windows machine.

11. Conclusions

This chapter elaborates on the results achieved by this project. The value that this project added to the stakeholders is also presented. Finally, this chapter also presents future work related to the project.

11.1 Results

The flowsheet design and the calculation of the heat and material balances is an important task that the process engineers have on every project. The main goal of this project was to improve the productivity of the process engineers. In order to improve the productivity of the process engineers the project aimed to: increase the comprehension of the structure and the state of the flowsheet design, decrease the number of errors, allow the process engineers to use predefined reusable sections that can be merged, allow the process engineers to work simultaneously on different plant parts, and integrate the editor and the solver into one tool.

According to the results of the survey in Section 9.1.1. the end product is very promising. More specifically, the process engineers agree that the new application will reduce the time required for the flowsheet design. The predefined sections that can be merged is the feature that adds the most value in the application according to the process engineers. Furthermore, the process engineers can use for the first time the same tool to edit and solve flowsheets. On the other hand, one of the weakest points of the application is the appearance of the diagrams and the visual representations. The appearance of the diagrams and the visual representations was a deliverable of the end product, although this deliverable is related more with graphic designing rather than software engineering. A comparison between the textual representations and the visual representations is presented in Appendix B: Comparison between textual representations and visual representations.

From the software design point of view, the system demonstrates usability, navigability, and extensibility. A reflection based on the design criteria is presented in Section 13.2

11.2 Future work

This section elaborates on future possibilities and improvements, as well as on features that were not designed or implemented in this project due to various constraints such as time and lack of knowledge.

Possible extensions are:

- Sirius provides functionality that can auto-arrange the elements of a diagram. The auto-arrange was not always ideal especially for diagrams with many elements. A customized auto-arrange function could be implemented.

- The streams are aligned in a default position that Sirius defines. The default position is not always the desired. The functionality about the default positioning could be overridden.

- All the streams have the same visual representation. The streams could have a different visual representation according to their items.

- The predefined sections are created on the flowsheet canvas by selecting them from the file system. Icons that represent each predefined section could be added to the palette of the flowsheet canvas.

- The history variable instances are used to display variable changes from free to fixed, or the opposite. The deletion of a history variable instance does not revert the changes. In order to revert the changes a new functionality could be implemented.

- The application logs the return values of limited kernel functions. The only messages that originate from the kernel and appear on the application screen are about the convergence of the simulation. As a future work a logging system and an error reporting system to the process engineers could be implemented.

- In order to save and load the structure and the state of a flowsheet design, a version control system could be added.

- The RCP can run in any major operating system (Windows, macOS, Linux) in both x86 and x64 architecture. However, the kernel can run only on Windows machines with x86 architecture. A kernel version that could run on the x64 architecture could improve the application performance.

- The RCP is based on the Eclipse platform, therefore menu items and toolbar buttons that are more useful for developers rather than process engineer exist. In order to simplify the UI it is recommended that a newer version of the RCP would hide those menu items and toolbar buttons.

- The application performance when opening a diagram for first time that contain a large piece of information is not ideal. For example, opening a diagram for first time that contains all the section variables of a complete plant varies from 7 to 14 seconds, depending on the information. As a part of this project performance issues related to the diagrams are mentioned as a bug in Eclipse Sirius. A workaround could be achieved by splitting the information into more diagrams with less information.

- The application is missing functionality that the previous flowsheet solver has. For instance, modify the step size of all the variables, the linstep, the damping factor, the case study, and the optima mode are missing.

- The kernel can only merge and simulate sections, which they have the stream items on the same position. As a future work a kernel which can merge and simulate section with stream item on different position is advised.

- The kernel instances are created by parsing a DAT file. The instances of the model are created by querying the kernel and the non-transient attributes are serialized in XMI files. As already explained in a previous chapter there is a synchronization mechanism for the kernel and the model instances. The synchronization mechanism will be omitted if the kernel instances will be created from the same XMI files that describe the model instances.

- The API of the kernel does not support functions that can reflect the creation of a model instance to a kernel instance. For instance, there is no JNI function that would reflect the creation of a node or a stream instance from the model to the kernel. In the current product it is not possible to create a flowsheet diagram from scratch, a DAT file should always be used. As a future work function calls that would reflect the creation of all the model instances to the kernel is advised.

- The API of the kernel currently supports setters for the attributes of the label, stream variable, and auxiliary stream variable instances. Any change made in any other model instance, for example, in a calculation function instance, will not be reflected in the kernel. Any change that is not reflected in the kernel is not taken into consideration in the simulation. As a future work new API calls that would allow the modification of all the attributes of kernel instances is advised.

