Process modelling tools and their application in design and optimization of modern decarbonized energy systems

Paweł Gładysz, PhD

pawel.gladysz@agh.edu.pl

paweljakub.gladysz@unifi.it

Scope of the presentation

- Short academic CV
- Modelling and simulations of energy systems
- Process modelling tools
- Selected past and on-going R&D projects at AGH University – application of different process modelling tools
- Discussion

Short academic CV (1)

- **AGH University of Science and Technology, Faculty of Energy and Fuels, Department of Fundamental Research in Energy Engineering, Kraków, PL**

- Silesian University of Technology, Faculty of Energy and Environmental Engineering, Department of Thermal Technology, Gliwice, PL

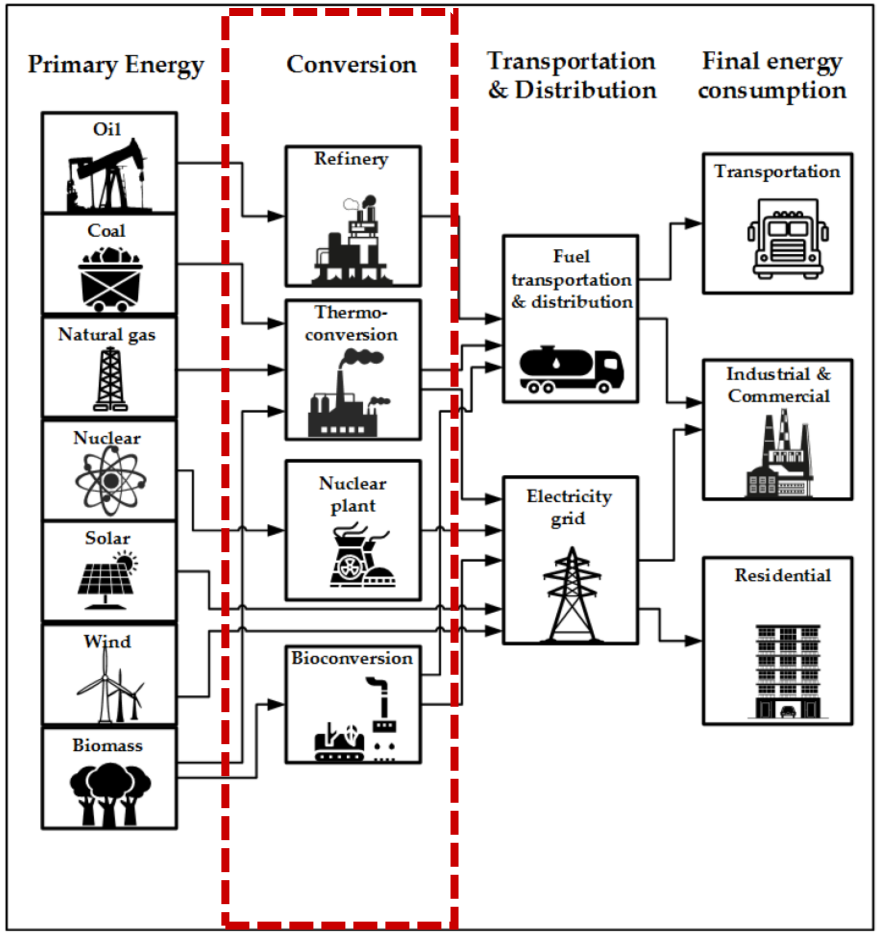
Short academic CV (2)

Research interests:

- **Modelling and optimization** of thermal processes (2010 – present)
- Geothermal energy including **enhanced geothermal systems** (2017 – present)
- **Exergy analysis** and optimization (2012 – 2015 & 2020 – present)
- **Thermo-ecologic cost** analysis including LCA (2010 – present)
- **Techno-economic** analysis (2010 – present)
- **Carbon capture, storage and utilization** technologies (2011 – present)
- Coal-to-Nuclear and Gas-to-Nuclear **retrofits** (2020 – present)
- **Machine learning** and AI in predictive and prescriptive maintenance (2019 – present)
- **Cogeneration** technologies (2010 – 2012 & 2017 – 2020)
- Thermal engineering in **iron & steel** industry (2016 – 2020)

Modelling and simulation of energy systems (1)

