Project information

Project title	Coordinating Optimisation of Complex Industrial Processes
Project acronym	COCOP
Project call	H2020-SPIRE-2016
Grant number	723661
Project duration	1.10.2016-31.3.2020 (42 months)

Document information

Deliverable number	D4.6
Deliverable title	Modelling guideline document and demonstration development kit (update)
Version	1.0
Dissemination level	Public
Work package	WP4
Authors	VTT
Contributing partners	TUDO, OPT
Delivery date	31.1.2019
Planned delivery month	M28
Keywords	Modelling, tools, workflow, digital maturity, human factors

This project has received European Union's Horizon 2020 research and innovation funding under grant agreement No 723661.

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VERSION HISTORY

Version	Description	Organisation	Date
0.1	Skeleton	VTT	22.11.18
0.2	Added MOSAIC	VTT	22.11.18
0.3	Digital Maturity, simulators, HF Milestones	VTT	14.12.18
0.4	Cleansing	VTT	19.12.18
0.5	Executive summary & cleansing	VTT	2.1.2019
0.6	Updates per review comments	VTT	21.1.2019
1.0	Final checks	VTT	28.1.2019

EXECUTIVE SUMMARY

This deliverable continues the work reported in deliverable D4.4 "Modelling guideline document and demonstration development kit". The work has progressed on two fronts, simulation tools supporting COCOP and the COCOP implementation workflow. On the former, we present a review of numerous simulators and delve deeper into the most promising ones. On the latter, the workflow has been extended with two activities: the Digital Maturity Analysis and Human Factors Milestones.

While investigating available modelling approaches and simulators and their applicability for COCOP, an extensive list of process simulators was compiled. It became apparent that the process simulation software market is significantly fragmented. There are numerous options aiming at restricted engineering domains, and it is not always straightforward to understand the strengths of a certain tools or differences compared to another tool. Thus selecting the best modelling tool, based on public material, for a new type of COCOP application, is demanding. Tools technical specifications are typically insufficient, when one has specific requirements in mind. Many commercial tools do not offer trial/demo versions for evaluation. On the other hand, open source tools often lack technical support and tool future maintenance may be uncertain. The adoption of simulation interoperability standards is limited, but it exists (mainly CAPE-OPEN, but also FMI for the Modelica-based tools). Whenever time and effort is needed to adopt a new modelling tool, it slows down the system development and accordingly, favour such applications, where solid modelling expertise already exists.

The Digital Maturity Analysis was evaluated with Finnish companies related to process industry in order to get an understanding whether it would be beneficial to the COCOP implementation workflow. Based on the study, this seems to be the case: it was regarded useful in finding out the current status of digital maturity of the companies/units. Decent up-to-date understanding of the project starting point is utterly important for allocating the development resources in the best way.

Human Factors Milestones are introduced in order to to promote value creation with the COCOP concept via emphasizing the role of the end users and the system development process itself. The development work is guided by actions, which are organized on a milestone-based timeline. This approach is demonstrated for a steel manufacturing plant which is one of the COCOP pilot cases.

This updated guideline extends the view to the holistic approach of COCOP. Together with the previous deliverable D4.4, this guideline pursues three important success factors for the COCOP installations: outstanding technical capability, full acceptance of the plant personnel, and environmental sustainability.

ABBREVIATIONS

Abbreviation	Full name
CAPE	Computer-Aided Process Engineering
CAPE-OPEN	Interface standard consisting of specifications to expand the range of application of process simulation technologies
FMI	Functional Mockup Interface
FMU	Functional Mockup Unit
HF	Human Factors
IT	Information Technology
ODE	Ordinary Differential Equation
OPC	OPen Connectivity via open standards
OPC UA	OPC Unified Architecture
P2P	Person-to-Person requirement
P2S	Person-to-System requirement
XML	Extensible Markup Language

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1 Introduction

As defined in the DoA, this deliverable and its previous version (D4.4 Modelling guideline document and demonstration development kit) will elaborate on

1. "a generic guideline for the modelling work related to decomposition-coordination optimisation of process operations, making the optimisation approach of the project more usable after the project in other processes
2. exemplify development of new or integration of existing software tools to be used to transform (legacy) models of different principles to the necessary form via e.g. such co-simulation approaches as FMI/ FMU standard and Simantics platform "

On these modelling related topics, this deliverable will present a review of tools that could help the COCOP-modellers. Further, this deliverable drills in to six of such tools.

Furthermore, as stated already in D4.4: "it has become evident that the guideline should not only relate to models, but rather try to answer the question: "What needs to be done when the COCOP concept is applied to a given plant?"." In this deliverable, the "COCOP implementation workflow" will be extended on two fronts: Digital Maturity Analysis and Human Factors Milestones. The former is a method and tool to analyze an organization's maturity in digitalization. This is relevant to COCOP since, in fact, the implementation projects are all about advanced digital technologies for plant-wide control of industrial projects. The latter topic is relevant because, in the end, the COCOP results will be used with organisations and people. Directions and actions to help in this are important for successful implementation.

This deliverable is divided into two major chapters. The first deals with modelling tools and the second with COCOP workflow updates.

2 Modelling tools

In D4.4 "Modelling guideline document and demonstration development kit", different methods for model simplification were reviewed. In this deliverable, we present a review of modelling tools that are especially relevant in the COCOP context, and delve into six selected tools a bit more deeply.

2.1 Simulation tool overview – State of the Art

The tool review looked into 82 simulation tools that target process engineering, see Appendix A. The list was based on the chemical simulators list in Wikipedia (https://en.wikipedia.org/wiki/List_of_chemical_process_simulators) with some additions. The focus was to check that these tools are still available, update the links to the corresponding websites and present key information for the features of the tools from the vendor's website. Especially of interest was how the tools could support COCOP-type modelling efforts. It is beneficial for the tools to support standards such as the CAPE-OPEN or the FMI standard for simulation model interoperability.

Some interesting observations while compiling this list are as follows:

- The process simulation market is significantly fragmented, there are many options and it is difficult to quickly understand the differences between the tools
- Most commercial tools do not specify the cost for licensing the software, the user needs to contact a dealer
- Many commercial tools do not offer trial/demo versions for evaluation, if there is such option, it has to be arranged with a dealer
- Some tools offer their functionality as a service (the user sends the inputs and the vendor replies with the solution)
- The adoption of simulation interoperability standards is limited but it exists (mainly CAPE-OPEN, FMI for the modelica-based tools)

2.2 Drill in to selected tools

In this section we focus on process simulation tools that are free, or free and open source, and they support either the CAPE-OPEN or the FMI standard for simulation model interoperability. The goal here is to get an overview of the tool. The tools to be examined are the

1. COCO simulation environment
2. DWSIM chemical process simulator
3. EMSO simulator
4. JModelica

5. OpenModelica
6. MOSAICmodelling.

The first five are looked into on a general level and are interesting with respect to COCOP due to their CAPE-OPEN and FMI capabilities. Finally, the last one, MOSAICmodelling, is analysed more deeply by conducting a case simulation and then exporting the resulting model. In the following subchapters we present screen shots of the simulators. These figures are intended only to illustrate some main features of the simulators, not to be fully readable.

2.2.1 COCO simulation environment

The COCO (CAPE-OPEN to CAPE-OPEN) simulation environment (https://www.cocosimulator.org/) is a free (but not open source) simulation platform for steady state calculations. COCO consists of 4 main components:

- COFE (CAPE-OPEN Flowsheet Environment), this component provides the user interface and the solution algorithm
- TEA (Thermodynamics for Engineering Applications), this is based on the thermodynamic library of ChemSep. It includes a data bank with chemicals and a set of calculation methods.
- COUSCOUS (CAPE-OPEN Unit-operations Simple package), this is based on unit operations provided by ChemSep-LITE (limited number of compounds and process stages) in the free version but it can be extended to use the paid version of ChemSep.
- CORN (CAPE-OPEN Reaction Numerics) for the specification or kinetic or equilibrium reactions.

The figure below presents an example flowsheet in the graphical user interface of COFE. New energy, material and information streams alongside unit operations and controllers can be added using menu commands

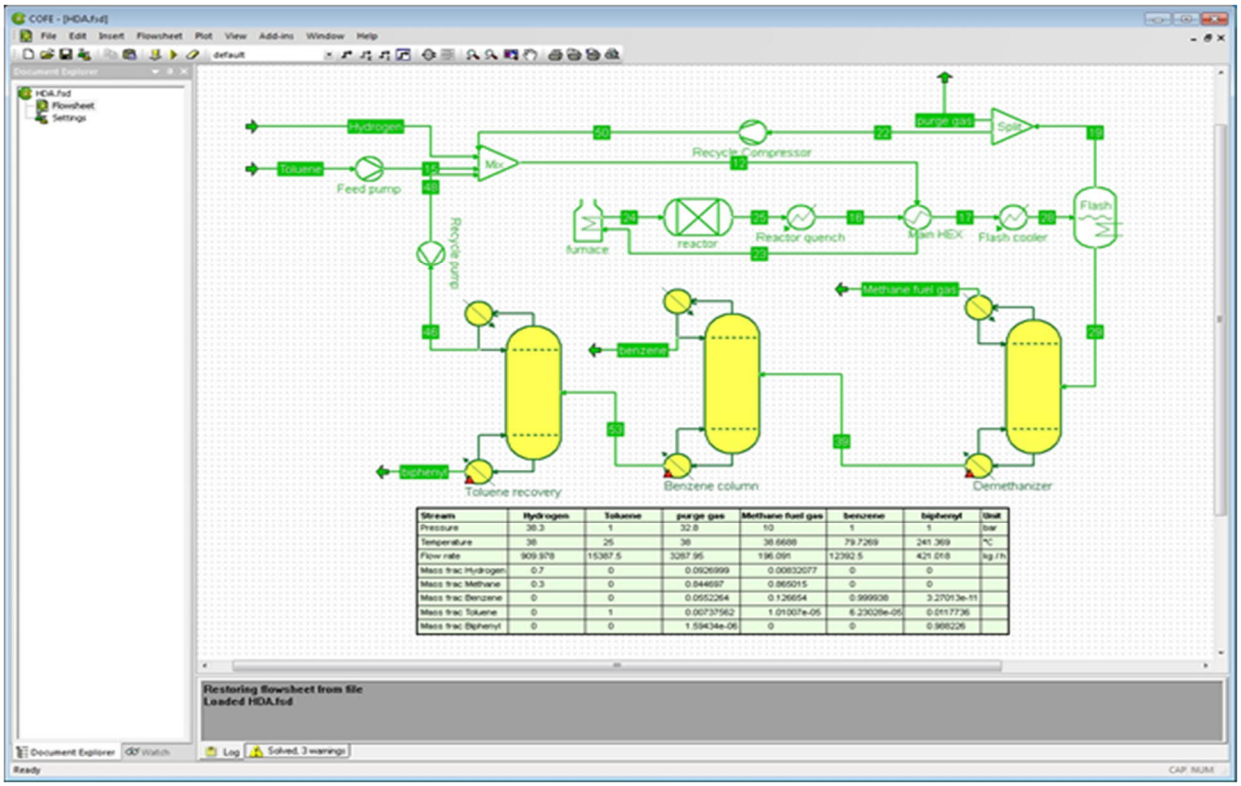

Figure 1 COFE simulator UI and a flowsheet

Many sample flowsheets in the COCO's website (https://www.cocosimulator.org/index_sample.html) help the evaluation of the tool and provide a starting point for modelling. A flowsheet can be solved and it is easy to get the steady state results in the form of tables or as plots as shown in the figure below.

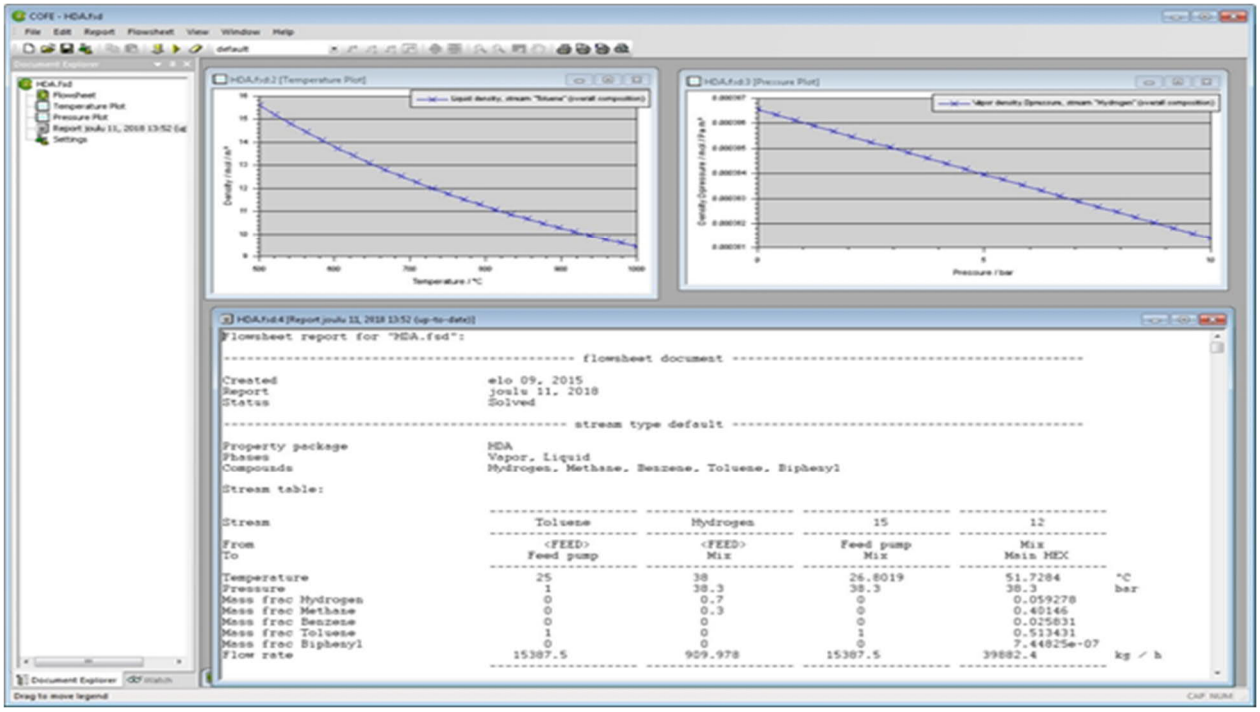

Figure 2 A view of results visualizations

Overall experimenting with the COCO tool was a good experience, one limiting factor of the free version of the toolchain is the use of ChemSep-LITE. The flowsheet is saved in a proprietary binary format, there is no option to export it in a more open form, e.g. as an XML file.

2.2.2 DWSIM - Open Source Process Simulator

The DWSIM - Open Source Process Simulator (https://sourceforge.net/projects/dwsim/) is an open source tool that can be used for steady state calculations. Some key features (as presented in the tool's website) are:

- CAPE-OPEN support
- High parallelization support, use of CUDA and OpenCL libraries
- Based on ChemSep component database
- Extensible through Python scripts
- User defined components.

The figure below presents the user interface of DWSIM and an example of a simple flowsheet. Energy and material streams as well as components can be added using drag and drop operations from a visual library.

