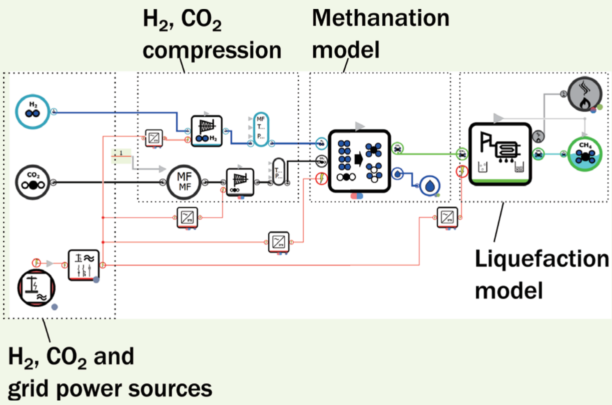
Decision Support Platform for Resource Optimization and Sustainable Energy

Renewable Gas R&D group at Kanadevia Inova AG (KVI) has been developing a software tool (DSP: Decision Support Platform) for conceptual and early design evaluation and optimization of complex, coupled waste management and energy systems. The tool fully integrates process, economic and environmental/social life cycle analyses. This report gives an overview of the tool design and features, with illustrative examples from application cases executed in KVI and Kanadevia Corporation (KVC). The next phase of the development will focus on expanding the simulation libraries, and user interface enhancements for transfer from R&D environment to wider use in engineering, project development and sales.



DSP4ROSE: Illustration of a simulation setup of a methanation and liquefaction plant in DSP4ROSE

The design of waste treatment and energy system has become increasingly complex, due to the need to consider wide range of technological, process, economical and life cycle criteria. Besides technical challenges, this increases the need to apply state-of-the-art techniques to support associated decision-making processes as well as communication with customers and stakeholders. This furthermore requires that underlying analyses are executed and evaluated in rigorous, transparent, and straightforward-to-understand manner.

DSP/DSP4ROSE (**D**ecision **S**upport **P**latform for **R**esource **O**ptimization and **S**ustainable **E**nergy) has been developed at the RG R&D group in Zürich as a process simulation and optimization tool. The objective is to create a unified, yet flexible environment in which we can setup a simulation, such as the methanation layout in the title Figure, and execute process simulation, with fully integrated economic and life cycle analyses, together with built-in capabilities for integration, optimization and reporting tasks.

■ Tool: “Concept”

Although the need for such a tool is clear, it is not obvious whether there are commercial options available, or in-house development is required. The DSP project decided to initiate custom development due to the following:

- We require a multi-domain tool, that allows simulation of variety of units, including chemical, electrical, mechanical, logistics and transportation operations, among others, since all such components are important parts of the systems of interest.
- The tool should integrate design steps that are currently split over variety of tools: block diagram design (often in a form of pdf), process and business cases calculations (instead of a number of excel sheets), unit simulations of sub-processes (e.g., in ASPEN), and external tools for life cycle analysis (such as OpenLCA). Interfacing such a set of tools becomes difficult when analyzed systems are complex and time-variable operations need to be considered, which leads to possible errors and increased loads on personnel and the new tool should simplify the overall process.
- Tool should allow time-variable analysis, from second scale to seasonal variations.
- The economic analysis should cover conventional elements, but allow also evaluation of life-cycle economic impacts, which are rarely considered in simulations but are critical in real systems, such as equipment degradation or economic impact of unplanned shutdowns.
- For decision-making support, the tool should include all “three pillars” of sustainability life cycle assessment: economic, environmental and social. For this, the simulation results need to

provide inventories for each of the pillars. This requires highly customized structure of the unit and system models.
- Since KVI focuses on waste treatment systems, the material streams involved in the simulations are complex, such as waste streams or products, with variety of possible contaminants. The tool has to inherently handle such streams, for example in order to estimate the economic impact of impurities in the products, or to integrate proper cleaning equipment in the process and related costs.

Given the unique combination of the above targets, the project initiated development of a new in-house tool.