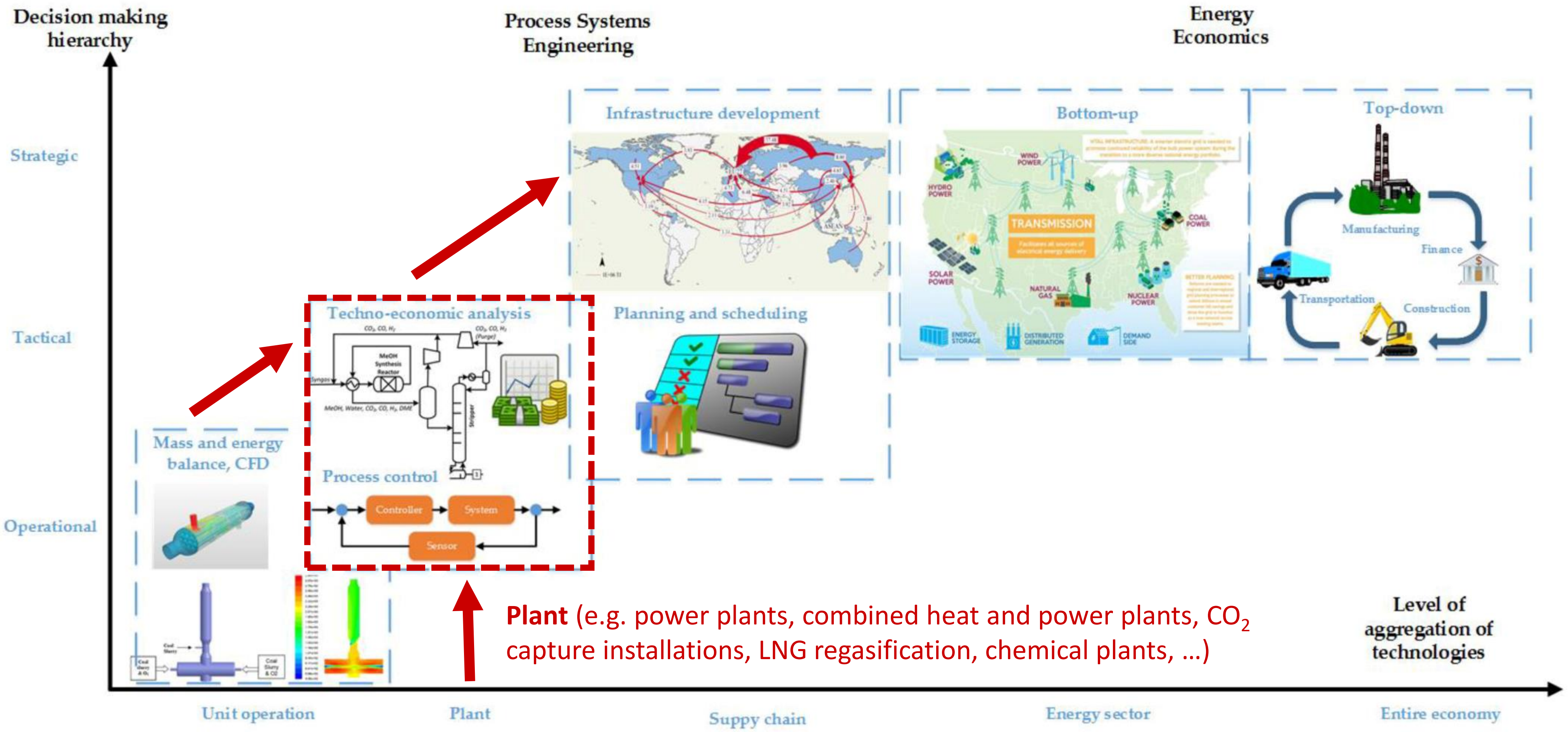
- **Primary Energy**: energy stored in natural resources (e.g. fossil fuels, uranium, renewable resources).
- **Conversion**: wide range of processes to transform energy to more usable forms (e.g. electricity, liquid fuels).
- **Transport & Distribution**: large number of infrastructure components and processes depending on the energy carrier.
- **Final Energy Consumption**: can be disaggregated into homogeneous categories of users such as transportation, residential, industrial, and commercial users.