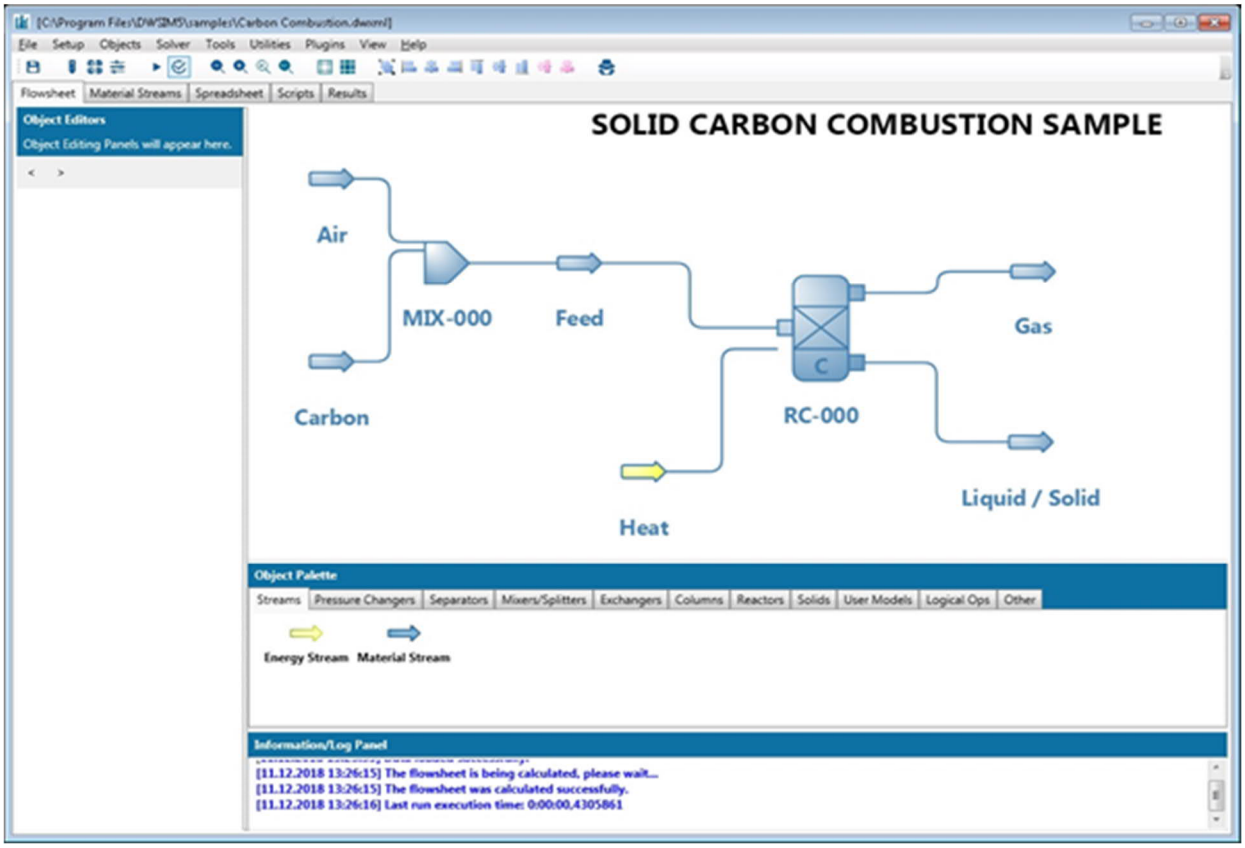

Figure 3 DWSIM user interface

The DWSIM also includes a set of sample flowsheets to help new users to familiarize with the tool and use them as a starting point. After the simulation/solution of the flowsheet, the results are presented in a text report to the user. Finally, the flowsheets can be exported as XML files that is human and machine readable, which provides significant flexibility for interoperability with other tools. Overall, the DWSIM was an easy tool to start using and the experience was positive. The fact, that it is supported by an active open source community, makes it a very interesting tool for steady state simulations.

2.2.3 EMSO - Environment for Modeling, Simulation, and Optimization

The Environment for Modeling, Simulation, and Optimization (EMSO) simulator is an equation-based process simulator for dynamic and steady state processes. It is a more academic-driven approach. The tool is not open source, but a version for academic use is free. The tool does include comprehensive manuals and many sample flowsheets.

One modelling approach is text-driven, where the equations describing the process are the main modelling artifact (see example in the figure below).

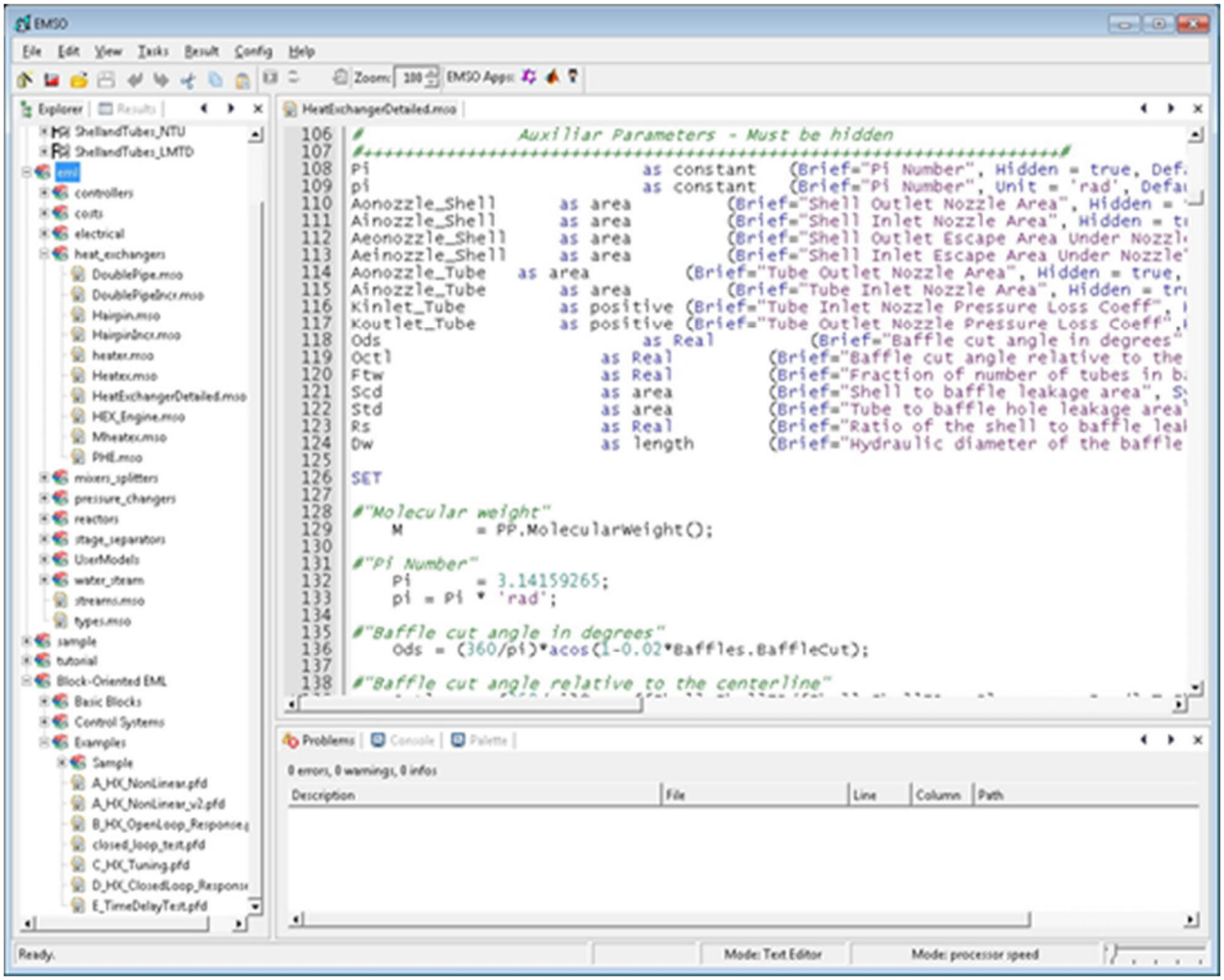

Figure 4 Text driven modelling approach of EMSO

A graphical block-based approach is also available, as shown in the figure below. This can also be used to visualize the dynamic simulation results.

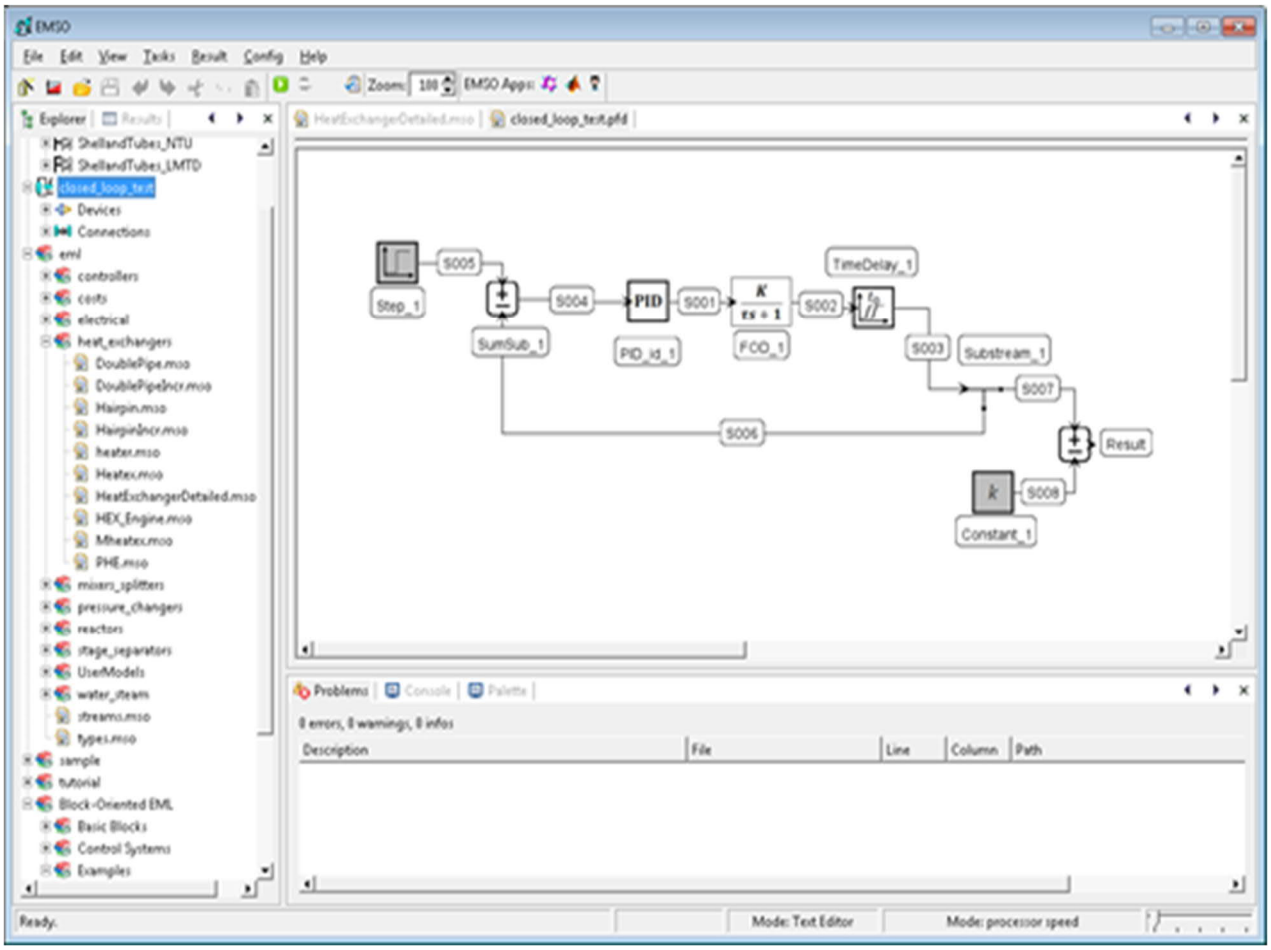

Figure 5 Graphical user interace of EMSO

The EMSO platform has links to Matlab and Simulink and can provide an OPC interface. Overall the EMSO is an interesting tool that can handle also dynamic simulations. The connection to Matlab and the OPC interface significantly add its potential for COCOP.

2.2.4 Modelica-based simulation tools: JModelica and OpenModelica

The Modelica modeling language is an established powerful language for modelling complex systems. It has been used as the basis for a number of free tools like the JModelica and OpenModelica. A common element in all these tools is the support of the FMI standard for interoperability of simulation models and the fact that they are open source. The Modelica langauage has also commercial implementations, such as Dymola and SimulationX.

2.2.4.1 JModelica

JModelica is a free open source platform for dynamic simulation, compliant with the Modelica Standard Library. It supports OPC connectivity via an OPC DA based OpenOPC

(http://openopc.sourceforge.net/about.html) package. JModelica uses Python scripts to interface with users (no visual user interface).

In the figures of Table 1 below, we can see the user interface of JModelica and the results of two example simulations, a bouncing ball (demonstrating the FMI interface) and the Hicks-Ray Continuously Stirred Tank Reactor (CSTR, demonstrating the the CasADi interface). “CasADi contains a facility to import dynamic system models formulated in the Modelica modelling language as well as in the Optimica extension of Modelica to optimal control” (http://casadi.sourceforge.net/v1.7.0/users_guide/html/node9.html).

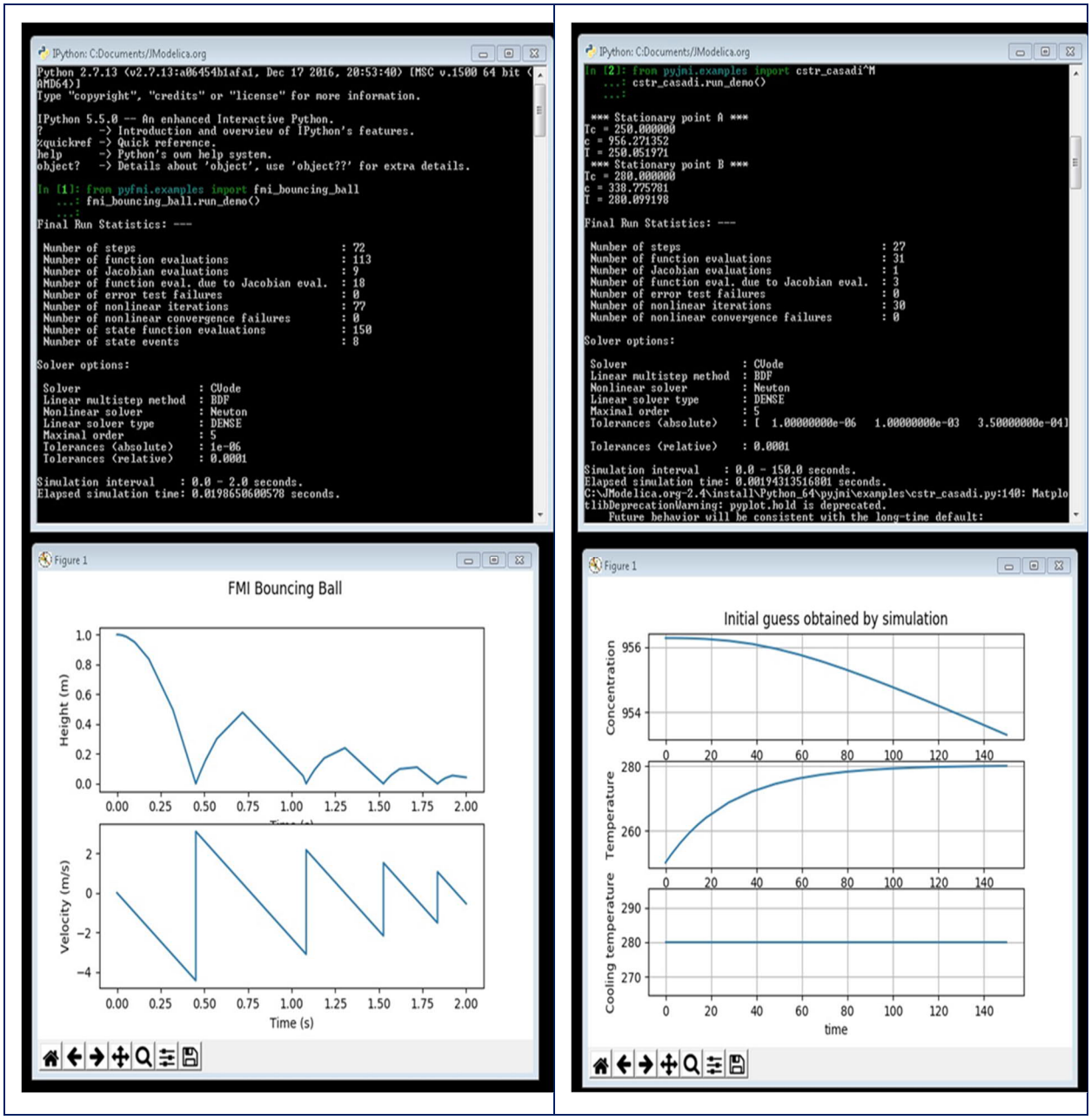

Table 1 JModelica UI and results example

The JModelica tool provides a good platform for running Modelica code and FMI support. It includes a powerful Python interface, but it is important to note that the user interface is text-driven, which may discourage some new users.

2.2.4.2 OpenModelica

OpenModelica is an open source platform for dynamic simulations similar to JModelica (but more popular). In contrast to JModelica, OpenModelica has a graphical user interface that facilitates the modelling process. It also includes a large set of libraries which also contain examples.

The graphical user interface is exemplified in the figure below which shows a model of a steam plant in OpenModelica.