- The test cases that implemented in this project cover only the JNI functions. Test cases for the model and the visual presentations is left as a future work.

12. Project Management

This chapter elaborates on the project management process that was conducted during the lifetime of the project.

12.1 *Way of working*

The system was developed under the agile methodology. The agile methodology suggests iterative and incremental development. Each iteration is called a sprint. The duration of each sprint for this project was two weeks. At the end of each sprint a deliverable had to be produced. The different phases of the sprint involve: the plan, the design, the development, a prototype with the new functionality, and the evaluation of the progress.

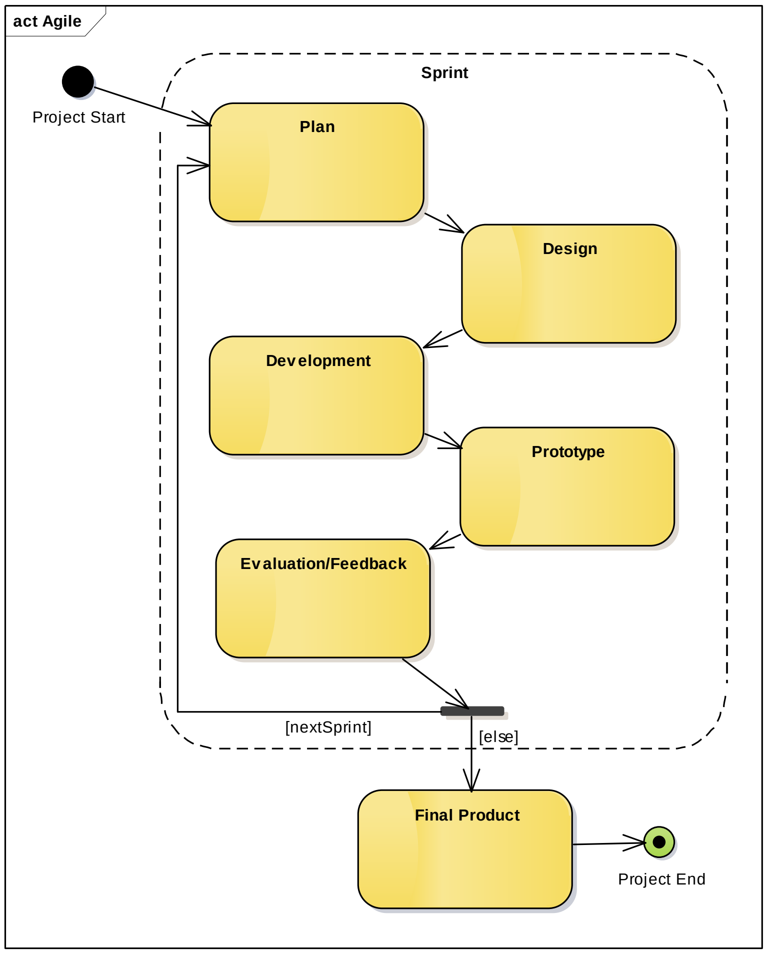


Figure 33 Agile lifecycle

The definition or the refinement and the prioritization of the requirements was held during the planning phase of each sprint. The next two sprint phases involved the software design and the software development of the application. The next phase involved a prototype and a new version of the product. The last phase involved the evaluation and the feedback about the sprint.

12.2 *Work-Breakdown Structure (WBS)*

The work-breakdown structure is presented on this section. The WBS is the way in which the project has been decomposed. The project is divided into four main activities as follows:

- Domain research: Research and study about the elements used in the flowsheet diagrams for the calculation of the heat and material balances.
- Technology research: Research about the technologies picked by stakeholders for the project.
- Design and implementation: Usage of the research and study of the previous two activities in order to build the software solution of the project.