Energy system showing the flow of energy from primary energy supply to final energy consumption

Source: Subramanian, A.S.R.; Gundersen, T.; Adams, T.A., II. Modeling and Simulation of Energy Systems: A Review. Processes 2018, 6, 238. https://doi.org/10.3390/pr6120238

Modelling and simulation of energy systems (2)



Classification of energy system models according to discipline and level of technological aggregation

Source: Subramanian, A.S.R.; Gundersen, T.; Adams, T.A., II. Modeling and Simulation of Energy Systems: A Review. Processes 2018, 6, 238. https://doi.org/10.3390/pr6120238

Modelling and simulation of energy systems (3)

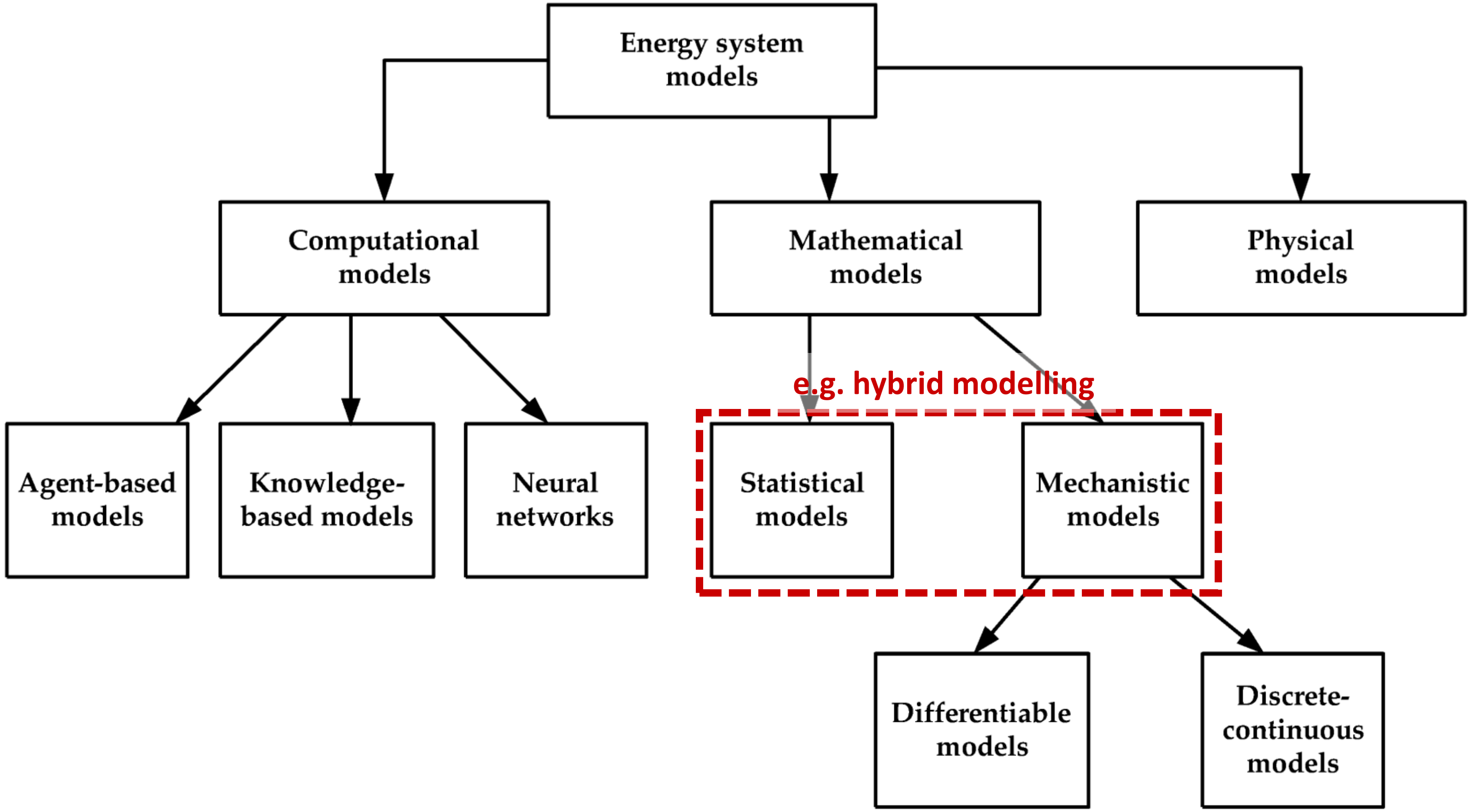
Classification of energy system models according to field

Field		Process Systems Engineering		
Nature of variables	Endogenous	Technological (e.g. temperature, pressure, enthalpy, Gibbs free energy, process size)		
	Exogenous	Economic (e.g. raw material prices, equipment prices, product demand, interest rates) Environmental (e.g. Global Warming Potential, Ecotoxity, resource depletion, terrestrial acidification)		
Theoretical underpinnings		Thermodynamics, Fluid mechanics, Kinetics		
Level of aggregation		Unit operation, Processing plant, Supply chain		
Spatial scale		Local, Regional, National, Global		
Decision making hierarchy		Strategic	Tactical	Operational
Temporal scale		Several years	Days-Weeks	Seconds-Hours
Classic purposes		Process design & integration Supply chain design/infrastructure	Production Planning and Scheduling	Process control Flexible operation
Recent trends		Multi-scale systems engineering Sustainable process analysis and design		