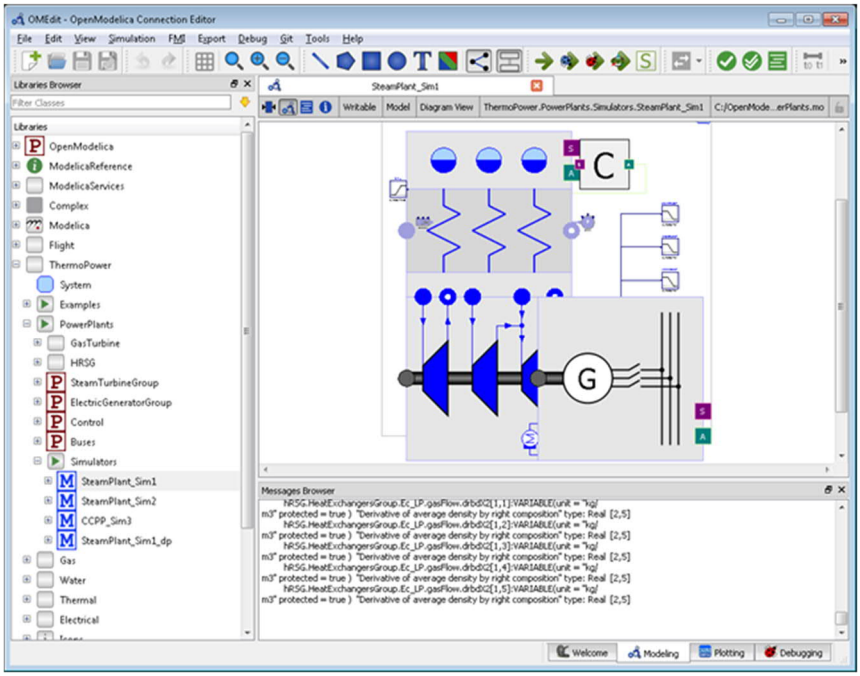

Figure 6 Graphical user interface of OpenModelica showing a steam power plant model

Like in many other tools the simulation results can be visualized on the user interface. Overall, OpenModelica is probably the best choice for a free and open source platform for dynamic simulation with FMI support and graphical user interface. An important beginner's observation is related to the responsiveness of the tool, i.e. many times it seemed that the tool was unresponsive when launching and when a simulation was requested. After some experience, the user can adapt to this behavior, but it may be an issue for new users.

2.2.5 MOSAICmodelling

When a mathematical model is developed for a process, an opportunity for mathematical optimization is opened too. It is common, however, that the simulation model is not straightforward to embed into an optimization algorithm or tool. Thus, reformulation of the model equations are required according to the requirement of the optimization environment. To

overcome the need to develop separate models in different software for simulation and optimization of a process, Technische Universität Berlin have developed MOSAIC platform (http://www.mosaic-modeling.de/). MOSAIC is a web based modelling, simulation and optimization platform (Esche et al. 2017). MOSAIC allows algebraic and differential equation systems to be build LaTex style and stored in MathML. The model codes formulated in MathML can be exported to different modelling and optimization platforms. MathML being a standard in mathematical publications, it is easier for a new model developer to start using MOSAIC with her or his colleagues. The reason for delving deeper into MOSAIC is that, in the COCOP context, it can provide to essential features: i) easy implementation of model/optimization equations and ii) easy way to export them to external solvers. There are several servers available worldwide for the modelling database, but to guarantee fluent use of the software in the testing, a standalone MOSAIC server installation was done in VTT.

2.2.5.1 Workflow in MOSAICmodelling

Model development in MOSAIC start with LaTex style notation defining. The notation explicitly state each variable name, super- and subscript and index. Next, equation system is build from separate equations written with the determined notation. MOSAIC determines the equation type (algebraic/differential/partial differential). The equation system is initialized and then simulated either in MOSAIC or in an external simulation software, e.g. Matlab. For differential algebraic equation and purely algebraic equation systems MOSAIC provides code generation for multiple different solvers, such as C++, Fortran, Matlab or gProms to say a few. Simulations based on C++ solvers can be made within the MOSAIC tool using solver installations on the MOSAIC's server. The exported code simulations are solved on user's local machine. Basic workflow of using MOSAIC is presented in the next figure. Results obtained from the simulation can be imported back into MOSAIC and used as initial guesses for the possible optimization activities.

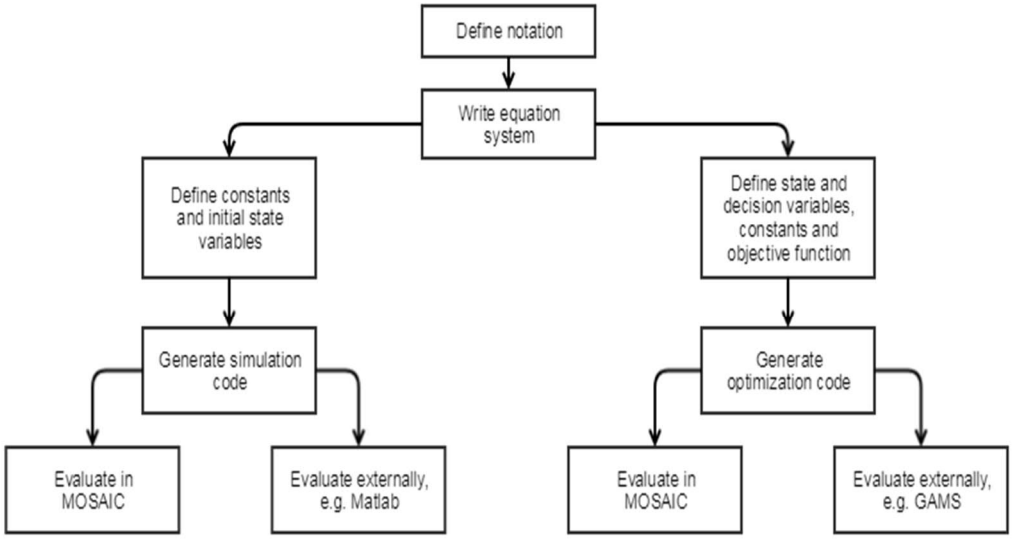

Figure 7 MOSAICmodelling workflow

Optimization can start from stored variable specifications and results of simulation. In optimization environment the objective function, the decision variables with lower and upper bounds and binary and integer variables are selected. All other specifications (design variables, parameters and state variables) are given by the stored results of simulation. Optimization code can then be generated for different programming languages, AMPL and GAMS being the most popular options. The generated code can either be used at local machine or exported to the University of Wisconsin's NEOS server. Generated optimization code can be either linear programming, mixed integer linear programming or nonlinear version of these.

2.2.5.2 Distillation column test case

A binary distillation column model was chosen for a test case for MOSAIC study. A bachelor of Science work (Järvelä, 2017) was used as the background material for the study. Before the actual modelling in MOSAIC, instructional videos on the MOSAIC web page were used as learning material to MOSAIC modelling. The video tutorials cover the basics of the software providing a few example cases (algebraic and ODE equation systems).

Standalone MOSAIC server was set up in VTT in early 2018. The software tutorials and the distillation column test case were studied on this server. There are some limitations on standalone servers, which are discussed later.

The dynamic simulation model for the distillation column consists of 20 distillation trays. On each tray, two differential equations and two algebraic equations are solved. Combined with the condenser, return flow and column bottom equations there were in total 87 equations. Number

of variables in the model is 91. Four variables (return flow, boil up rate, bottom product flow and distillate flow) were either controlled by PI controller or kept as constants.

Total implementation time for simulation ready model was around three to four hours, for a first time MOSAIC user. Before this, the initial familiarization and the learning video experiments took about 3 hours. Some time was lost with inaccurate notation presented in the bachelor thesis used. Also, there were some undocumented features in MOSAIC which needed guidance from the personnel of Technische Universität Berlin.

The generated simulation code was exported to Matlab, as the C++ based evaluation was not supported on the VTT standalone server. The exported code was more or less working right away, but some initial value manipulation was still done in the Matlab environment, mostly because the users had better know-how of Matlab than MOSAIC.

It was convenient that the generated Matlab code included also plotting of the output variables, here shown without any modifications. Firstly, the model was run to achieve steady state with constant inputs, as illustrated in the figure below (left picture) with vapour composition at column bottom (yB in the figure on the left).

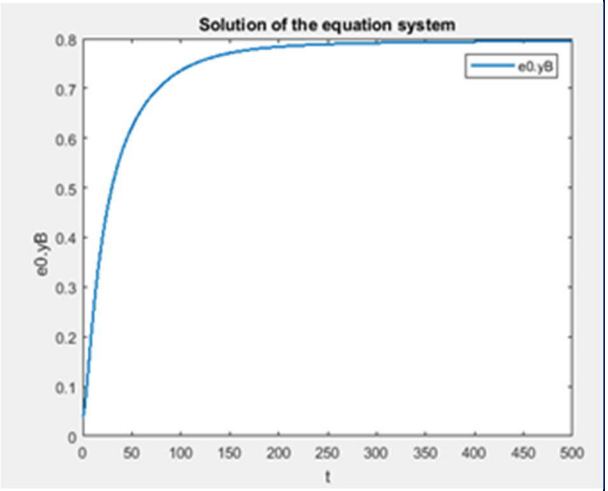

Figure 8 Initial simulation to steady state. yB is the bottom vapour composition as molar fraction, time is in seconds.

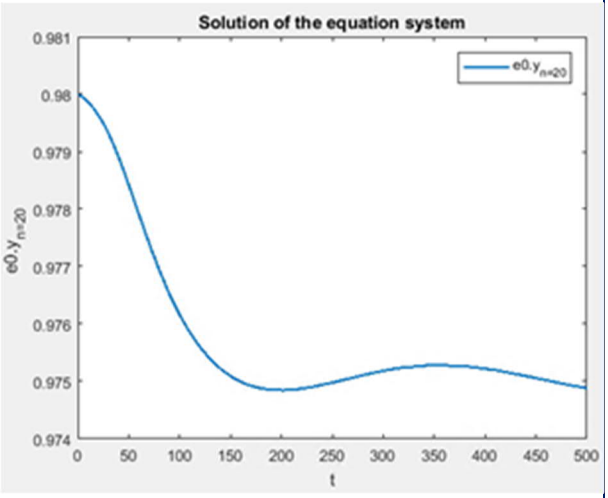

Figure 9 Control test simulation, yn=20 is the top vapour composition which is controlled to a new value of 0.975.

Secondly, a transient simulation was initiated by changing the top vapour composition set point for the PI-controller, which controls the return flow. At time t = 0 s, the set point was changed from 0.98 to 0.975. The behaviour of top vapour composition can be seen in the right part of the figure above.

The background and strongest application area for the MOSAIC environment is chemical engineering, so we consider it could fit rather well in possible new COCOP applications. The method is easy to start using, and certainly provides added value especially for those application developers, who inherently work with several modelling and optimization platforms, and benefit from using a same notation and equation system formulation for all tools. The approach does

not, however, offer any special tools for transforming the equations for the most COCOP-friendly, linear form.

MOSAIC was found to be a useful tool for future trials. Due to limited and partly outdated tutorial material, a training session by expert users would be needed. Also, features (e.g., optimization, CAPE-OPEN, etc.) of the tool that were not studied yet, need more attention. Our expectation is that with more experience MOSAIC might prove to be very useful tool for various engineering tasks related to COCOP.

3 COCOP workflow updates

The deliverable D4.4 "Modelling guideline document and demonstration development kit" presented the COCOP implementation workflow, which is here reviewed. Extensions to the workflow, shown in the figure below, have been investigated. They are:

1. Digital Maturity Analysis
2. Human Factors Milestones

The modelling methodology forms one of the COCOP cornerstones. In the previous Chapter, this was addressed from the point of software tools, pointed out in the figure as well.

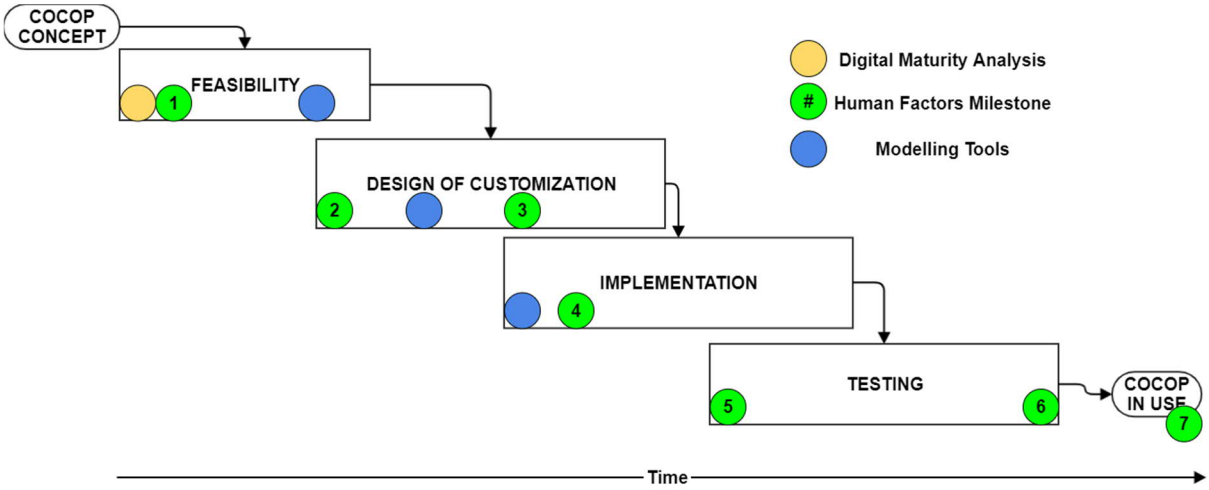

Figure 10 COCOP workflow with two extensions: Digital Maturity Analysis (Orange) and Human Factors Milestones (green). Also included are the modelling tools (blue).

The Digital Maturity analysis has been added to the feasibility part of the workflow in order to provide the COCOP implementation team and the plant in question a baseline of current digitalization state. This baseline can be used to evaluate whether the plant is digitally mature enough for the COCOP implementation to continue. The results help to identify, where especially efforts are needed to achieve the adequate competence. The human factors milestones, on the other hand, pertain to several of the steps of the workflow. As alluded in deliverable D4.4, this extension deepens the workflow on the implementation phase. In this respect, the current view is that once the COCOP system has been deemed feasible and customization is designed, the rest of the workflow will closely follow a standard industrial automation implementation project's workflow. As the COCOP project is moving towards its implementation phase at the writing of this deliverable, this is the working hypothesis.

In the following sections the two methodological extensions in the workflow are described in detail.

3.1 Digital Maturity analysis

3.1.1 Introduction

The content of COCOP clearly is a part of digitalization of a company. While the main emphasis is focused on technology at process-level functions - taking into account the human factors within the framework of social innovation of co-creation and co-development - it is beneficial also to take a more holistic look on the prerequisites of digitalization in an organisation.

In digitalization, the first step is to understand organisation's digital maturity level. Thereafter, selecting potential improvement steps becomes possible. The digital transformation path in each industry (and organisation) depends on the current digital maturity, status in the value chain and models of the focus markets. In the context of digital maturity, we refer to the definition of Sommarberg (2016) for the concept of digitalization: "The use of digital technologies to create value for a firm". Furthermore, according to Tihinen et al. (2016) digital transformation is defined as a change to models of working, roles and business offerings, occasioned by the adoption of digital technologies by an organisation or its operating environment. This refers to changes at process, organisational, business and societal levels. It involves a change in leadership, encouragement of innovation and new business models, the incorporation of digitisation of assets, and an increased use of technology to improve the experience of organisation's employees, customers, suppliers, partners and stakeholders. From the technical perspective, digitalization utilizes the processes of changing analogical data into a digital form (Sommarberg, 2016). However, it does not mean just converting existing data digital, but it is an opportunity to rethink, and (re)create new processes as well.

Regarding digitalization, the notion of maturity means two slightly different things. Firstly, it refers to organization's readiness for digitalization: Organization's capability, willingness (mindset) to change its function, processes, organization and capability to effectively adopt new technology/-ies. Secondly, maturity refers to organisation's performance based on digital technology. Therefore, digital maturity is built as a systemic combination of business, technology and socio-technical totality, where the balance between business development and information technology is essential. Maturity models have long history and many models can be found in literature directed to various topics. Recently, for example, several maturity models have been proposed in the area of Business Process Management (Tarhan et al., 2016) and PLM implementations (Silventoinen et al., 2013). However, based on our literature survey, maturity models with the proposed wide digitalization scope being tightly linked to business perspective are lacking.

In WP4, the project investigated a generic VTT Model of Digimaturity (Leino & al., 2017) with respective public free-of-charge online tool developed by VTT to help in understanding and structuring the concept of digitalization. The online tool, based on self-assessment, gives an estimate of organisation's current maturity level in six dimensions, as well as general guidelines towards the desired maturity level. The objective was to find out its potential as part of the

COCOP implementation workflow, as defined in D4.4. First, the online tool was demonstrated interactively at COCOP General Meeting (16-17.10.2018). The quick feedback stated that the tool itself is easy to use and the result presentation is clear. Subsequently, the tool's potential was studied with a group of process industry -related companies in Finland.