Basic environments

DSP4ROSE is built on three main interacting environments (**Figure 1**):
- **Modelica** simulation language is a modern language for simulation of multi-physics systems. It is maintained by the Modelica Association (Modelica), and open-source editor OpenModelica (openmodelica.org) is used. DSP4ROSE uses Modelica as an efficient environment for development of unit and system models, and as a powerful numerical solver.
- **Python** language ecosystem is used to create the overlying DSP4ROSE system from which the simulations are controlled. Additionally, variety of Python libraries are used for data analysis, and for pre- and post-processing tasks, which are together combined into DSP4ROSE Workflows.
- Data, ranging from unit characteristics to weather and economic data, are managed in **SQL database** environment.

Additional components may be used to enhance the functionalities, such as commercial life cycle impact database ecoinvent (ecoinvent.org). However, the design principle of DSP4ROSE is that all functions are in principle implemented with open source or in-house components.

(Modelica) https://modelica.org/
(openmodelica.org) https://openmodelica.org/
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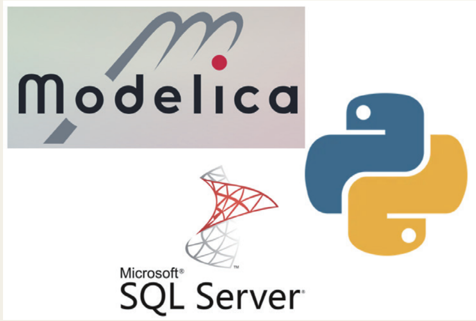

Figure 1　Three main environments of DSP4ROSE

FIT Modelica package

The simulation structures of DSP4ROSE are embodied in an in-house Modelica package, called **FIT** (**F**ast **I**ntegration **T**ool). The FIT package consists of a hierarchy of stream definitions, unit model library and system models. Currently the package includes about 140 stream definitions, such as H_2, CH_4 or municipal solid waste. Each unit model is then defined by inflow and outflow streams, and physical/chemical models that reflect the simulated unit behavior (**Figure 2**). Importantly, models can continuously evolve from simple implementations to any level of details.

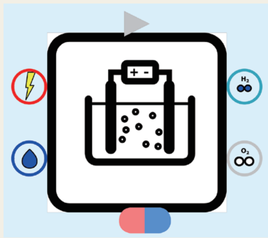

Figure 2　Example of "icon" representation of an electrolyzer model in FIT. The model provides calculation of the outlow connectors (H_2 and O_2 on the right) from the inflows (power and water on the left). Note that the streams include not only basic state properties such as temperature and pressure, but also detailed composition, covering details of the stream state

Besides physical and chemical models, each unit model also includes:
- Calculations of economic variables, such as capital costs, operating costs associated with any stream. In total, 41 of economic indicators are available for each unit model, which include also structures to estimate degradation of the equipment given the simulated operation pattern, or variety of subsidy or tax structures.
- Calculations of inventories required for environmental and societal life cycle analysis, for example, pollutant emissions, physical

footprint indicator, or labor requirements associated with each unit.

Unit models can be assembled in FIT to system models such as flue gas treatment model in **Figure 3**. DSP4ROSE Workflows provide variety of tests to ensure that such modular connectivity is maintained throughout the tool.

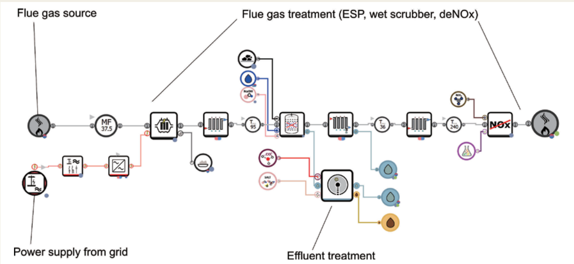

Figure 3　Example of flue gas treatment system in FIT

■ DSP4ROSE Workflows

In DSP4ROSE, pre-processing, simulation/optimization control, post-processing analyses and reporting are organized into Workflows implemented in Python, using Jupyter Notebook environment. Custom graphical user interfaces are in development. The DSP team maintains a set of main Workflows that cover typical tasks, such as mass and energy analysis, economic summary, or environmental impact report. Additionally, custom Workflows can be created.