Source: Subramanian, A.S.R.; Gundersen, T.; Adams, T.A., II. Modeling and Simulation of Energy Systems: A Review. Processes 2018, 6, 238. https://doi.org/10.3390/pr6120238

Modelling and simulation of energy systems (4)

- **Computational models**: a sequence of instructions that can be executed by a computer.
- **Mathematical models**: a series of equations that denote relationships between different meaningful variables and parameters.
- **Physical models**: a phenomena of the real-world system actually occur at a smaller scale or with less complexity.



Classification of energy system models according to modelling approach

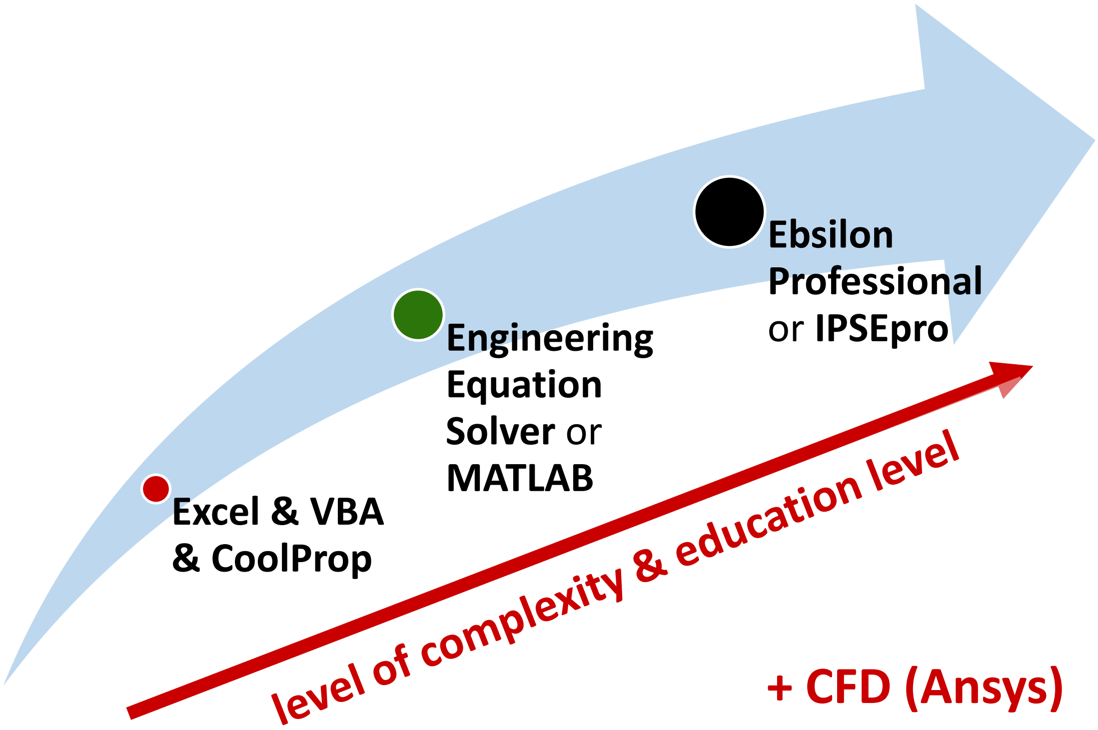
Source: Subramanian, A.S.R.; Gundersen, T.; Adams, T.A., II. Modeling and Simulation of Energy Systems: A Review. Processes 2018, 6, 238. https://doi.org/10.3390/pr6120238

Process modelling tools (1)

Process modelling tools used (so far) in research activities:

- F-Chart Software: **Engineering Equation Solver**
- MathWorks: **MATLAB**
- GE: **GateCycle™**
- **THERMOFLEX®**
- STEAG: **EBSILON®** Professional
- SimTech: **IPSEpro**
- Siemens PSE: **gPROMS** to be discussed

Process modeling tools used in teaching activities at AGH University of Science and Technology:



+ CFD (Ansys)

Engineering Equation Solver

F-Chart Software - **Engineering Equation Solver**:

- a general **equation-solving program** that can numerically solve thousands of coupled non-linear algebraic and differential equations;
- can also be used to solve **differential and integral equations**, do **optimization**, provide uncertainty analyses, perform linear and non-linear regression, convert units, check unit consistency, and generate publication-quality plots;
- includes high accuracy **thermodynamic and transport property database** that is provided for hundreds of substances in a manner that allows it to be used with the equation solving capability.