3.1.2 VTT Model of Digimaturity and related online DigiMaturity tool

Previously, VTT has developed a generic VTT Model of Digimaturity (Leino & al., 2017) and respective public free-of-charge online tool to help directors, managers and experts in digitalization efforts of organizations. The tool will guide to consider various dimensions that are important in digitalization, to support the development actions in the organizations, and to benchmark organizations against others. In short, to assess the digital maturity of the respective organization. The baseline of digital maturity is a valuable piece of knowledge for the decision makers and digitalization leaders in organizations. However, further understanding and concretization is required in order to allocate the development resources and activities so that best possible impact and value can be created. This concretization phase may depend on domain.

The online Digimaturity tool was published in the end of 2017 and there are now over 200, mostly Finnish, respondents. It has several purposes, functionalities and benefits. Firstly, it can be used as a free of charge self-assessment tool, which produces a basic analysis for an organization. It gives the baseline of current digitalization capabilities and maturities in six main dimensions which can be used for recognizing the most important and urgent development targets which depend on nature of the business and size of the organization. Secondly, it helps in understanding and structuring the ambiguous concept of digitalization. Thirdly, especially in larger organizations it can be used for collecting different views for digitalization. Persons from several departments and several organization levels can fill the enquiry in order to get different perspectives to maturity and digitalization. Fourthly, in the long run the online tool includes data that can be used in order to compare and benchmark for instance different organizations in same domains, same size, same location, etc.

The tool includes registration, self-assessment data entry and the result diagram display with own and reference data. It includes 4-5 questions of each 6 dimensions, mostly including one basic question with the rest focusing on digitalization from the viewpoint of the dimension. The dimensions and categories addressed in each dimension are summarised in the following table.

Strategy	**Organization and processes**
Strategy defined	Process organization
Digitalization as part of the strategy	The digital degree of information
Strategic objectives for digitalization	Digital integration of processes
Following the benefits of digitalization	Roles and functions
Business model	**People and culture**

Business model described	Readiness for change
Digitalization as part in the business model	Organization culture
New business models based on digitalization	Digitalization competences
The effect of digitalization in the result	Encouraging ideation
Customer interface	**Information technology**
Using digital channels	IT architecture
Digital services in engaging customers	IT complience within organization
Digital follow-up of customer satisfaction	IT complience with partners
Customer access to process/usage data	Roadmap for IT development
Customer-specific tailoring opportunities	Utilization of IT systems

Table 2 Dimensions addressed by VTT's DigiMaturity tool

The self-assessment is done by selecting the most suitable option of the presented alternatives in each category. The results diagram includes comparison to all organizations in the database. More thorough comparisons based on branch, turnover or personnel can also be made.

Figure 11 An example of result diagram of VTT's DigiMaturity tool.

3.1.3 Case studies in process industry -related units

In addition to testing the DigiMaturity tool at COCOP General Meeting, it was tested in four finnish process industry -related units. The aim was to examine the current state of digital maturity and applicability of the tool in case studies. The objective was to gather opinions broadly from the units to find out 1) the holistic view of different areas of digitalization in one picture - the general level of each digital maturity dimension, 2) the potential differencies between departments, 3) more detailed information about digital maturity based on the distribution of answers to the 25 individual questions, 4) comparison to other case units and all respondents of the public online tool, and if there are similarities across the units' results. Furthermore, an

objective was 5) to find out the tool's potential in early phases of the COCOP implementation workflow as baseline of the current digital maturity against (digitalization) strategy, and to evaluate whether the plant is digitally mature enough for the COCOP implementation to continue.

Regarding the six dimensions of the tool, the main emphasis was planned to be put on Organisation & Processes, People & Culture, and Information Technology dimensions, those being the most relevant under the COCOP framework. In addition to gathering information from the units with the online tool, a workshop with each participating unit was held in order to both discuss the results and get feedback from the use of the tool in them. The study was implemented in three process industry -related units with 15-18 respondents and 4-6 functions (departments), and in one engineering office unit. One of the former units operates mainly within B2B environment, one mainly in consumer business, and one is mainly internal supplier.

The process included filling the online tool questionnaire, and presenting and discussing the results in a unit-specific workshop.

Digital Maturity Results

The digital maturity of different dimensions in case units varied somewhat as can be seen in the following figure. The engineering office unit evaluated itself to be on slightly higher level than the other case units, which was not surprising as they are industry consultants. The unit with lowest scores has internal customer, and thus the questions were a bit harder to answer (resulting also to lower scores), which can be seen especially in Customer Interface figures. The smallest variation within the case units and compared to the average of all public tool respondents was in People and Culture dimension. All case units gave best scores to Information Technology - which is also in line with all respondents to the public online tool. The amount of case units was too small to make any conclusions regarding process industry in general.

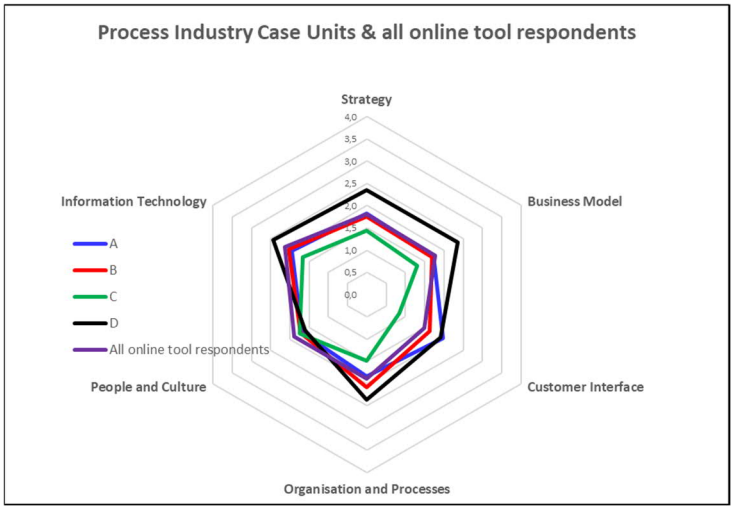

Figure 12 Digital maturity results in the six dimensions (case units and average of all online tool respondents).

In the workshops, the departmental averages and question-specific distributions were also worked through. Following figure shows an imaginary example of how the departmental averages can differ from each other.

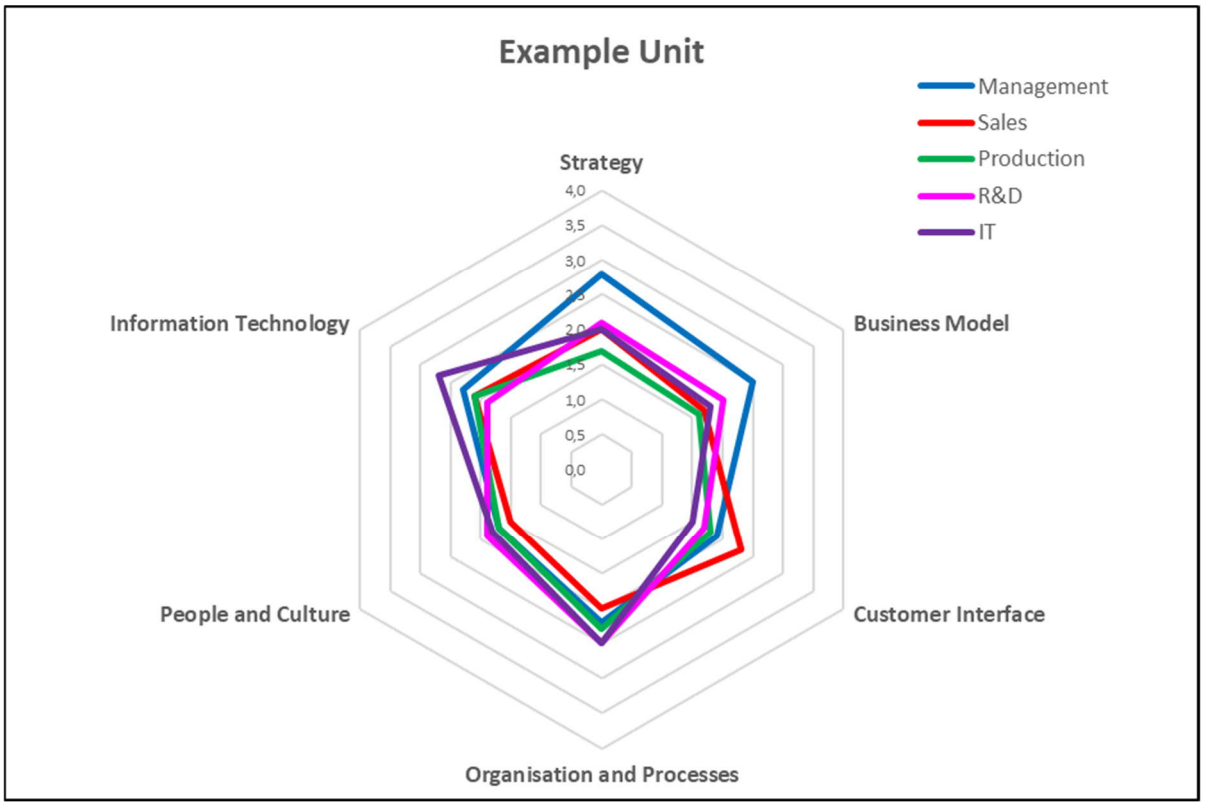

Figure 13 Imaginary example of departmental variation of digital maturity results.

Feedback of the digital maturity case studies

The general feedback from the DigiMaturity tool was that it is useful in finding out the current status of digital maturity of the units, firstly in opening up the holistic view into different dimensions of digitalization, secondly showing the digital maturity levels in each dimension and thirdly pointing out the potential differences between departments. Comparison to other units would have needed more background information of them - or more selected reference group as in this study they were quite different from each other.

The related workshop clarified concepts both regarding the digital maturity tool and in the unit. In addition to the overall and departmental averages, it was regarded vital to go through individual questions with the written choices, and the distribution of answers of all respondents to them. The results initiated a lively discussion and brought up more focused information and ideas thus assisting in reaching common understanding which is the baseline for development actions. It was regarded as a must to include the workshop in the exercise.

The exercise (DigiMaturity tool and related workshop) was regarded as a good starting point and a catalyst for ideating development actions. In COCOP framework, digital maturity analysis would

suit well in early phase COCOP implementation workflow in order to discover the general digital maturity status in the unit and it's departments as preconditions for digitalization development, as well as in the end as one indicator of the change. In the following stage, a more detailed analysis with more focused questions of e.g. process automation would be beneficial.

The achievement of the objectives of case studies is presented in the following table in more detail.

Objective	**Result**
Holistic view of different areas of digitalization in one picture - the general level of each digital maturity dimension.	This was achieved and was regarded useful. The case units stated that the tool and related workshop brought clearer view of digitalization and digital maturity. One said that it is a good way to find out e.g. if the strategy is clear for everyone and the attitudes towards (digitalization) development. All in all, it makes you think where to strive for.
Potential differences in digital maturity levels between unit's departments.	This was achieved. The results and differences initiated discussion about what digitalization means at different departments, and contributed to joint perception of the digital maturity status in the unit.
More detailed information about digital maturity: distributions of the answers to the 25 individual questions.	This was achieved. The distribution of answers to individual questions also catalysed lively discussion, including also that some terms within the tool were understood a bit differently.
Comparison to other case units and all respondents of the online tool, and if there are similarities across the units' results.	This was achieved. However, the benefit of anonymous comparison was not regarded as high as against identified ones - or more focused comparison to similar units. It was also discussed that internal benchmarking within the company could be beneficial.
To find out the tool's potential in early phases of the COCOP implementation workflow as baseline of the current digital maturity and to evaluate whether the plant is digitally mature enough for the COCOP implementation to continue.	The results of both this study and previous experience imply to this. However, as this was not worked out with the COCOP companies, it remains to be seen.

Table 3 The achievement of the objectives for digital maturity analysis.

Following observations were made and development ideas presented at the workshops.

Observation	Development ideas
The background and part of the vocabulary of the tool were unclear to some respondents.	Some kind of introduction would be beneficial before using the tool, e.g. a short video.
Some dimensions may be challenging depending on the nature of the unit; e.g. customer interface when the customer of the unit is internal, or the person does not have knowledge or experience of the matter.	Organization-specific “translation” of some of the tool’s concepts, e.g. what is meant by organization or management in the specific unit. The version of the tool used already had an option of not answering all questions.
The questions were at quite general level and the tool did not have any process automation specific questions.	In the next phase there could be potential extention(s), i.e. more detailed questions, regarding e.g. process automation.
The questions in the tool suit the better the higher in the organization the respondent is, i.e. some questions are challenging in the floor level.	The floor level questions could be more concrete, e.g. about what is happening in practice.

Table 4 Observations and development ideas of the Digimaturity Tool and related workshop

Feedback was gathered in the end of each workshop from the attendees via a short feedback questionnaire. The results are shown in the following figure and written answers after that.

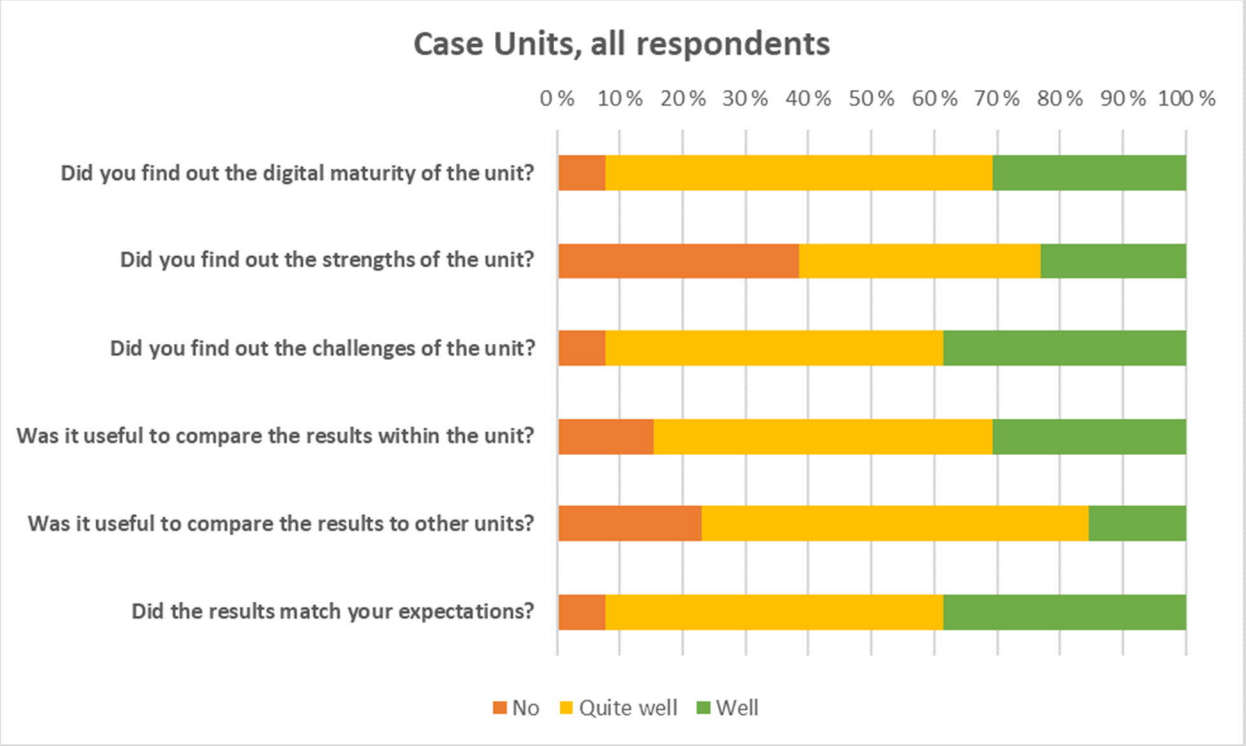

Figure 14 Feedback gathered after the workshops (at this stage from 2 out of 4 units).

According to the respondents, the biggest benefits from the exercise were getting the overall picture and different viewpoints within the unit, initiation of discussion, in addition to identification of challenges and initial development ideas. The DigiMaturity tool and the results raised the general awareness level and gave a snaphot of the current state, and catalyzed the discussion in the workshop. The workshop was needed for common understanding - in order to give more background information and examples of the digital maturity model and dimensions, clarifying both digital maturity tool concepts and what digitalization means in the unit and it's departments, and initiating discussion of the current state & challenges - baseline for development. Showing the actual questions and distribution of answers when going through the results was needed, as it opened the discussion and clarified the viewpoints.