When the model is created in FIT, pre-processing, input data assembly from SQL database, and compilation are performed, after which the simulation case is ready for execution. All simulations are executed as time variable, and most typically, systems are simulated over 1 year period with 1 hour time step. The results include energy, mass, economic, environmental and societal inventories (**Figure 4**).

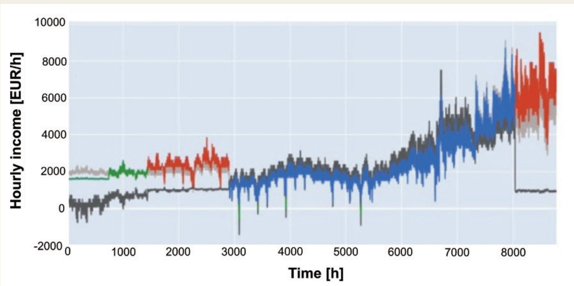

Figure 4　Example of "economic inventory": This example shows revenues profile from a KVI study that compared four different carbon capture technologies

Based on the results, DSP4ROSE performed standard and custom analysis. Illustrations of analyses available in the Workflows are illustrated graphically on the following set of Figures (note that the frames intend to illustrate the types of reports, but are collected from several unrelated studies, and results have no context within this article):

1) Energy and mass flow analysis

Figure 5 shows a Sankey diagram with mass flows for a amine carbon capture system. Black boxes represent process units, and mass flow of various materials is graphically visualized. Explicit labels are shown for water (blue) and MEA (mono-ethanol amine solvent in orange), but FIT simulations can track wide variety of contaminants and components. The relative thickness of the colored bands represent the mass flow of each compound. Labeled in the diagram are the desorbed, absorber, and water wash units, with visible water and amine circulation patterns. Similar type of visualization is performed for energy forms (heat, power).

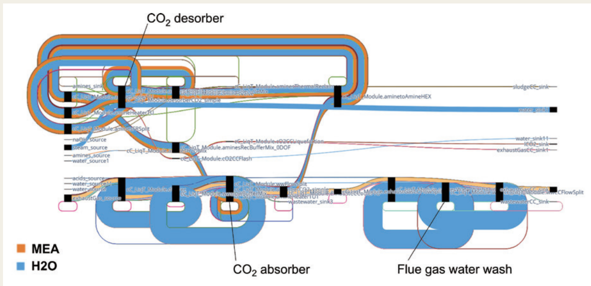

Figure 5　Sankey diagram example of mass flow analysis from carbon capture study. shows flow of the main compounds (water in blue, and amine in orange) as well as range of impurities and amine degradation products

2) Thermal integration

DSP4ROSE includes Workflow for analysis and improvement of thermal integration of the simulated system. **Figure 6** shows the composite curves of simulated system as the basis for such analysis.

3) Exergy analysis:

Besides the mass and energy analysis, DSP4ROSE includes exergy analysis, suitable for improvement of simulated systems.

4) Economic balance

As a highly common part of techno-economic studies, DSP4ROSE presents several types of economic analysis, for example cost/revenue breakdown. **Figure 8** shows top level of such

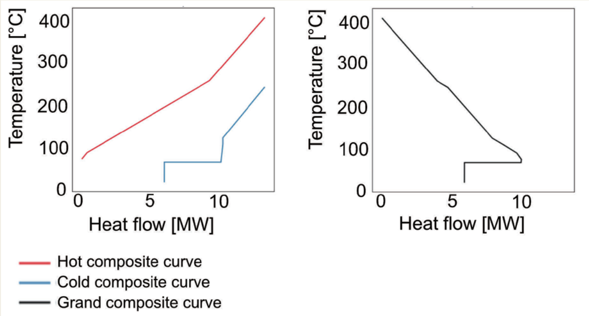

Figure 6 All of FIT models can include structures to allow heat integration analysis. At each step of the design process, for example, the engineer can explore possible improvements using the composite curves, as shown here