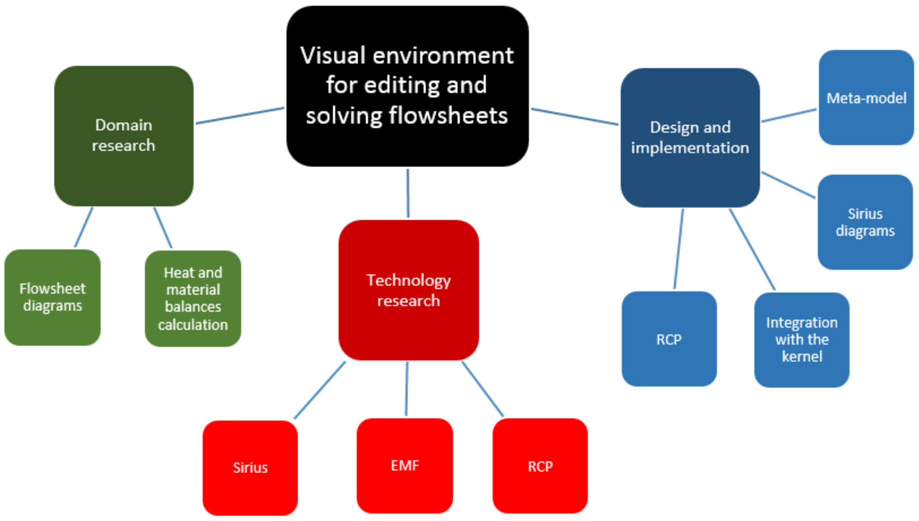

Visual environment for editing and solving flowsheets
Domain research
Flowsheet diagrams
Heat and material balances calculation
Technology research
Sirius
EMF
RCP
Design and implementation
Meta-model
Sirius diagrams
RCP
Integration with the kernel

Figure 34 Work-breakdown structure of the project

12.3 *Project Planning*

According to the work-breakdown structure a project plan was formulated. The initial version of the project plan was formulated during the first weeks of the project. Adjustments were introduced during the whole period of the project, as the knowledge and the understanding about the project deepened.

12.3.1. Initial version

The initial version of the project plan involved four activities: the domain analysis, the design and implementation, the technical report, and the final presentation. As it is visible in *Figure 35* there is overlapping between the activities.

The domain analysis activity involves the domain research, the technology research, and the requirements. The domain analysis was expected to last until the first week of April.

The design and implementation was expected to last from mid-January to mid-August. The design of EMF, the design of Sirius and the integration with the kernel was expected to last from mid-January to late-May.

The writing of the technical report and the preparation for the final presentation were expected to last from mid-May until the end of the project.

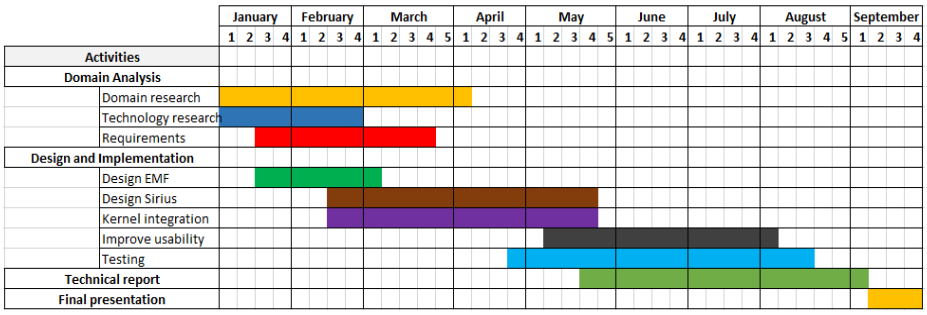


Figure 35 Initial project planning

12.3.2. Final version

The final version of the project plan displays what actually happened during the project. The only activities that remain the same or almost the same are the writing of the technical report and the preparation for the final presentation.

In the domain analysis phase, the domain research lasted less than expected; however, new requirements were introduced in June. The new requirements affected the design and implementation of the project. More specifically, because of the new requirements, the design of the EMF and the design of Sirius lasted longer. In addition, a new activity called a performance check added in the project plan. The integration with kernel also lasted longer than what was initially expected.

Finally, it is worth mentioning that the testing was developed and applied iteratively in different time periods. This incremental-iterative development approach is better aligned with the agile way of working that the approach planned in the initial project plan.