3.2 Human Factors Milestones

Human factors (HF) aims to add value to the COCOP concept by increasing system value for the users and by improving the developed system. The work is performed by defining requirements and by executing actions that aim to fulfill requirements. In this section we present the goals of these requirements and actions, as well as, present how the actions are scheduled on a milestone based timeline. More information about human factors requirements is given in deliverable D2.4 Characteristics of operator work and user acceptance in the process industry. Further details will be presented in deliverable D6.1 Co-Creation, combining technological and social innovation.

The HF works in the context of a socio-technical system, where organisational and personnel goals are aligned with technical system. End users have sufficient understanding of plant processes and skills to operate the COCOP system. Eventually, this has an impact on the end user system usage, which is a key factor in determining the added value of a COCOP system. In other words, if end users are reluctant to use the system, the system may not reach the expected added value. Furthermore, the HF work aims to improve the COCOP system development by involving relevant stakeholders, and in combination with HF expertise, find aspects that improve the usability and the functionality of the system.

The HF related requirements aim at supporting and facilitating an effective usage of the system, such as considering user acceptance, usability and competence related matters. The system brings the most added value, when the attitude of users towards the system is positive, the users understand the role of the system and the system is in harmony with both user's personal goals and company goals. In general to reach this, the end user involvement in the development process is crucial. End users should be given good understanding of the purpose and place of the system. Skill gaps and fears of failure should be overcome, for example, with training. The usability of the system supports user acceptance, but it is equally important in pursuing the added value for the company and end users. Aspects that increase the usability include: the user interface should be intuitive, features that support working memory should exist, system feedback should be helpful, the system should make end users work easier and detailed information about the system should be easily available in order to understand the system behavior. In general to reach this, end users should be able to impact the system that is being developed. Also the company, where the COCOP system is implemented, has responsibilities in facilitating the usage of the new system. This is done by organising training about plant-wide processes to end users and by ensuring that organisational practices, such as a bonus system, does not hinder the usage of the COCOP system. The human factors team supports the company in collecting and implementing the requirements.

3.2.1 Collecting and defining requirements

The human factors requirements were first gathered through user interviews and human factors work in collaboration with technical developers. A framework was created that divides the requirements based on if they were result (R) or process (P) oriented. A result oriented requirement has a measurable goal which is typically true when end users can test and use the system. The process oriented requirement goal is more difficult to measure, and it typically considers aspects during the development. Furthermore, the requirements are divided into two categories, the ones between the user and the new system (person-to-system requirements, i.e., P2S), and the ones between users and the usage context (person-to-person requirements, i.e., P2P).

3.2.2 Requirement format example

We give an example of requirement P-P2P-2.1. The process oriented requirement (P) is of type person-to-person (P2P) and has an identification number (2.1). The requirement description is as follows:

> Trainings SHOULD be defined and developed to close the skills gap between needed and existing skills.

Action to be performed is as follows:

> A workshop with human factors team, developers, end user representative, process expert and training expert.

Note that the use of term SHOULD, among other capitalized words, has a precise definition that is given in deliverable D2.3 "System Requirements Specifications". The categorization was performed in order to obtain a better overview and find synergies between the actions.

3.2.3 Milestones

One or more actions are specified for each requirement that aims to fulfill the requirement. The actions are organized on a milestone based timeline and the following list defines the milestones:

1. Setting up the project (building a project team)
2. Use case definition and requirement specification. During this milestone key persons are identified, attitudes of future users are analyzed and an HF action plan is made.
3. A final or mature version of a mock-up or similar is sent to the customer. No functionality is required in the mock-up and it should be sent before the main software development (coding) effort starts.
4. Introduction of a prototype with some functionality.
5. Testing period of the release candidate that is expected to be final. The testing period should be initiated with an evaluation of the system by HF experts. Most or all functionalities are included.
6. Final system delivery
7. Maintenance

The milestones are defined in order to ease the burden to track when actions should be executed. Actions should be executed at latest immediately after a milestone is reached, but in many cases it is preferable to execute them during the milestone activity. The actions can and should be syncronized with the other project activities so that synergies can be utilized. Milestone 1 was predefined at the start of the implementation COCOP project and therefore does not contain any actions. However, we acknowledge the importance of this milestone and recommend to give it

attention when implementing the COCOP concept in the future. For example, time should be reserved for HF work throughout the project and commitment of relevant stakeholder participation should be guaranteed. In the following table, an action plan is presented for one of the COCOP pilot studies as an example of the HF work. The pilot case is Sidenor's steel manufacturing plant in Spain (see detailed descriptions in deliverable D2.1 "Use case definition document"), hereafter called steel pilot case. The HF work is ongoing and the table shows the current status.

In the table, the status column contains abbreviations with the following interpretation:

1. (U) - Unhandled
2. (I) - In progress
3. (C) - Completed
4. (P) - Partially completed
5. (F) - Failed to execute
6. (N) - Will Not be executed

From the table we can see that for the steel pilot case, the HF milestone 2 has almost been completed and milestone 3 contains the next actions to be executed. For each milestone ID, an action type is given, which is of one of the following 5 types:

1. COCOP internal work or triggering an activity
2. Questionnaires
3. Interviews
4. Skype Meeting
5. Regular meetings or workshops

Milestone-ID	Action	Requirement-ID	Estimated time consumption on customer side	Status
M2-1	Kick-off workshop at pilot plant.	P-P2P-7 (Common understanding) R-P2S-3.1 (UI related) R-P2S-3.2 (UI related) R-P2S-3.3 (UI related) R-P2S-3.4 (UI related)	2 days	P-P2P-7 (C) R-P2S-3.1 (I) R-P2S-3.2 (I) R-P2S-3.3 (I) R-P2S-3.4 (I)
M2-2	Interviews	P-P2P-1.1 (Future work content) P-P2P-1.2 (New skills) P-P2P-6.2 (End users needs)	2 days (up to 1 hour per interview)	P-P2P-1.1 (C) P-P2P-1.2 (C) P-P2P-6.2 (C)
M2-3	Questionnaires	R-P2P-1.1 (Operator training) R-P2P-1.2 (Understanding processes) R-P2P-2 (Job satisfaction) P-P2P-6.1 (End user involvement) P-P2P-6.2 (End users needs)	20 min per person	R-P2P-1.1 (C) R-P2P-1.2 (C) R-P2P-2 (C) P-P2P-6.1 (C) P-P2P-6.2 (C)
M2-4	Workshop	P-P2P-3 (Organisational practices)	0,5 day	P-P2P-3 (C)
M3-1	COCOP internal work	R-P2S-3.1 (UI related) R-P2S-3.2 (UI related) R-P2S-3.3 (UI related)	0	R-P2S-3.1 (U) R-P2S-3.2 (U) R-P2S-3.3 (U)

Milestone-ID	Action	Requirement-ID	Estimated time consumption on customer side	Status
		R-P2S-3.4 (UI related) R-P2S-8 (UI related)		R-P2S-3.4 (U) R-P2S-8 (U)
M3-2	Workshop	P-P2P-6.3 (Feedback on mock-up) P-P2S-2.1 (Effects of decisions)	0,5 day	P-P2P-6.3 (U) P-P2S-2.1 (U)
M3-3	Regular meetings	P-P2S-1.1 (Practical knowledge)	0,5 day	P-P2S-1.1 (U)
M4-1	Workshop	P-P2P-1.1(New skills) P-P2P-1.2 (New skills) P-P2S-2.1 (Effects of decisions)	1 day	P-P2P-1.1 (I) P-P2P-1.2 (I) P-P2S-2.1 (I)
M4-2	Workshop	P-P2P-2.1 (Plan training)	1 day	P-P2P-2.1 (U)
M4-3	Triggering decisions of the company	P-P2P-4 (Scope of decisions)	To be discussed	P-P2P-4 (U)
M4-4	Triggering level of flexibility	R-P2S-7 (Flexibility of use)		R-P2S-7 (U)
M4-5	Triggering decision about detailed information	R-P2S-11.1 (Detailed information)	To be discussed	R-P2S-11.1 (U)
M4-6	Regular meeting	P-P2S-1.1 (Practical knowledge) P-P2S-1.2 (Reliability of practical knowledge)	1 day	P-P2S-1.1 (U) P-P2S-1.2 (U)

Milestone-ID	Action	Requirement-ID	Estimated time consumption on customer side	Status
M4-7	Internal COCOP work	R-P2S-6 (Memory supporting features)	0	R-P2S-6 (U)
M4-8	Triggering decision about detailed information	R-P2S-11.1 (Detailed information)	To be discussed	R-P2S-11.1 (U)
M5-1	Skype Meeting	P-P2P-2.2 (Education)	0,25 days	P-P2P-2.2 (U)
M5-2	Skype Meeting	P-P2P-3 (Organisational practices)	0,25 days	P-P2P-3 (U)
M5-3	COCOP internal work	P-P2P-4 (Validation scope of decision) R-P2S-1.1 (Acceptance ratio) R-P2S-6 (Memory supporting features) R-P2S-8 (UI related) R-P2S-12 (Differences between shifts)	0	P-P2P-4 (U) R-P2S-1.1 (U) R-P2S-6 (U) R-P2S-8 (U) R-P2S-12 (U)
M5-4	Interview	P-P2P-5 (Communication channels) P-P2P-3 (Organisational practices) R-P2P-1.1 (Operator training) R-P2P-1.2 (Understanding) R-P2P-2 (Job satisfaction) R-P2S-1.2 (Acceptance)	2 days (1 hour per interview)	P-P2P-5 (U) P-P2P-3 (U) R-P2P-1.1 (U) R-P2P-1.2 (U) R-P2P-2 (U) R-P2S-1.2 (U)

Milestone-ID	Action	Requirement-ID	Estimated time consumption on customer side	Status
M5-5	Questionnaire	P-P2P-6.1 (Involvement tracking) R-P2P-1.1 (Operator training) R-P2P-1.2 (Understanding) R-P2P-2 (Job satisfaction) R-P2S-1.2 (Acceptance)	20 min per questionnaire	P-P2P-6.1 (U) R-P2P-1.1 (U) R-P2P-1.2 (U) R-P2P-2 (U) R-P2S-1.2 (U)
M5-6	Questionnaire	P-P2P-6.4 (Training)	20 min per questionnaire	P-P2P-6.4 (U)
M5-7	Regular meeting	P-P2S-1.1 (Practical knowledge) P-P2S-1.2 (Practical knowledge)	1 day	P-P2S-1.1 (U) P-P2S-1.2 (U)
M5-8	Workshop	P-P2S-2.1 (Prototype evaluation) R-P2S-3.1 (UI related) R-P2S-3.2 (UI related) R-P2S-3.3 (UI related) R-P2S-3.4 (UI related) R-P2S-7 (Flexibility and efficiency) R-P2S-9 (System errors) R-P2S-10.2 (Help documentation) R-P2S-11.2 (Detailed information)	1 day	P-P2S-2.1 (U) R-P2S-3.1 (U) R-P2S-3.2 (U) R-P2S-3.3 (U) R-P2S-3.4 (U) R-P2S-7 (U) R-P2S-9 (U) R-P2S-10.2 (U) R-P2S-11.2 (U)
M5-9	Triggering	P-P2S-2.2 (Simulate process) P-P2S-2.3 (Track process)	0	P-P2S-2.2 (U) P-P2S-2.3 (U)

Milestone-ID	Action	Requirement-ID	Estimated time consumption on customer side	Status
		R-P2S-2 (Provide relevant data) R-P2S-9 (System errors)		R-P2S-2 (U) R-P2S-9 (U)
M6-1	Interview	P-P2P-6.1 (Involvement) R-P2P-1.1 (Operator training) R-P2P-1.2 (Understanding) R-P2P-2 (Job satisfaction)	2 days (1 hour per interview)	P-P2P-6.1 (U) R-P2P-1.1 (U) R-P2P-1.2 (U) R-P2P-2 (U)
M6-2	Questionnaire	P-P2P-6.1 (Involvement) R-P2P-1.1 (Operator training) R-P2P-1.2 (Understanding) R-P2P-2 (Job satisfaction)	20 min per questionnaire	P-P2P-6.1 (U) R-P2P-1.1 (U) R-P2P-1.2 (U) R-P2P-2 (U)
M7-1	Triggering	P-P2P-5 (Communication channels) P-P2S-1.3 (Practical knowledge) R-P2P-3 (Support team)	To be discussed 30 min	P-P2P-5 (U) P-P2S-1.3 (U) R-P2P-3 (U)
M7-2	Interview	P-P2P-3 (Organizational practices) R-P2S-1.2 (Acceptance) R-P2S-2 (Relevant data)	1 hour per interview	P-P2P-3 (U) R-P2S-1.2 (U) R-P2S-2 (U)
M7-3	COCOP internal work	R-P2S-1.1 (Acceptance)	0	R-P2S-1.1 (U)
M7-4	Questionnaire	R-P2S-1.2 (Acceptance)	20 min	R-P2S-1.2 (U)

Table 5 Action plan for human factors work at the steel pilot plant.

4 Conclusions

This deliverable continues the work reported in D4.4 "Modelling guideline document and demonstration development kit", on two fronts. Firstly, the modelling toolkit idea is investigated through a survey of potential simulator tools and a deep dive to the most interesting ones. Secondly, the COCOP implementation workflow is deepened with the Digital Maturity analysis and Human Factors Milestones. Of these, the former clearly pertains to the very early phases of the workflow, whereas the latter cover several parts, including implementation. The final parts of the workflow are foreseen to resemble a standard process automation implementation project. This hypothesis will be investigated in the coming months of the project where implementation to the steel and copper (another pilot study in COCOP) pilot cases will commence.

The process simulation tool overview showed that there is a plethora of options available and it is not always clear, without thorough evaluation with the collaboration of the tool vendor, what are the exact features, strengths and weaknesses of each tool. There is limited support for simulation model interoperability standards like the CAPE OPEN or the FMI, which leads to the models created in a tool to be usable only in that context (with the exception of communication interfaces that are mostly proprietary). There are tools that are both easy to evaluate (they are free, or free and open source) and do support open interoperability standards. Out of them the COCO, the DWSIM and the EMSO provide a friendly user interface and support the CAPE OPEN standard, while the OpenModelica and the JModelica support the Modelica language and the FMI standard. The advantage of the OpenModelica over JModelica is its graphical user interface. In the future we hope that the simulation tool ecosystem will evolve towards supporting standards in simulation models (CAPE-OPEN, FMI) but also for communication (like the OPC UA). Furthermore on the simulation tool front, we found that the MOSAICmodelling tool seems promising in the COCOP modelling context, since models created there can be quite easily exported to various simulation or optimization languages/tools. The tool does require some initial efforts to master it, but this is typically the case with any modelling and simulation tool. Its tutorial material is rather limited, but the support available from the developers helps to overcome this deficiency.

On the COCOP implementation workflow front, we conclude that Digital Maturity analysis, when properly adapted to the process industry is useful to form a picture of COCOP implementation's feasibility with respect to the targeted company's organisation and assets. The general feedback from the DigiMaturity tool was that it is useful for finding out baseline of the digital maturity in an organization. The exercise with case units (DigiMaturity tool and related workshop) was regarded as a good starting point and a catalyst for ideating development actions, but wishes were presented for more focused questions regarding process automation/optimization -related issues in the following stage. The related workshop was regarded as a must in order to go through the answers, open up the concepts of the tool and where the figures within the unit and compared to other units arise from.

Finally, we have defined Human Factor Milestones to promote value creation with the COCOP concept. System improvements are reached by emphasizing the role of the end users and the system development process itself. The work is guided by actions, which are organized on a milestone based timeline. We demonstrated this by showing in detail the status of actions for the steel pilot case. The steel pilot case development work is still in progress, and the status assessment shows that milestone 2 has almost been completed. Milestone 3 represents the next actions to follow. This work will continue towards the end of the COCOP project.

Together with the previous D4.4, this document works as a guideline to assess, whether the COCOP methodology fits in the targeted industrial plant. And when found promising, these guidelines help with the practical work in the system development, commissioning and maintenance.