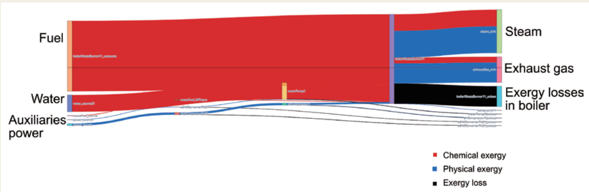

Figure 7 DSP4ROSE includes also possibility to equip unit models with exergy calculations at input and output, which allows visualization of process efficiency. (Red: chemical exergy contained in the streams; Blue: physical exergy; Black: exergy loss into heat. Each vertical column represents a simulated unit or source/ sink)

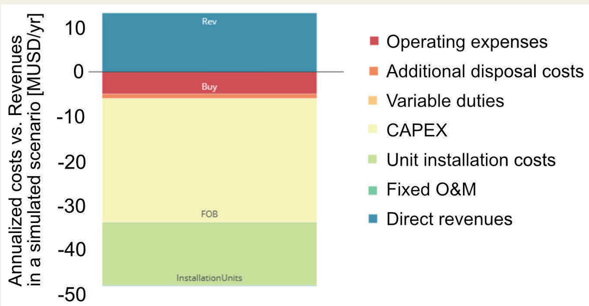

Figure 8 Economic results are assembled to variety of indicators, here for example comparing operating and annualized capital costs for several alternatives of flue gas treatment systems

analysis, which can be broken down to subprocesses and any of the calculated economic indicators.

5) Environmental life cycle impacts

The focus of DSP4ROSE on calculation of detailed inventories and in particular detailed consideration of the composition of simulated streams allows direct integration of the simulation results with life cycle analysis. For that, ISO14040 is followed, in which the calculated inventories are processed into standardized form of mid-point and end-point impacts, defined by various methods, which show for example impacts on human health, or global warming. **Figure 9** shows calculated impacts in four shown impact indicators, in the form of DALY (disability adjusted life years).

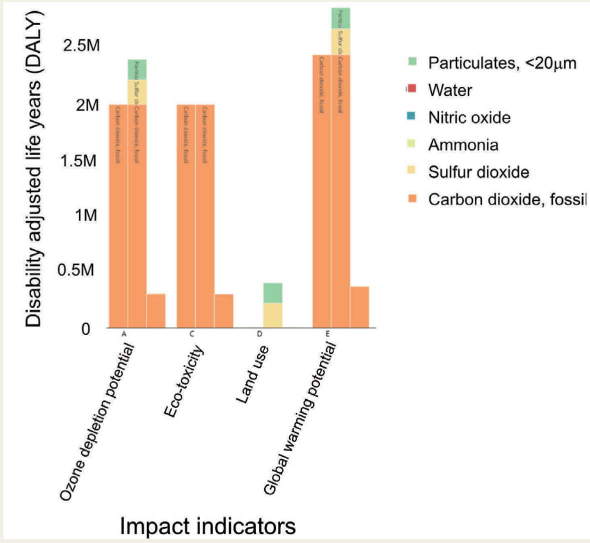

Figure 9 Environmental and social impacts can be analyzed using selectable methods, following the ISO14040 LCA standard. Example shows gate-to-gate analysis of human health impacts in DALY for carbon capture systems comparison

Optimization Workflows

Since all of the above inventories and analyses are generated directly in DSP4ROSE simulation, an added advantage is that any of the calculated quantities can be assembled into single- or multi-objective optimization. This allows to directly co-optimize for example process design parameters with economic performance and with environmental impact in selected category.

An example in **Figures 10** and **11** show an illustration of a real-life electrolysis+methanation+liquefaction case, with such combined optimization. In this case the task was to find a solution that simultaneously combined optimal sizing of all process storage tanks (reducing CAPEX), the lowest costs due to forced shutdowns of methanation and liquefaction units, the lowest costs of purchased grid power, while maximizing the green premium of the LPG product and maximizing usage of power from PV and wind plants with time-variable prices. Besides optimization of the above variables, improvement in such situations can be also achieved by selection of the most suitable control strategy. The simulation therefore additionally includes a set of controllers, which are included in the four pentagons at the top of the frame. These controllers function as distributed programmable controllers: they collect system inputs, and use an algorithm to send control signals to controlled components, for example to set a mass flow.