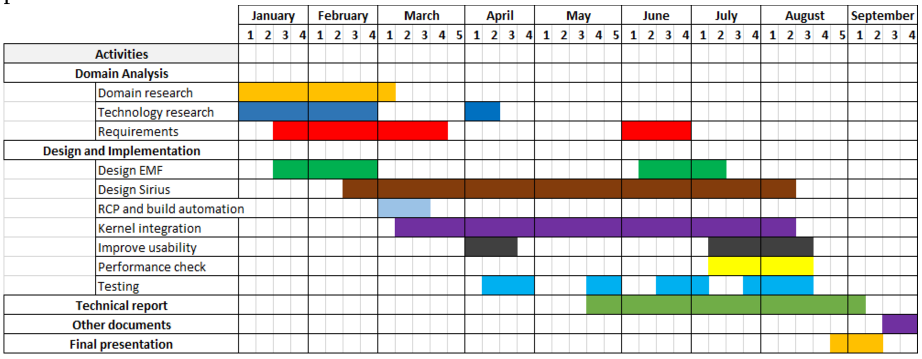


Figure 36 Final project planning

12.4 Project execution

The execution of the project followed a structured path based on the project planning. The first days of the project involved meetings with the stakeholders in order to familiarize the PDEng trainee with the domain and the high-level requirements. The agile way of working aimed on a prototype that it is iterative and incremental implemented. The domain analysis and the design and implementation of project have been executed simultaneously.

Every three weeks a Project Steering Group (PSG) meeting was held. The project progress and a live demonstration of the prototype was presented by the PDEng trainee during the PSG meetings. The prototype allowed the stakeholders to have a clear view of the project progress. During these meetings the stakeholders were giving feedback about the project and the product. The feedback worked as a method of validation about the product and advocated on keeping track of the project direction.

The prioritization of the requirements at the end of each iteration was the main reason that the project execution was significantly different from the initial project plan.

13. Project Retrospective

This chapter presents a reflection of the project based on the candidate's perspective. At the end of the chapter a reflection is presented based on the design criteria set in Chapter 3.

13.1 Reflection

In the project conducted over the past nine months I faced several challenges from both technical and non-technical perspective. For me as a software engineer it was a great experience and it helped to improve my technical and soft skills.

At the beginning of the project I had two main concerns regarding to the project. The first concern was related to the project domain and the second was related to the technology constraints of the project. About the first concern, my knowledge about chemical engineering and more specifically about the flowsheet solving was zero prior to this project. I was able to gain the domain knowledge from the user manual of the old flowsheet simulator and from my stakeholders. Luckily for me most of the times it was easy to arrange a meeting with my stakeholders and I could gain the needed information for my project. About the second concern, I had low to zero experience with the technology constraints. My knowledge about Eclipse Modeling Framework was limited. During my first year as a PDEng trainee I participated in a one week workshop about model driven software engineering. However, this was the first and last experience that I ever had with EMF prior to this project. In addition, I had no experience with Eclipse Sirius, although I found the tool relatively easy to use. Finally, I had no knowledge about what an RCP is and how could I build one.

The tasks that required the most time was the design of the EMF meta-model and the kernel integration. The design of the EMF meta-model was probably the most crucial task of the project. The majority of the code is automatically generated from the meta-model. The model instances have to reflect the kernel instances, although I had no access in the kernel. I was using the user manual of the flowsheet simulator as a reference to understand elements needed for the heat and material balances calculations. However, there were some inconsistences between the user manual and the kernel. For instance, the kernel adds additional information for all the variables, although according the user manual only a specific number of variables have additional information. I was able to bypass such a problem by communicating with my stakeholders. About the kernel integration it is mentioned that he API of the kernel was extended in parallel with my project. The return values of the new API functions were not always correct. That was the main reason that I spent more time on kernel integration than I expected. The extra time was spent mostly on debugging.

At a late stage of my project I identified performance issues in the application. The issues were related to the creation of new sections and to the simulation of the flowsheet. The performance issues were noticeable in the creation and the simulation of a complete urea plant. In order to optimize the application I used the Eclipse debugger, two profilers, and I contacted the Eclipse Sirius community. Thanks to their help I managed to solve the performance issues. In order to contribute back to the community I created a video tutorial about how to create an Eclipse Sirius based RCP[1]. In this project I managed to create the RCP and automate the build of the RCP in a week. I believe that if there was a tutorial similar to the one that I created I would have achieved the task in one or two days.

[1] https://www.youtube.com/watch?v=ZmUrTlzqCXcv

Apart from the project design and implementation, the project management was another important part of the project that I had to satisfy. I was responsible for updating the requirement list and estimating the time needed for each requirement. Although the initial project plan differed significantly from the final plan, my sort-term time estimations for the tasks were quite accurate. In addition to project management, I was also responsible for the organization of the majority of the meetings, for instance, the meetings with the process engineers and the project steering group meetings. All those meetings helped me to improve my soft skills, for example, my presentation and organization skills.

In conclusion, this project was a great experience. I had the opportunity to gain experience in a new domain. The Eclipse modeling tools that I used (EMF and Sirius) broaden my experience and knowledge about model driven software engineering. On top of that, the cooperation with the stakeholders and the project management responsibilities helped me to improve my soft skills.