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Appendix A. Process simulators

The following table summarizes the simulation tools that were found and briefly reviewed. The list is based on the chemical simulators listed in Wikipedia (https://en.wikipedia.org/wiki/List_of_chemical_process_simulators), but it was further extended. We also included those simulators that seem to be without current maintenance or activity, but which Wikipedia has listed. For most of the tools, we have referred the vendor's web site. Accordingly, the description texts contain commercial formulation.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
ASCEND	http://ascend4.org/Main_Page	Free and open source	Free and open source	Features • Developed at Carnegie Mellon University since 1978 • Main uses have been in the field of chemical process modelling although its capabilities are general • ASCEND can solve systems of non-linear equations, linear and nonlinear optimisation problems, and dynamic systems expressed in the form of differential/algebraic equations. • Its architecture helped to inspire newer languages such as Modelica • GPL (free software)
MOSAICmodelling	http://www.mosaic-modeling.de/	Free	Free	MOSAICmodeling is a free, web-based modeling, simulation, and optimization environment. Based on a LaTeX-style entry method for algebraic and differential equations, equation systems can be built and

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				subsequently used for simulation and optimization. Based on a steadily growing library of existing models of chemical engineering applications large-scale flowsheets, optimization problems, etc. can be built. MOSAICmodeling provides an automatic code generation for numerous simulation and optimization environments, such as AMPL, Aspen Custom Modeler, GAMS, gPROMS, MATLAB, Modelica, and for solvers interfaced via C++, FORTRAN, Python, etc.
Matlab / Simulink	https://uk.mathworks.com/products.html?s_tid=gn_ps	Commercial	Trial	A powerful and widely used simulation platform with libraries addressing multiple domains and also with applications for process modelling (see https://uk.mathworks.com/academia/books/process-dynamics-bequette.html)
Mirror Plant	https://www.yokogawa.com/solutions/solutions/industrial-iot/iiot-efficiency/iiot-mirror-plant/	Commercial	no info	Mirror Plant (Plant Simulator) provides visualization of “present” and “future” by predicting behaviors of the cyber physical system. Challenges • Detect process failure in advance during normal operation • Reduce off-specification products as much as possible • Need considering operations with varieties of fuels • Improve operators’ and staffs’ skills and techniques Solutions

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Analyze plant's behaviors based on the rules and principles • Measure the plant's internal information which cannot be detected or measured in reality • Predict the dynamic behaviors of the processes several hours in advance • Consider changing operating conditions, not just steady-state operation but also dynamics included Benefits • Realize safety operation by avoiding critical state by predictive alarms • Realize flexible operations (e.g. production volume control, accommodating with varieties of raw materials) • Sublimate operation skills into technology
Avtech Scientific - Advanced Simulation Library	http://asl.org.il/	Free and open source	Free and open source	Advanced Simulation Library is a free and open source hardware accelerated multiphysics simulation platform and an extensible general purpose tool for solving Partial Differential Equations. Transport processes in focus, chemical reactions: only electrode reactions. Features http://asl.org.il/features/

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
ProSim - ProSim DAC	http://www.prosim.net/en/software-prosim-dac-18.php	Commercial	no info	ProSim DAC (Dynamic Adsorption Column Simulation) is a dynamic simulation software for adsorption columns. Both adsorption and regeneration steps (TSA, PSA, VTSA…) can be modeled. ProSim DAC is a decision support tool to conduct in-depth analysis of solid-gas adsorption operations including refinery hydrogen purification, isotopic separation, VOC emission control, solvent recovery... The software is mainly used in nuclear, air treatment and hydrogen studies. Features • Easy simulation and cyclic process management • In-depth analysis of solid-gas adsorption operations • A property database containing more than 2,200 components • A full set of thermodynamic models • A full set of isotherm models
ProSim - Simulis Thermodynamics	http://www.prosim.net/en/software-simulis-thermodynamics-3.php	Commercial	no info	Mixture properties and fluid phase equilibria calculations. Interoperability, integration, reusability. Simulis Thermodynamics allows anyone in industry, engineering or research to run high quality thermophysical properties calculations. These calculations can be plugged in any software of wider application range (equipment sizing, system modeling, etc) and properties are available for any kind of fluid. Simulis Thermodynamics makes open simulation a practical reality.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Features • Reliable and accurate thermophysical properties; • Extensive set of services (flash, data regression, phase envelopes, etc.); • Powerful pure-compound physical properties prediction tool; • Automatic splitting of user added molecules into appropriate functional groups for the predictive models (various UNIFAC, PSRK ...); • Easy plug in common 32- and 64-bit applications (Microsoft Excel®, MATLAB®, etc.); • Flexible and CAPE-OPEN compliant solution.
ProSim - ProPhyPlus	http://www.prosim.net/en/software-prophyplus-8.php	Commercial	no info	Based on Simulis Thermodynamics, ProPhyPlus is a stand-alone calculation software to run all the calculations, without any programming. ProPhyPlus software performs fast, interactive, fluid phase equilibria and fluid properties directly from its own user-friendly graphical interface. ProPhyPlus is specifically for users who prefer an easy-to-use graphical user interface to set up and run their calculations.
ProSim - ProSimPlus	http://www.prosim.net/en/software-prosimplus--1.php	Commercial	no info	ProSimPlus is a process engineering software that performs rigorous mass and energy balance calculations for a wide range of industrial steady-state processes. It is used in design as well as in operation of existing plants for process optimization, units troubleshooting or debottlenecking, plants revamping or performing front-end engineering analysis.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Features • Comprehensive set of unit operations including complex models • Powerful thermodynamic package able to model highly non-ideal systems and a wide range of processes. • Unique graphical user interface allowing instant usability, convenient drawing of the flowsheet and quick access to results. • Open system to expand capabilities (user defined unit operations, Visual Basic scripting, CAPE-OPEN thermo and unit operation interfaces...). • Solution widely used by world's leading oil, gas, chemicals and engineering companies.
ProSim - ProSimPlus Energy	http://www.prosim.net/en/software-prosimplus-energy-14.php	Commercial	no info	ProSimPlus Energy is tailored for the energy managers, energy auditors, eco-efficient facilities designers, and all other engineers responsible to solve these important challenges. Features • Specific unit operations dedicated to energy efficiency improvement (heat pumps, ORC...), utilities production (boilers, fuel turbines...) and waste recovery (combustion, methanization…). • Energy audit tool for an entire process using the pinch analysis technology to maximize energy savings.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Exergy analysis capability. • Process economic evaluation (CAPEX and OPEX). • Easy-to-use and open software to expand capabilities.
ProSim - BatchColumn	http://www.prosim.net/en/software-batchcolumn-9.php	Commercial	no info	BatchColumn is for the simulation and optimization of batch distillation columns. Features • Rigorous dynamic model that is fully configurable (semi-batch, multi-fraction operation …) • Detailed representation of the heating system, hydrodynamics of the column, condenser / decanter and associated controls • Optimization of the most complex separations (azeotropic, extractive, reactive …) • Reliable description of the production recipe (filling, total reflux, variable reflux …) • User-friendly interface, fast calculation and easily exploitable results
ProSim - BatchReactor	http://www.prosim.net/en/software-batchreactor-4.php	Commercial	no info	BatchReactor is for the simulation of chemical reactors in batch mode. Features

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• A detailed modeling of the reactor (heating/cooling system, condenser…). • A reactional model fitted on available experimental results. • A thermophysical model suited to the problem to be addressed. • A reliable description of the production recipe. • A user-friendly interface, fast calculations and easily exploitable results.
APMonitor	https://omictools.com/apmonitor-tool http://apmonitor.com/	Free web-service	Free web-service	Advanced process monitor (APMonitor), is a modeling language for differential algebraic (DAE) equations. Permits users to optimize mixed-integer and differential algebraic equations. APMonitor is able to: • construct model, • fit parameters to data, • optimize over a future predictive horizon, and • transform differential equations into sets of algebraic equations. It employs a model to byte-code and is based on analysis of the sparsity structure of the model. This tool is able to solve the differential and algebraic equations using a simultaneous or sequential solution approach.
Apros	http://www.apros.fi/en/	Commercial	Demo license	Apros is a comprehensive, accurate and user friendly software for modelling and dynamic simulation of power plants, energy systems and industrial processes. The key uses of Apros include safety analysis, engineering

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				support (e.g. development of control strategies, verification of design), automation testing and operator training. Apros provides easy user interface for configuring and running the simulation models, efficient solution algorithms and model libraries for full-scale modelling and dynamic simulation of industrial processes. Besides the process, also automation and electrical systems can be modelled in detail. The model libraries have been comprehensively validated against data from physical process experiments. Input data for a plant scale dynamic simulation model are typically process connections, physical dimensions of process equipment and pipelines, equipment-specific parameters (e.g. pump and valve curves), automation concept diagrams, control parameters and nominal condition information. Apros has been developed since 1986 by VTT and Fortum.
Aspen Plus / Aspen Plus Dynamics	https://www.aspentech.com/en/products/engineering/aspen-plus	Commercial	no	To maximize profits using a plant-wide simulation solution that combines unparalleled accuracy and engineering collaboration with time-saving workflows. Aspen Plus is for steady state simulation, Aspen Plus Dynamics for dynamic simulations.
Aspen HYSYS	https://www.aspentech.com/en/products/engineering/aspen-hysys	Commercial	online trial	To maximize safety, throughput and profits by optimizing the entire site in one environment using industry-validated simulation accuracy and time-saving workflows.
ASSETT	https://kongsberg.com/?sc_mode=nor	Commercial	no	Features

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
	mal&sc_itemid={AB98D6B1-A838-4955-82F3-E0F08AA346CE}&sc_lang=en https://www.ksat.no/en/kog/news/2004/may/0524assett-basedprocesssimulation/ https://www.ife.no/en/ife/departments/process_and_fluid_flow_tech/files/assett-users-seminar-2000-1			• Dynamic process simulation system • Interactive, graphical operation • Extensive process model library • Flexible thermodynamic package • Efficient (single phase) network solver for large simulators • Selected as the platform for the Field Simulator implementation
BATCHES	http://www.bptechs.com/	Commercial	no	BATCHES is a proven, most comprehensive and versatile simulation system to manage multiproduct batch/semicontinuous processes in the pharmaceutical, specialty chemical and food industries. BATCHES has been successfully used worldwide to improve the profitability of batch/semicontinuous processes. The BATCHES recipe modeling constructs are similar to the batch manufacturing concepts described in the ANSI/ISA-S88.1 standards. By combining the operational and design features of a process, a BATCHES simulation model allows you to evaluate

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				alternative system configurations and operating procedures, to size process equipment, and to evaluate scheduling strategies. Features • Hybrid simulation methodology (Discrete and Dynamic Simulator) • Library of process dynamics models • Logic to implement operating decisions • Graphical user interface for model building and analysis
D-SPICE	https://www.kongsberg.com/en/kongsberg-digital/news/2008/august/0829_expands_to_meet/	Commercial	no	D-SPICE has been superseded by the K-SPICE tool (see the next row)
K-SPICE	https://www.kongsberg.com/en/kongsberg-digital/news/2009/june/0625_kpice/	Commercial	no	Enhanced dynamic simulation tool enables more confidence in system and process design. Kongsberg Oil & Gas Technologies has launched K-Spice, its next generation dynamic process simulation tool. In addition to a wealth of sophisticated new and improved features for system management, thermodynamics, solvers and a flexible and intuitive graphical user interface, K-Spice combines the very best of the proven, class leading D-SPICE and ASSETT lifecycle simulation solutions.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
CADSIM Plus	https://www.aurelsystems.com/cadsim-plus/	Commercial	no	CADSIM Plus is chemical process simulation software that can perform mass and energy balances and simulate dynamic conditions. It is a first-principles dynamic chemical process simulator and a full-featured Computer Assisted Drawing (CAD) front-end in one package. CADSIM Plus includes a comprehensive set of generic process modules and has a number of optional module libraries for various applications. It performs precise heat and material balances of any chemical process. It can also be used to develop complex dynamic simulations with control logic and batch operations. Here is a partial list of applications: • Designing a process • Finding solutions for process bottlenecks • Tracking product grade changes • Energy Tracking • Identifying process and operation problems • Reducing energy and/or materials usage • Improving process efficiency • Online Dynamic Data Reconciliation • Real-time optimization • Advanced process control

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
ChromWorks	https://www.ypsofacto.com/services-chemical-software-chromworks.php	Commercial	no	Chromworks helps you make the best use of your experimental data to design, secure, and optimize purification processes. You can then fine-tune all your process parameters, get performance, analyze the influence of dead volumes, etc. Applications • Single column systems • Multi-Column Chromatography • Short-cut tools for quick process design Typical examples of use • Select the best equipment for your separation • Create a recipe and optimize a purification process • Troubleshooting • Train your team on chromatography
CHEMCAD	https://www.chemstations.com/CHEMCAD/	Commercial	Trial	CHEMCAD is an integrated suite of intuitive chemical process simulation software that fits into the chemical engineering workflow and supercharges an engineer's efficiency. Perhaps most significantly, it continues to evolve to meet the ever-expanding needs of chemical engineers. Features • Highly customizable, flexible, and affordable

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• All modules work within a single graphical user interface for seamless interaction • Adapts to how you approach engineering challenges • Appealing graphics and reports are easy to export to third-party software • Easily integrates into chemical engineering computing environment • Personalized technical support second to none
Cycle-Tempo	http://www.asimptote.nl/software/cycle-tempo/	Commercial	Demo	Cycle-Tempo is a flow sheeting for the thermodynamic analysis and optimization of energy conversion systems. It is suited for conventional power plants, compression refrigeration and cooling systems, unconventional energy systems like: • solar ORC power plants, • tri-generation systems, • absorption-cooling and refrigeration systems, • fuel cells, • Kalina-cycle power plants, • scCO2 -turbine power plants, • IGCC power plants.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Cycle-Tempo is one of the few software packages that allows for exergy analysis. It has been around for more than a decade and has a large user community, including major energy companies, consultancy firms and research and development institutes. The main feature of Cycle-Tempo is the calculation of all relevant mass and energy flows in the system. It has a particularly robust and efficient computational method, which means that you can depend on it to quickly obtain a reliable solution even in the most demanding situation. Additional features allow for more detailed analysis and optimization of the system. Cycle-Tempo allows also for real-time integration within existing plant-wide data monitoring systems for performance analysis and trouble-shooting.
COCO	https://www.cocosimulator.org/index.html	Free	Free	COCO (CAPE-OPEN to CAPE-OPEN) is a free-of-charge CAPE-OPEN compliant steady-state simulation environment consisting of the following components: COFE - the CAPE-OPEN Flowsheet Environment is an intuitive graphical user interface to chemical flowsheeting. COFE has sequential solution algorithm using automatic tear streams. COFE displays properties of streams, deals with unit-conversion and provides plotting facilities. COFE flowsheets can be used as CAPE-OPEN unit operations; so you can use COFE Flowsheets as unit operation inside COFE (flowsheets in flowsheets) or inside other simulators. TEA - COCO's Thermodynamics for Engineering Applications, is based on the code of the thermodynamic library of ChemSep and includes a data bank of over 430 commonly used chemicals. The package exhibits more

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				than 100 property calculation methods with their analytical or numerical derivatives. COUSCOUS - the CAPE-OPEN Unit-operations Simple package is shipped with COCO. It contains a splitter, a mixer, heat exchangers, pumps and reactors amongst other unit operations. ChemSep-LITE, a limited version of ChemSep with a maximum of 40 compounds and 300 stages, can serve as an equilibrium distillation unit operation in COCO. A full version of the equilibrium and non-equilibrium column simulator can be obtained at http://www.chemsep.com/. ChemSep-LITE is included in the COCO installation. CORN - the CAPE-OPEN Reaction Numerics package that comes with COCO facilitates specifying any kind of kinetic or equilibrium reaction. Simple reactor units, like conversion reactors, CSTRs and plug flow reactors that can use the CORN package come with the COUSCOUS package.
Design II for Windows	https://www.winsim.com/design.html	Commercial	2 week trial	With a forty-five plus year history of continued development and refinement, DESIGN II has long been a leader in process simulator innovation. It performs complete heat and material balance calculations for a wide variety of pipeline and processing applications. The simulator's easy-to-create flowsheets allow process engineers to concentrate on engineering, rather than computer operations. It offers advanced features, such as sizing and rating of heat exchangers and separators, within the flowsheet. The database contains 1,200 pure components, and others can be added via CHEMTRAN. Also included is a crude library with 38 world crudes, already characterized and at your fingertips.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Applications: • Physical Properties • 2 Phase Pipeline Modeling • Expander and Lean Oil Plants • Glycol Units / TEG dehydration • Amine Units (Single and Mixed) • LNG Liquefaction • Gathering & Transmission • Rigorous Refinery Columns • Petrochemical, Hydrocarbon, Refrigeration, Chemical, Ammonia, Methanol, Sulfur and Hydrogen Plants • Heat Exchanger Sizing & Rating • Separator Sizing & Rating • VLE, VLLE and LLE Data Regression • Fuel Cell Systems • Relief Valve Simulation over Time