However, selection of optimal control strategy is complex in this type of plants. To find the best solution, the controllers in the given example include several possible control strategies that are co-optimized with the previously mentioned performance targets.

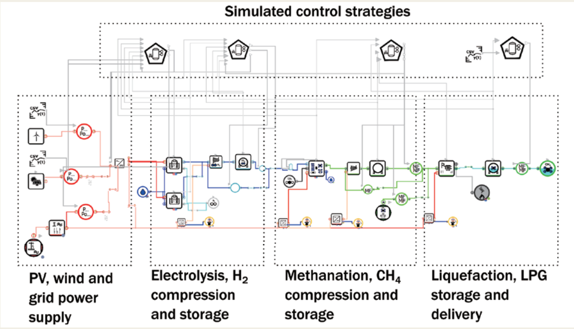

Figure 10　Example of combine process simulation with controllers. The shown system draws electric power (red line) from PV and wind plant (on the left), uses two electrolyzers to produce H_2 (blue line), which is further converted to methane (green line) and liquefied to LNG (azure line), delivered on the right

Result of optimization in the above example for one of the analyzed scenarios is in **Figure 11**, in which the aggregated objective function is plotted against the ratio of electric power purchased from the grid to the electric power sourced from PV and wind plants. The result shows that although the grid power is overall more expensive than renewable power, purchase of about 39% is favorable to minimize shutdowns of the process and save CAPEX (Capital Expenditure) on sizing of intermediate

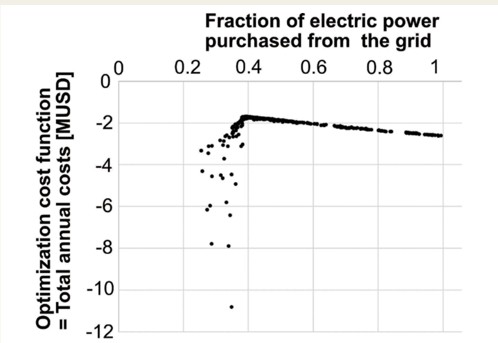

Figure 11　Example of optimization result from system in Figure 10

storage tanks that are otherwise needed to prevent the interruptions caused by intermittent renewables.

■ DSP4ROSE uses and future plans

Although illustrated types of analysis are available in different commercial and academic tools, we believe that integration of these steps into DSP4ROSE can result in better accuracy, consistency and reliability of the results. This can help to improve the technical solution itself, reduce safety margins embedded in the design due to uncertainties, and facilitate interaction with customers and stakeholders.

DSP4ROSE has been already applied in variety of research and commercial cases, and KVI is in collaboration with users at KVC, as well as with several university partners.

The future use of DSP4ROSE is expected to grow to the following areas:

- preparation of solutions and plant designs for evaluation with customers, including scenario analysis and multi-objective optimization
- reduction of CAPEX in optimized designs
- optimization of operating costs and performance for customers and for own operations
- environmental life cycle analysis is increasingly demanded and appreciated by customers and regulatory bodies, and demonstrating high levels of competence is important

At this point, the project has demonstrated all the above functionalities in R&D environment. In the next phase, the tasks will focus on improving reliability and usability. This will include in particular:

- more user-friendly interfaces for expansion of the user base.
- substantial future work is required to create reliable library with all models of interest. In some cases, significant effort may be also needed for collecting required data (for example, data and good models of equipment degradation and other operating costs are very rare).
- Several expansions of Workflows are also planned. For example, economic and environmental analysis will be expanded beyond the simulated time period (typically

1 year of operation), to cover complete project timeline, including construction and decommissioning periods. Additionally, optimization workflows will be expanded to cover not only a single plant, but to allow robust optimization across fleets, with the intention to find (for example) an optimal product size for a given range of scenarios or application situations.

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