13.2 Design criteria revisited

This section presents a reflection of the project based on the design criteria that were introduced in Section 3.6

Usability
Usability should be addressed by means of making the product easy to understand and use. Functionality that could reduce the steps that a process engineer needs in order to perform an action is implemented. A wizard that simplifies the creation of a new urea plant project is implemented. With the wizard the number of clicks required in order to create a new project, create a root instance of the model in the project, select the viewpoints for the project, and create the representations for the root instance, reduced from more than 40 to 7. In addition to the wizard, functionality that automatically generates diagrams is implemented. For example, in a complete urea plant design more than a hundred diagrams are generated automatically.

Navigability
In the previous tools the process engineers had to scroll and search for keywords in the text files in order to find the desired piece of information, in the new application all the information is structured in diagrams. In order to increase the navigability options and to provide all the necessary information in the diagrams, extra associations are added in the meta-model. An example is given in Section 8.2.3. In addition, the diagrams provide information that wasn't available with the previous tools, for instance, the history tracking of the free and fixed variables.

Extensibility
The plug-in based architecture that is used in this project is ideal for an extensible application. New diagrams can easily be created by modifying the Tisflo Sirius plug-in. The domain model can be extended by modifying the Tisflo meta-model plug-in. New plug-ins that contain other domain models or functionality could simply be added on the Tisflo feature project and be deployed in a future version of the RCP.

Glossary

This chapter presents the terminologies used in this report.

Term	Definition
API	Application Programming Interface
BEP	Basic Engineering Package
DAT	File extension of the text files that the process engineers are storing the information needed for urea plant designs
DLL	File extension of dynamic-link library files
Eclipse IDE	Eclipse Integrated Development Environment
EMF	Eclipse Modeling Framework
EPC	Engineering, Procurement, and Construction
H&MB	Heat and Material Balances
JDK	Java Development Kit
JNI	Java Native Interface
JVM	Java Virtual Machine
MDE	Model-driven engineering
MOF	Meta-Object Facility
MoSCoW	The framework for prioritizing requirements by four groups: Must, Should, Could, Would
OMG	Object Management Group
OSGi	Open Service Gateway Initiative
PDEng	Professional Doctorate in Engineering
PDP	Process Design Package
POM	Project Object Model
PSG	Project Steering Group
RCP	Rich Client Platform
Sirius	Eclipse plug-in for creating visual representations
ST	Software Technology
Stamicarbon	The company name
Tisflo	The software program name of the flowsheet solver
TU/e	Eindhoven University of Technology
UI	User Interface
UML	Unified Modeling Language
VSM	Viewpoint Specification Model
VSP	Viewpoint Specification Project
WBS	Work-Breakdown Structure
XMI	XML Metadata Interchange
XML	Extensible Markup Language

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Appendix A: The complete meta-model