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Ammonia Plants
Distillation expert trainer	https://www.environmental-expert.com/training/complete-distillation-training-system-132808	no info	no info	Distillation Expert-Trainer has been used to train and qualify hundreds of operators worldwide. This system has aided companies in their qualification of thousands of operating personnel regarding the operation of distillation units. The Expert Trainer is an integrated computer-based training system composed of self-paced interactive lessons, drills, quizzes and a comprehensive exam. The trainee also has access to a number of resources as well as a dynamic simulation process. Students work at their own pace in either in a structured learning environment or through on-demand access to the system.
DWSIM	http://dwsim.inforside.com.br/wiki/index.php?title=Main_Page	free	free/OSS	DWSIM is a multiplatform, CAPE-OPEN compliant chemical process simulator for Windows, Linux, Android, macOS and iOS. Built on the top of the Microsoft .NET and Mono Platforms and featuring a rich Graphical User Interface (GUI), DWSIM allows chemical engineering students and chemical engineers to better understand the behavior of their chemical systems by using rigorous thermodynamic and unit operations' models with no cost at all. Features • CAPE-OPEN features: Thermo 1.0/1.1 Property Package Socket, Thermo 1.1 Property Package Server, Unit Operation Socket and Flowsheet Monitoring Object support. Additionally, DWSIM exposes its

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Python Script (Custom) Unit Operation for all CAPE-OPEN compliant simulators. • Thermodynamic models: CoolProp, Peng-Robinson, Soave-Redlich-Kwong, Lee-Kesler, Lee-Kesler-Plöcker, UNIFAC, Modified UNIFAC (Dortmund), UNIQUAC, NRTL, Extended UNIQUAC, Chao-Seader, Grayson-Streed, Raoult's Law, IAPWS-IF97 Steam Tables, IAPWS-08 Seawater, Black-Oil and Sour Water; • Unit Operations: Mixer, Splitter, Separator, Pump, Compressor, Expander, Heater, Cooler, Valve, Pipe Segment, Shortcut Column, Heat Exchanger, Reactors, Component Separator, Orifice Plate, Distillation/Absorption Columns, Solids Separator, Cake Filter, Excel, Script and Flowsheet Unit Operation; • Utilities: Phase Envelope, Hydrate Calculations, Pure Component Properties, Critical Point, PSV Sizing, Vessel Sizing, Spreadsheet and Petroleum Cold Flow Properties; • Tools: Binary Data Regression, Compound Creator, Bulk C7+ and Distillation Curves Petroleum Characterization and Reactions Manager; • Process Analysis: Multivariate Constrained Optimization and Sensitivity Analysis utility; • Extras: Scripting System and Plugins Interface.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
DynoChem	https://www.scale-up.com/ (website is down atm)	Commercial	no info	no info
EMSO	https://www.revolvy.com/page/EMSO-simulator	free	free	EMSO simulator is an equation-oriented process simulator with a graphical interface for modeling complex dynamic or steady-state processes. It is CAPE-OPEN compliant. EMSO stands for Environment for Modeling, Simulation, and Optimization. The ALSOC Project - a Portuguese acronym for Free Environment for Simulation, Optimization and Control of Processes -, which is based at the UFRGS, develops, maintains and distributes this object-oriented software. Pre-built models are available in the EMSO Modeling Library (EML). New models can be written in the EMSO modeling language or a user can embed models coded in C, C++ or Fortran into the simulation environment
EQ-COMP	https://www.eq-comp.com/	Commercial	no	EQ-COMP is a chemical process simulation software for calculation of bubble point, hydrocarbon dew point, water dew point, phase envelope, compressibility factor, McCabe Thiele curves, gas hydrate equilibrium curve, CO2 freezing and frost curve and other binary / multicomponent vapor liquid equilibrium (VLE) properties for hydrocarbon mixtures / oil and natural gas mixtures. Oil and natural gas samples comprise primarily of non-polar and mildly polar hydrocarbon compounds. EQ-COMP has been developed considering these non-polar and mildly polar hydrocarbons.
Dymola	https://www.3ds.com/products-	Commercial	free trial with	Dymola, Dynamic Modeling Laboratory, provides multi-engineering modeling and simulation based on Modelica and FMI. It is a complete tool

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
	services/catia/products/dymola/		limitations	for modeling and simulation of integrated and complex systems for use within automotive, aerospace, robotics, process and other applications. Rapidly solve complex multi-disciplinary systems modeling and analysis problems, using Dymola's best-in-class Modelica and simulation technology. Dymola is a complete environment for model creation, testing, simulation and post-processing.
Flowtran simulation	no product page was found	no info	no info	Academic papers from the 70's do exist. The tool doesn't seem to be in development/supported anymore.
gProms	https://www.psenterprise.com/products/gproms/platform	no info	no info	There are three major environments: gPROMS ProcessBuilder, gPROMS FormulatedProducts and gPROMS ModelBuilder. The core environment you start with depends on your specific modelling needs: • ProcessBuilder is an advanced process flowsheeting simulator for optimising process design and operation of primarily vapour-liquid processes. • FormulatedProducts is an integrated environment for design & optimisation of formulated products & their manufacturing processes, primarily for particulate processes. • ModelBuilder is an advanced process modelling environment for expert modellers to build, validate and execute steady-state and dynamic custom process model libraries. In addition to the desktop environments, PSE provides a number of Operational Excellence Solutions that deploy gPROMS models for

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				operational monitoring, optimisation and planning. Features • World-leading custom modelling • Steady-state and dynamic simulation within the same environment • Advanced parameter estimation, including model-based data analysis • Powerful optimisation tools for large-scale steady-state, dynamic and mixed-integer (MINLP) optimisation • Global system analysis tools for systematic sensitivity and uncertainty analysis • Model export and packaging … and many more. • Equation-oriented solution power • High-performance computing for rapid parallel execution on multi-core, cluster and cloud configurations • Advanced materials modelling • Advanced thermodynamics The platform also contains utilities and execution environments, including: • Links to CFD tools in various ways, for example the multizonal CFD interface

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Toolkits for implementing gPROMS models behind custom interfaces (MS Excel, web) • The gPROMS Objects for execution within MATLAB, CAPE-OPEN environments, etc.
HSC Chemistry	https://www.outotec.com/products/digital-solutions/hsc-chemistry/	Commercial	no	Outotec's HSC Chemistry Software carries out thermodynamic and mineral processing calculations on a standard computer quickly and easily. Essential software toolkit for process research, development, design, and digitalization, as well as for estimating process efficiencies, yields, and environmental footprints. Features • Develop new processes and improve existing ones through modeling and simulation • Develop process flowsheet models and test ideas prior to lab or pilot stages • Estimate the environmental footprint of processes for Life Cycle Assessment • Apply complex process theory in an easy-to-use format • Apply complex calculations in minutes • All the tools and databases you need in a single package

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
HYD-PREDIC	no product page was found	no info	no info	no info
HYDROFLO	http://www.tahoesoft.com/html/hydroflo.htm	Commercial	15 days trial	HYDROFLO 3 is a powerful, yet easy to use Pump and Piping System Analysis software tool. Any type of incompressible liquid flow can be analyzed. Many types of conveyance systems can be modeled including open source/discharge, closed re-circulating and gravity flow systems. Industrial process, water supply, wastewater treatment, fire protection, sprinkler systems, chemical process, mine de-watering, swimming pool, pond/irrigation and HVAC systems can be quickly created, analyzed and solved for steady-state flows and pressures and operating parameters. Virtually any type of piping system element can be described using the wide variety of hydraulic modeling components available. Custom element head losses can be described using flow vs. head loss curves, fixed head losses (at any flow) or by specifying custom friction coefficient values. Systems are built in a unique vertical workspace that offers easily viewable suction and high-head conditions along with Hydraulic Grade Line elevations and pressures. The Hazen-Williams and Chezy-Manning equations are available for use with water systems and the Darcy-Weisbach equation is available for use with any type of incompressible fluid of known viscosity (a full database of liquid properties is available for selection).
INDISS	http://www.corys.com/en/indiss-plusr	Commercial	no	IndissPlus is the latest generation dynamic simulation platform developed by CORYS. Based on First Principles of Chemical Engineering, IndissPlus models accurately match process behavior at normal operations or during transient periods, whether the models are part of a dynamic study or

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				incorporated into an Operator Training Simulator (OTS) solution. The application has a rich library of Thermodynamics Packages, Pure Components, and Unit Operation Modules. However, if 3rd party proprietary components, thermodynamics packages or chemical reactor models are required they can be seamlessly integrated within the Indiss Plus platform, by taking advantage of the multi-layer component architecture. Integration of Cape-Open thermo package into IndissPlus® for use in Simulation.
ICAS	http://www.pseforspeed.com/icas/	Commercial	no	ICAS, Integrated Computer Aided System, provides a framework through which a collection of tools developed with the latest theories and data are made available to users for a range of problem solving, such as, property estimation, process modelling, separation process design, and many more. The algorithms, methods & models are based on generic and systematic solution approaches. ICAS is dedicated to managing the complexity through a systems approach.
ICAS/Model Test-bed (MoT)	http://www.pseforspeed.com/icas/mot/	Commercial	no	Model Test-bed (MoT) is part of ICAS toolbox and it was designed with the objective of minimizing the amount of effort to specify, solve, and visualize the solution of a system of Algebraic equations (AEs), Ordinary and Partial Differential equations (ODEs or PDEs) without sacrificing power and flexibility. It is a mathematical modeling solver designed for personal computers running Microsoft Windows. It is an equation based modeling /simulation tool and allows the user to perform simulations of a process without having to write any source code. External models written in text-format and/or XML-format can be imported to MoT. The translated model

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				can be solved, after satisfying mathematical consistency requirements, equation by equation in the debug-mode or simultaneously in the solution-mode. The solvable model can also be exported through a model transfer feature (COM*-objects) to other simulation engines and/or external software. The Modelling framework in ICAS also includes a tool for model creation (ModGen) and a tool for model reuse (ModTem).
IDEAS	https://www.andritz.com/automation-en/downloads/ideas-simulation-software	Commercial	no	IDEAS is the leading dynamic simulator for the global kraft pulp industry, oil sands operations, potash operations, and hard rock mining, helping industrial operations reduce risk.
ITHACA	https://elementprotech.com/	Commercial	Free Trial	A low-cost, general-purpose dynamic process simulator for all industries
iiSE Simulator	no product page was found	no info	no info	no info
LIBPF	https://libpf.com/process_expert.html	Commercial	Demo	LIBPF is a new, flexible technology for the simulation of continuous industrial processes
JModelica.org	https://jmodelica.org/	Free	Free/OSS	Features • A free and open source software platform based on the Modelica modeling language for modeling, simulating, optimizing and analyzing complex dynamic systems

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• A Modelica compiler for translating Modelica source code into C or XML code. The compiler also generates models compliant with the Functional Mock-up Interface standard. • A Python package for simulation of dynamic models, Assimulo. Assimulo provides interfaces to several state of the art integrators and is used as a simulation engine in JModelica.org. • Algorithms for solving large scale dynamic optimization problems implementing local collocation methods on finite elements and pseudospectral collocation methods.
METSIM	https://www.metsim.com/	Commercial	Free demo	METSIM is a general-purpose process simulation system (steady-state and dynamic) designed to assist the engineer in performing mass and energy balances of complex processes. METSIM uses an assortment of computational methods to effect an optimum combination of complexity, user time, and computer resources usage. METSIM originated as a metallurgical process simulation program, written to perform mass balances around the major unit operations of complex process flowsheets. Application of the program proved so successful that it was expanded to include detailed heat balances, chemistry, process controls, equipment sizing, cost estimation, and process analysis. The unique nature of the programming language, APL, allows modification and expansion of the system with minimum effort and permits the incorporation of continuing technological innovations in process simulation.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Application examples: • SAG/Ball Milling and Flotation of Various Ores • Chloride Leaching of Molybdenum Concentrates • Hydrochloric Acid Leaching of Alumina Clays • Gold Cyanidation / Precipitation • Roasting/Flash Smelting of Copper Concentrates • Acid and Carbonate Leaching of Uranium and Vanadium Ores • Heavy Media Coal Preparation Plants • Base Metal Smelting • Gold, Nickel, Uranium, and Copper Heap Leaching
Mimic Simulation Software	https://www.emerson.com/en-us/catalog/mimic-simulation-software	Commercial	no	Mimic Simulation Software provides accurate and real-time simulation of plant behaviors. Made for the end-user or integrator with process automation experience, not simulation experts, Mimic integrates easily and automatically with your off-line control system. Use the same operator graphics and controls to train operators and test configuration.
Mobatec Modeller	https://www.mobatec.nl/web/	Commercial	Free demo	The process modelling methodology implemented in Mobatec Modeller is based on the hierarchical decomposition of processes into networks of elementary systems and physical connections. This process modelling

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				software combines two approaches to modelling: equation based modelling and flowsheeting. This makes it an advanced process modelling software which is best described as an Equation Based Flowsheeter. Equation based (white box) modelling is flexible, as users can create custom tailored models to their own needs resulting in a high fidelity simulations. Conventionally equation based modellers require a programming language, used by the user to transform (code) the model equations into lots of lines of code in order for solver to solve the model. This code is not transparent, and even experienced users need time to use, modify or improve existing models. With Mobatec Modeller no knowledge of code (programming) is required, equations are written almost as on paper and the code is generated automatically by the software.
NAPCON Simulator (NAPCON ProsDS)	https://www.napconsuite.com/product/napcon-simulator/	Commercial	no	NAPCON Simulator is a highly interactive training simulator that turns your plant into a safe yet intriguing training environment. It offers challenging and motivating training for both beginners and experts. Use NAPCON Simulator for • Energy Efficiency • Quality • Safety

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
Clearview	no product page was found	no info	no info	no info
OLGA	https://www.software.slb.com/products/olga	Commercial	no	OLGA Dynamic Multiphase Flow Simulator, is a tool for dynamic multiphase flow simulation. Successful production system design and operations requires a detailed understanding of multiphase flow behavior. Flow modeling and simulation provides valuable insights into flow behavior, including the physics describing flow through the entire production systems, from reservoir pore to process facility. The OLGA dynamic multiphase flow simulator models time-dependent behaviors, or transient flow, to maximize production potential. Transient modeling is an essential component for feasibility studies and field development design. Dynamic simulation is essential in deepwater and is used extensively in both offshore and onshore developments to investigate transient behavior in pipelines and wellbores. Transient simulation with the OLGA simulator provides an added dimension to steady-state analyses by predicting system dynamics such as time-varying changes in flow rates, fluid compositions, temperature, solids deposition and operational changes. From wellbore dynamics for any well completion to pipeline systems with all types of process equipment, the OLGA simulator provides an accurate prediction of key operational conditions involving transient flow. Application examples: • liquids handling,

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• sizing separators and slug catchers, • managing solids, • simulating key operational procedures including start-up, shut-down, and pigging, • modeling for contingency planning, • assessing environmental risk in complex deepwater drilling environments.
OLI Studio	https://www.olisystems.com/oli-studio-stream-analyzer	Commercial	Evaluation copy	OLI Studio (formerly known as Analyzer Studio) contains: • Stream Analyzer • ScaleChem • Corrosion Analyzer (with EVS)
Omegaland	http://www.omegasim.co.jp/contents_e/product/ol/	Commercial	no	The OmegaLand is the general term for integrated environment for dynamic simulators. It consists of functional modules to meet a large variety of applications of many industries. It is intended for the industries that are potentially demanded to solve problems of hazards to safety, environment, and resource/energy savings. Such industries are generally related to petrochemicals, chemicals, electric power, gas, steel, pulp and paper, food, and pharmaceuticals. The OmegaLand is useful for their various departments including research, technology, manufacturing, production management, maintenance, security, and personnel/labor. The OmegaLand provides dynamic simulation environments producing the maximum effect at

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				the minimum cost according to user's purposes such as designing, analysis, education, training, control, operation assistant, and optimization.
OptiRamp	http://optiramp.com/services#dynamic-study	Commercial	no	Dynamic studies may be conducted to verify process design and basic behavior, to analyze transient processes, and to understand complex turbomachinery equipment. The goals are to determine process stability, identify and avoid design issues and immediate risks, and ensure the proposed system functions as expected. Use cases • Provide technical support for assessing system behavior during design stage • Eliminate risks during performance tests • Confirm correct control system algorithm functionality or discover system dynamic behavior deviations • Provide continuous access to "what if" scenarios and predict an outcome before control action is taken
OpenModelica	https://www.openmodelica.org/	Free	Free/OSS	OpenModelica is an open-source Modelica-based modeling and simulation environment intended for industrial and academic usage. Its long-term development is supported by a non-profit organization – the Open Source Modelica Consortium (OSMC). The goal with the OpenModelica effort is to create a comprehensive Open Source Modelica modeling, compilation and simulation environment based