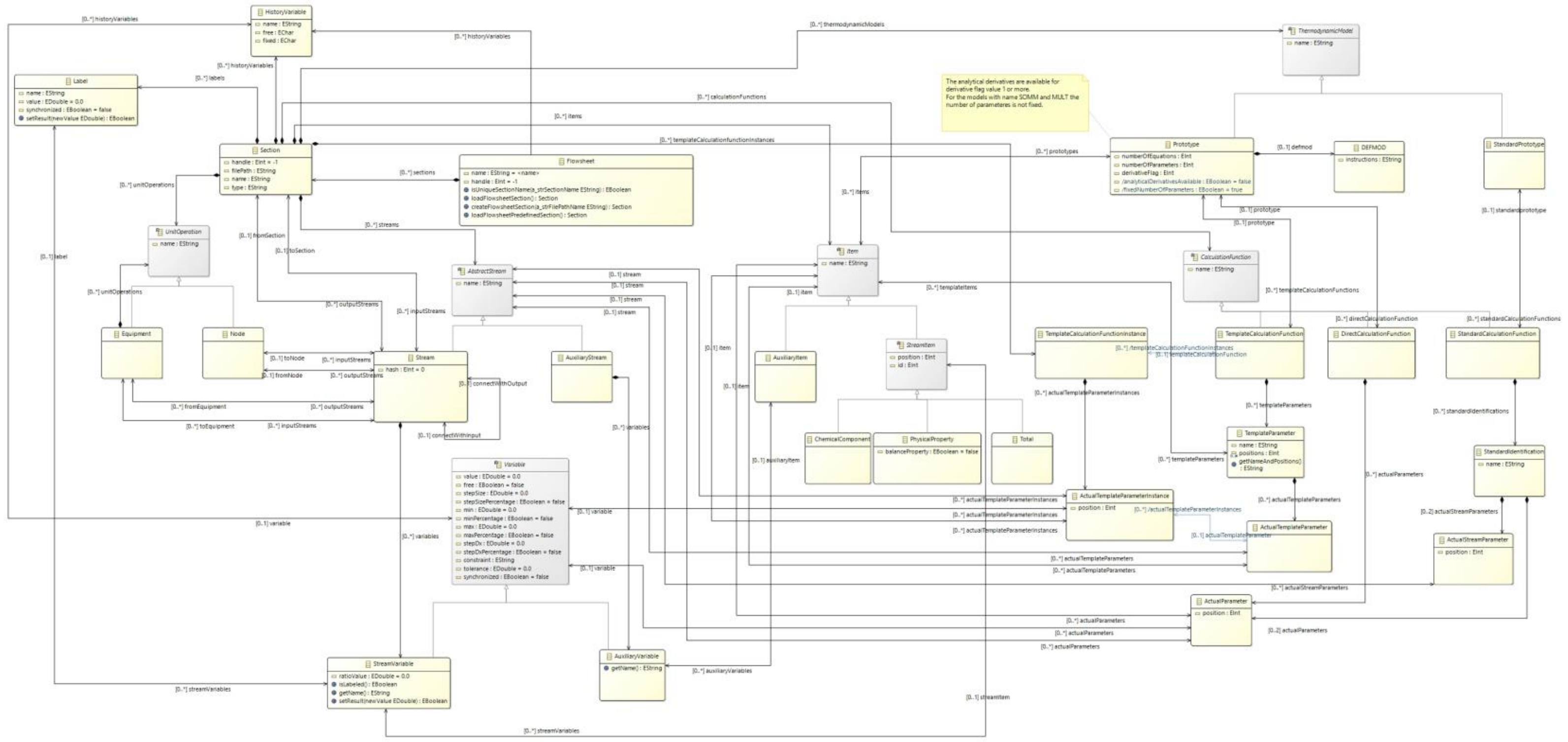
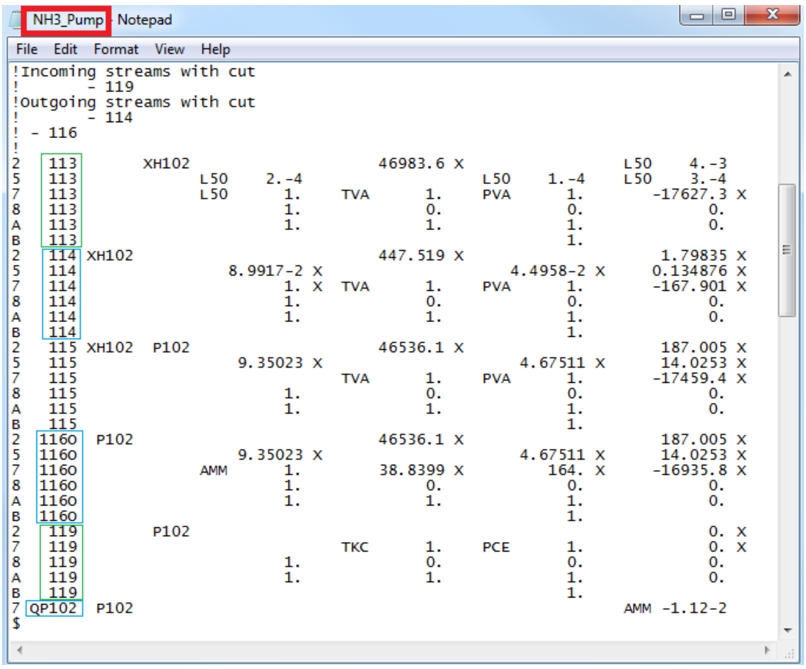


Figure 37 The complete meta-model

Appendix B: Comparison between textual representations and visual representations



```
!Incoming streams with cut
!       - 119
!Outgoing streams with cut
!       - 114
! - 116
!
2   113       XH102                    46983.6 X                 L50    4.-3
5   113             L50    2.-4                   L50    1.-4    L50    3.-4
7   113             L50      1.    TVA      1.    PVA      1.       -17627.3 X
8   113                      1.             0.             0.             0.
A   113                      1.             1.             1.             0.
B   113                                                    1.
2   114 XH102                          447.519 X                     1.79835 X
5   114                8.9917-2 X                    4.4958-2 X     0.134876 X
7   114                      1. X  TVA      1.    PVA      1.       -167.901 X
8   114                      1.             0.             0.             0.
A   114                      1.             1.             1.             0.
B   114                                                    1.
2   115 XH102  P102                    46536.1 X                     187.005 X
5   115                 9.35023 X                     4.67511 X      14.0253 X
7   115                            TVA      1.    PVA      1.       -17459.4 X
8   115                      1.             0.             0.             0.
A   115                      1.             1.             1.             0.
B   115                                                    1.
2  1160  P102                          46536.1 X                     187.005 X
5  1160                 9.35023 X                     4.67511 X      14.0253 X
7  1160             AMM      1.        38.8399 X         164. X     -16935.8 X
8  1160                      1.             0.             0.             0.
A  1160                      1.             1.             1.             0.
B  1160                                                    1.
2   119        P102                                                       0. X
7   119                            TKC      1.    PCE      1.             0. X
8   119                      1.             0.             0.             0.
A   119                      1.             1.             1.             0.
B   119                                                    1.
7 QP102  P102                                                    AMM -1.12-2
$
```

Figure 38 Input and output streams of a section in a textual representation

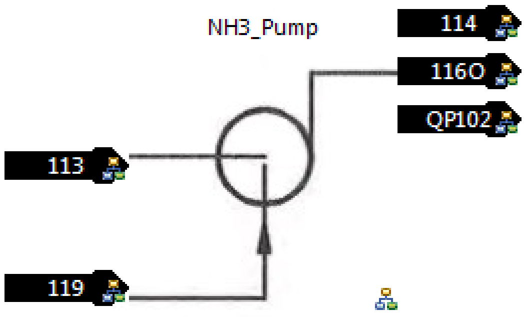
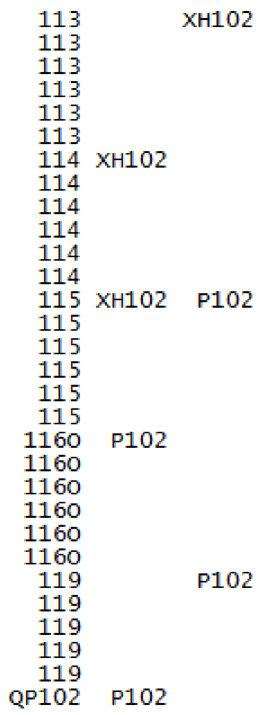


Figure 39 Input and output streams of a section in a visual representation



```
  113       XH102
  113
  113
  113
  113
  113
  114 XH102
  114
  114
  114
  114
  114
  115 XH102  P102
  115
  115
  115
  115
  115
 1160  P102
 1160
 1160
 1160
 1160
 1160
  119        P102
  119
  119
  119
  119
QP102  P102
```