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				on free software distributed in binary and source code form for research, teaching, and industrial usage.
PIPE-FLO Professional	https://eng-software.com/products/pipe-flo-professional/	Commercial	Demo	Engineered Software, Inc.'s PIPE-FLO Professional is the world's leading fluid flow analysis and design modeling software tool. These versatile tools provide value across multiple disciplines, industries and during all stages in the lifetime of a fluid piping system. They provide a common basis for operators, process and design engineers and management to understand, communicate and document their fluid piping systems and processes. Equally applicable to process, support and distribution systems in commercial, industrial and public facilities, PIPE-FLO products are an invaluable tool for the design, commissioning, operation and modification of fluid piping systems.
PEL Software Suite	http://www.pelsoftware.com/	Commercial	30d evaluation	PEL Suite is a highly effective, proven, technology solution for generating and managing process engineering data. It has been developed, used and tested in a manufacturing environment to enable engineers to design processes more quickly and more reliably with up-to-date and permanently available design data. Features • Fluid Flow: Quickly and reliably calculate the correct size of every part of pipelines, equipment, and pressure relief systems.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Physical Properties: Generate physical properties for pure components, aqueous solutions, and mixtures over a range of temperatures and pressures. • Datasheets & Equipment Lists: Access up-to-date design and plant data in a revision-controlled environment either on the desktop or via the web. • Engineers' Workbench: Perform validated chemical engineering calculations for fluid flow, heat transfer, equipment sizing and mixing. • CAPRE: Use Microsoft Excel to perform validated calculations for sizing relief devices and determining required relief rates. • Fault & Event Trees: Create fault tree and event tree diagrams quickly and easily to represent results of hazard analyses.
Petro-SIM	https://www.kbc.global/software/simulation-and-optimization/process-simulation	Commercial	no	Petro-SIM is the leading process simulation and optimization platform for driving excellence in facility performance and organizational productivity. At the core of Petro-SIM's technology, rigorous simulation models generate dependable for upstream, midstream and downstream refinery and petrochemical processes. Petro-SIM is a rigorous decision support tool. Its unique open platform architecture promotes exceptional levels of integration and collaboration between project teams. It allows date-based simulations and scenarios to be fully developed, making it a uniquely effective predictive and analytic tool. It closes the loop between monitoring and planning, allowing for real-time comparisons of plans, actuals and simulations. For upstream oil and gas, Petro-SIM is the only purpose-built simulation

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				software that can ensure facility processing capabilities meet long term reservoir needs. In oil refining and petrochemicals, Petro-SIM works in tandem with our world-leading SIM Reactor Suite to create the only proven simulator capable of scaling from reactor units to entire refinery petrochemical facilities. In other industries, Petro-SIM supports plug-ins for other 3rd party simulation tools. Features • Addresses each phase of the lifecycle of a facility • Integrates processes, pipelines and utility systems within a single environment, including highly detailed sizing and rating models for unit operations • Built to work in real-time, for monitoring unit health and profitability • Allows superior collaboration and version control, and the ability to build in your own design standards and checks • Contains all the infrastructure to connect and manage messy real-world data, including historian connections, data validation and reconciliation • Supports data and model analytics, with all simulation calculations stored in a database for historical analysis and datamining
PETROX	no info	no info	no info	Scientific articles only, no webpage

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
Power Plant Simulator & Designer	http://www.powerplantsimulator.com/?page_id=2406	Commercial	no info	Power Plant Simulator & Designer is a world standard program for designing steam generators. It is designed for engineering complex heat exchangers e.g. steam boilers, power stations…etc. The PowerPlantSimulator&Designer allows the user to build quickly a graphical schematic representation for a plant in a graphical user interface by selecting from a library of predefined power plant elements to simulate their operation. Element connections for fluid-flow paths, mechanical couples, or signal/logic flow paths are based on connectivity rules, defined for each element. Applications • Natural circulation boiler • Forced circulation • Force flow boiler (once through boiler) • Benson-boiler (supercritical) • Municipal waste incinerator • Fire tube boilers • Hot water boiler • Fluidized bed combustion • Heat exchangers, heat transfer fluids, etc.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
Process Studio	https://protomationsite.com/process-studio-4-7/	Commercial	no info	Simulation applications for the Process Industry including companies in the oil and gas, petrochemical, energy, the basic and specialty chemicals sector etc. High fidelity and robust dynamic (Process Studio) process models. Operator Training Simulators (OTS) which comply with the highest standards of quality.
Prode Properties / Prode simulator	https://www.prode.com/	Commercial	free limited version	Prode combines knowledge of process engineering and software technology to provide a range of competitive software products available in form of code libraries, standard and custom applications (for Windows, Unix, Android etc.). With more than 25 years of successful installations, the codes have been extensively tested in many areas including process simulation, fluid properties, phase equilibria, heat transfer, process optimization, realtime process controls etc. Since 1992 Prode Properties thermodynamic library adds advanced features to Windows, Linux, Android applications: • Properties of pure fluids and mixtures in Excel / Matlab • Multi phase equilibria in Excel / Matlab • Phase envelope in Excel / Matlab • Dew, bubble point in Excel / Matlab • Distillation column in Excel / Matlab • Hydrate formation temperature and pressure, inhibition, dissociation

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
ProSimulator	http://www.siminfosys.com/	Commercial	no info	ProSimulator - Operator Training Simulator systems are custom developed, high fidelity training systems and will enable the client to provide continuous training and development of operator and engineers. By using the OTS systems, the client will be able to improve operating experience, confidence and accuracy in normal and abnormal plant operations.
Pro-Steam	https://www.petromehras.com/petroleum-software-directory/project-management-software/prosteam-energy-suite	Commercial	no info	Energy-SIM consolidates years of consulting expertise in model construction into a standardised database structure. This makes model building and modification a simple case of populating databases of users and equipment. The Energy-SIM structure contains ready built reporting, historian plug-ins and is formulated ready for the optimiser module. This allows full automation of the entire process from data capture and reconciliation, simulation of the equipment, optimisation and reporting delivered into the hands of frontline operators, along with performance monitoring, and continuous improvement support tools. ProSteam applications: Utility systems usually offer the largest opportunities to improve site energy consumption. Benchmarking and gap analysis frequently shows this is where the biggest performance gaps lie, and the fact that utilities are more peripheral means that changes can be made without compromising the core production processes. Effective utility modelling poses many challenges, such as distributed systems spanning entire sites and including potentially dozens of turbines, and hundreds of steam users. Complex balancing logic, often with multiple marginal mechanisms which frequently change. Highly interconnected constraints,

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				often involving a need to simultaneously balance fuel, steam, power and hydrogen networks, as well as consider production process constraints.
ProMax	https://www.bre.com/	Commercial	no info	ProMax is a powerful and versatile process simulation software package that is used by engineers worldwide to design and optimize gas processing, refining and chemical facilities. The goal for the software is that it be highly customizable yet very robust, extremely powerful yet approachable and usable, and very accurate in its predictions without any need of regression or fitting on the part of the user.
PRO/II	https://sw.aveva.com/engineer-procure-construct/engineering-process-design/pro-ii-process-engineering	Commercial	Demo can be scheduled	PRO/II Process Engineering is a steady-state simulator that optimises plant performance by improving process design, operational analysis, and performing engineering studies
DYNSIM	https://sw.aveva.com/engineer-procure-construct/simulation-and-training/dynamic-simulation	Commercial	Demo can be scheduled	DYNSIM Dynamic Simulation is a comprehensive, dynamic process simulator that enables users to meet and beat the dynamic challenges of designing and operating a modern process plant safely and profitably. By assisting in process design, controls checkout, and control system design, DYNSIM Dynamic Simulation enables process yield improvement and reduction of capital investment costs. The DYNSIM Dynamic Simulation

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				operator training simulator provides safer operation while improving performance and productivity.
ROMeo	https://sw.aveva.com/operate-and-optimise/optimise-operations/romeo-process-optimisation	Commercial	Demo can be scheduled	Rigorous Online Modelling with Equation-Based Optimisation. Process Optimisation is industry-leading technology for real-time optimisation that can generate precise operating information to improve performance and give operators the ability to make informed decisions at an expedited rate.
RecoVR	webpage unreachable	no info	no info	no info
REX	http://www.optience.com/rex/software/index.asp	Commercial	15 day trial can be downloaded	Optience REX is a comprehensive software that aids chemists and chemical engineers to analyze chemical reaction systems and thereby develop strategies to maximize their yield performance. The software components in REX aid in decision making at every step of your workflow: You may start your journey with REX from reaction route evaluation, continuing on to experimentation, reasoning of the experimental data through kinetic modeling, evaluation of alternate strategies for the reaction system, and finally optimization of the reaction system to meet performance objectives. REX allows you to reason through the bottlenecks in your reaction system, identify the causes for yield loss and by-product formation, and devise strategies to maximize the performance of the reaction system.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
SimCreate	https://www.tscsimulation.co.uk/solutions-process-training-plant-operations	Commercial	no	TSC Simulation's process simulation models are designed for basic and advanced learning and competence assessment. They are widely used in colleges and training centres worldwide. Their engineering fidelity, including full thermodynamic integrity with heat and mass balance means that they are also used extensively for plant and control system verification. From individual process items to complete production systems they are all suitable for running stand alone, in classrooms, in our Virtual Control Room for teamwork training and now with the ability to connect to the 3D environment. Features • Uses industry proven accurate mathematical algorithms for modelling • There are no third party licencing costs - lifetime licencing • Runs on individual PCs, networked classroom or Virtual Control Room • Suitable for OPITO certified courses, including OIM Emergency Management level • Dynamic response (typically 10mS iterative looping) allows full performance checks on compressor anti-surge and other rapid response control systems • Site Specific simulation systems can use full emulations of most available DCS interfaces

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
SimCentral	https://sw.aveva.com/discover-simcentral-simulation-platform	Commercial	Demo can be scheduled	This new unified Simulation Platform supports the entire engineering lifecycle; from representation of actual P&ID, mapping each equipment object to a detailed engineering database; to building/testing the dynamic simulation early in the process design; to optimizing the process and control design, comparing capital versus operating costs; to the continuous improvement of operations, as the simulation model becomes the plant's Digital Twin.
SPEEDUP	no page, links to academic papers	no info	no info	no info
SuperPro Designer	http://www.intelligen.com/superpro_overview.html	Commercial	Demo	SuperPro Designer facilitates modeling, evaluation and optimization of integrated processes in a wide range of industries (Pharmaceutical, Biotech, Specialty Chemical, Food, Consumer Goods, Mineral Processing, Microelectronics, Water Purification, Wastewater Treatment, Air Pollution Control, etc.). The combination of manufacturing and environmental operation models in the same package enables the user to concurrently design and evaluate manufacturing and end-of-pipe treatment processes and practice waste minimization via pollution prevention as well as pollution control. It is a valuable tool for engineers and scientists in process development, process engineering, and manufacturing. It is also a valuable tool for professionals dealing with environmental issues (e.g., wastewater treatment, air pollution control, waste minimization, pollution prevention). It provides under a single umbrella modeling of manufacturing and end-of-pipe treatment processes, project economic evaluation, and environmental impact assessment.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				Features • Available for the Windows platforms • Models for over 140 unit procedures / operations, rigorous reactor modules • Material and energy balances • Extensive chemical component and mixture database • Extensive equipment and resource databases • Equipment sizing and costing, thorough process economics • Scheduling of batch operations • Throughput Analysis and Debottlenecking • Resource (utilities, raw materials, and labor) tracking as a function of time • Waste stream characterization • Environmental impact assessment • OLE-2 support • PFD customization through addition of your own graphics and text • Compatibility with a variety of graphics, spreadsheet, and word processing packages

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Option to export PFDs in DXF format (for incorporation into AutoCAD) and in WMF format
SysCAD	https://www.syscad.net/products-and-software/	Commercial	Trial	SysCAD is a powerful and versatile plant simulation software, and can be used to simulate the simplest processing circuit through to a complex full plant operation. It can be operated as a steady state solver or in dynamic mode. When used to its full potential, it can serve in every aspect of the plant life cycle from feasibility studies, to design, commission, operations and maintenance to expansion and more. It is an invaluable process design tool that will help users gain tremendous insight into their process operations. This knowledge can translate into: • Better decision making • Improved plant operation performance • Cost saving • More efficient and knowledgeable operators
System7 / SINET	http://www.epcon.com/sinet.html	Commercial	no info	The industry's most powerful and proven flow network analysis computation engine. Robust mathematical engine solves systems with hundreds of pipes in less than a second. Features • Unlimited pipes and equipment and multiple models can be open at the same time

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				• Incompressible and Compressible flow capabilities in a single software solution • Equation of state accurately determines the density of non-ideal gases • Tested and perfected in industry on hundreds of systems over the past 20 years • Intuitive and efficient graphical user interface • Analyze mode highlights the root-causes of system flow and pressure bottlenecks • Integrated equipment sizing programs with high quality physical property data • AIChE DIPPR® database of over 2000 components (DIPPR is a registered trademark of AIChE and is used by permission) • Model any process or utility system using one software and interface (Petroleum streams, Natural gas, Steam and condensate, Refrigerants, Instrument and compressed air, Cooling water and firewater, Any process or utility system)
UniSim Design Suite	https://www.honeywellprocess.com/en-US/explore/products/advanced-	Commercial	Trial	Honeywell's UniSim® Design Suite is an intuitive process modeling software that helps engineers create steady-state and dynamic models for plant design, performance monitoring, troubleshooting, business planning, and asset management.

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
	applications/unisim/pages/unisim-design-suite.aspx			
UniSim Competency Suite	https://www.honeywellprocess.com/en-US/explore/products/advanced-applications/unisim/unisim-competency-suite/pages/default.aspx	Commercial	no info	Honeywell UniSim® Competency Suite enables industrial companies to plan, deploy and manage a structured program for operator competency. It offers robust solutions to train plant personnel for safe, incident-free and efficient startups to achieve operational excellence. With comprehensive field and console operator training, plant operators can gain the knowledge and skills to be the Ultimate Operator.
Usim Pac	http://caspeo.net/usimpac	Commercial	no info	USIM PAC enables to model and simulate in a single tool the whole industrial transformation raw materials: • Mass, energy, water and CO2 balances • Industrial process audit • Plant optimisation or comparison of scenarios • Technical and economic feasibility studies • Libraries of unit operation models dedicated to the following industrial fields: mineral processing, food processing & biorefining

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
Virtuoso	https://www.woodgroup.com/__data/assets/pdf_file/0020/28811/Virtuoso.pdf	Commercial	no info	Wood Group provides robust, real-time online and offline software systems for the efficient management of oil and gas operations. Virtuoso is a field proven suite of software products, with more than 20 years' successful track record of performance in the field. Our technology supports engineering studies, operator training and simulation wells, pipelines and processing facility operations onshore and offshore. We address the most complex single and multiphase gathering, productions, transportation and processing issues with our technology solutions. The software suite includes offline packages: Engineering simulator, Operator training system. And online packages: Operations monitoring, Operations advisory, Leak detection system, Operations control, Operations optimization and planning, Virtual metering system, Data analysis and processing.
VMGSim	https://virtualmaterials.com/vmgsim	Commercial	trial	VMGSim is a world-class, rigorous and comprehensive steady-state process simulator developed with an integrated flowsheet design in a user-friendly, modern environment. It is used around the world to model existing processes and to design new facilities from the ground up. With over 20,000 chemicals, more than 80 thermodynamic property packages and hundreds of unit operations, VMGSim provides unparalleled model sophistication and precision, giving you more time to solve processing challenges creatively. It builds your models based on rigorous thermodynamic relationships and needs only the information absolutely required to do so, saving you time and processing power. Experiment with different equipment configurations in your simulation models to see the effects of changes to the whole system instantly and economically. VMGSim does this by instantly calculating

Name	Website	Commercial / Free / OSS	Demo / trial available	Description from vendor (normal font) and/or comments (in italics)
				process changes, intelligently propagating information, and continually monitoring degrees of freedom when you modify any unit operation parameters or process conditions. VMGSim is a true Gibbs-based simulator that is capable of monitoring each variable's state and its thermodynamic significance. By means of the Gibbs phase rule, with enough degrees of freedom fulfilled, calculations are automatically completed and the results transmitted throughout your flowsheet.
Wolfram SystemModeler	http://www.wolfram.com/system-modeler/	Commercial	trial	Wolfram SystemModeler is an easy-to-use, next-generation modeling and simulation environment for cyber-physical systems. Using drag and drop from the large selection of built-in and expandable modeling libraries, you can build industrial strength, multidomain models of your complete system. Adding the power of the Wolfram Language gives you a fully integrated environment for analyzing, understanding and quickly iterating system designs.

Table 6 Simulator list