Figure 40 Streams and nodes in textual representation

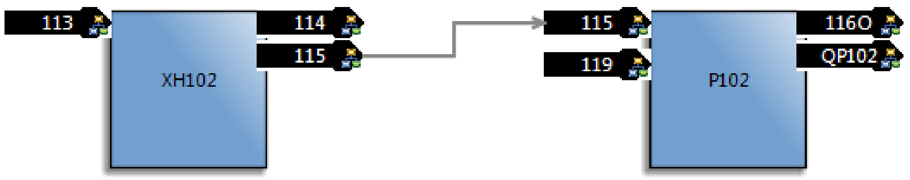
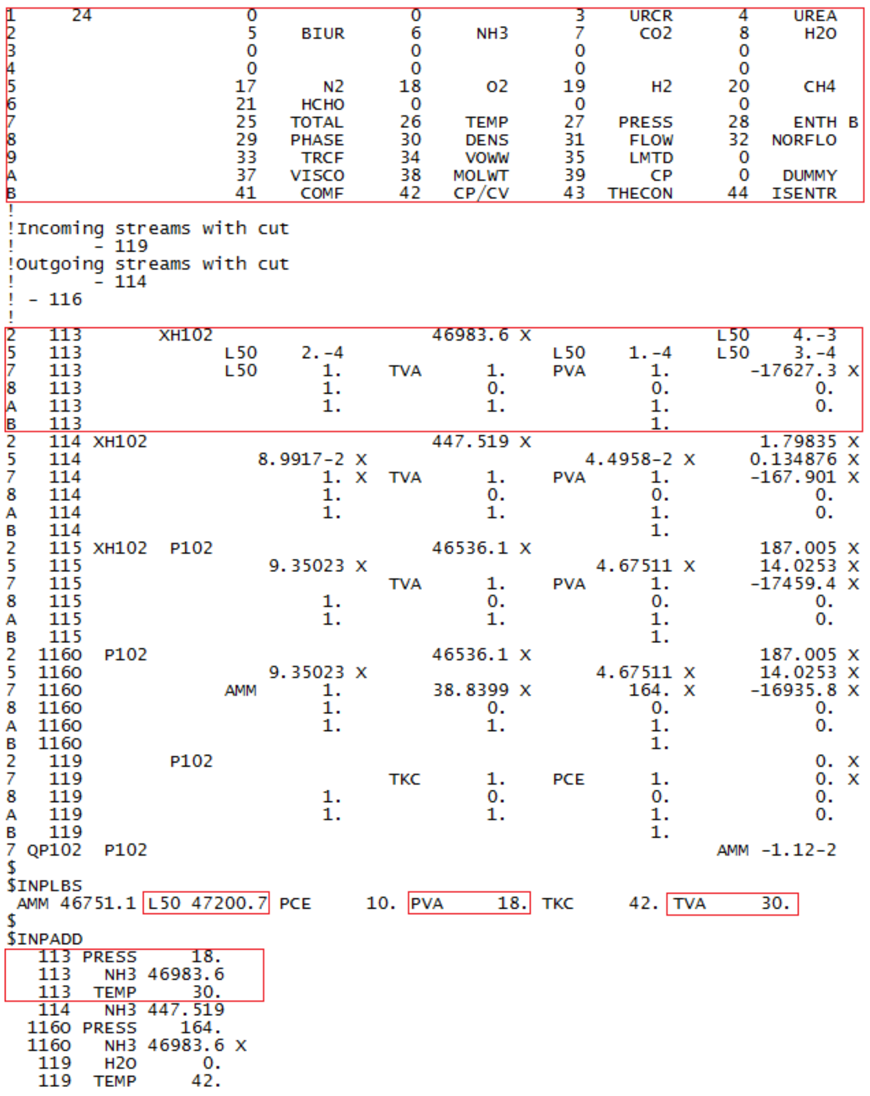


Figure 41 Streams and nodes in visual representation



```
1     24              0              0              3     URCR     4     UREA
2                     5     BIUR     6      NH3     7      CO2     8      H2O
3                     0              0              0              0
4                     0              0              0              0
5                    17       N2    18       O2    19       H2    20      CH4
6                    21     HCHO     0              0              0
7                    25    TOTAL    26     TEMP    27    PRESS    28     ENTH B
8                    29    PHASE    30     DENS    31     FLOW    32   NORFLO
9                    33     TRCF    34     VOWW    35     LMTD     0
A                    37    VISCO    38    MOLWT    39       CP     0    DUMMY
B                    41     COMF    42    CP/CV    43   THECON    44   ISENTR
!
!Incoming streams with cut
!       - 119
!Outgoing streams with cut
!       - 114
! - 116
!
2   113       XH102                    46983.6 X                 L50    4.-3
5   113             L50    2.-4                   L50    1.-4    L50    3.-4
7   113             L50      1.    TVA      1.    PVA      1.       -17627.3 X
8   113                      1.             0.             0.             0.
A   113                      1.             1.             1.             0.
B   113                                                    1.
2   114 XH102                          447.519 X                     1.79835 X
5   114                hFILLER
```

About the Author

Konstantinos Raptis received his diploma in Electrical and Computer Engineering from the Aristotle University of Thessaloniki, Greece in 2015. During his studies, he focused on Software Technology and Computer Science. He is also interested in Game Theory and he has won many poker and sports tipster competitions. His diploma thesis is titled "Real-time Online Betting Analysis – The THMMY Case-Study." In his thesis, he created an interactive Ruby on Rails betting platform with a MySQL database that encompasses a sophisticated algorithm for real-time betting analysis on the dynamic calculation of profit margins. He invited the students to bet on what they thought that the average grade in a course would be.

From September 2015 until September 2017, he worked at the Eindhoven University of Technology as a PDEng trainee of the Software Technology program from the 4TU.Stan Ackermans Institute. During his graduation project, he worked at Stamicarbon on a project focused on visual editing and solving flowsheet models.