Source: https://www.fchartsoftware.com/ees/

MATLAB

MathWorks - **MATLAB**:

- programming and numeric **computing platform**;
- desktop environment tuned for **iterative analysis and design processes** with a programming language that expresses matrix and array mathematics directly - creating scripts that combine code, output, and formatted text in an executable notebook;
- a lot of **dedicated toolbox** (professionally developed, rigorously tested, and fully documented) – e.g. Deep Learning, Machine Learning, Predictive Maintenance, ...;
- perform **large-scale computations and parallelize simulations** using multicore desktops, GPUs, clusters, and clouds.

Source: https://uk.mathworks.com/products/matlab.html

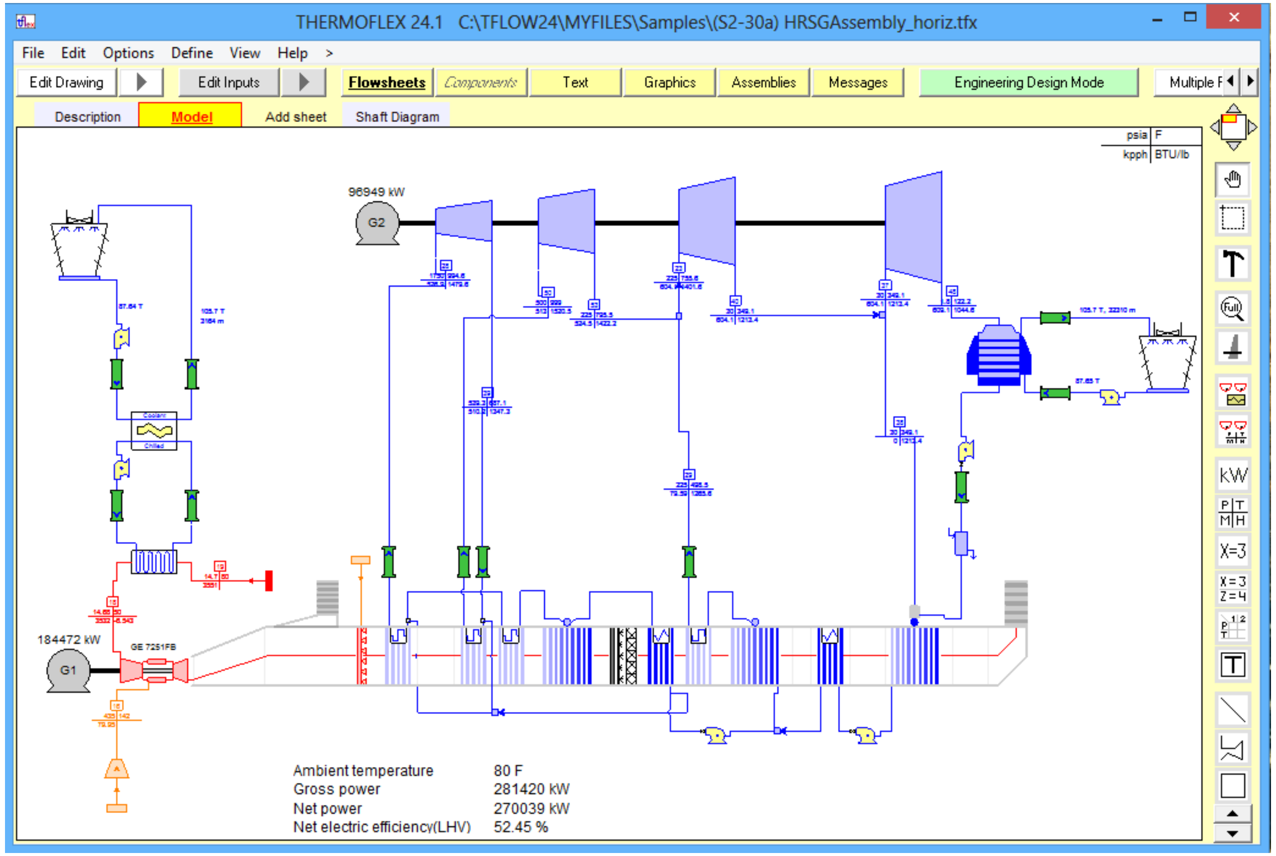
THERMOFLEX® (1)

Thermoflow - **THERMOFLEX®**:

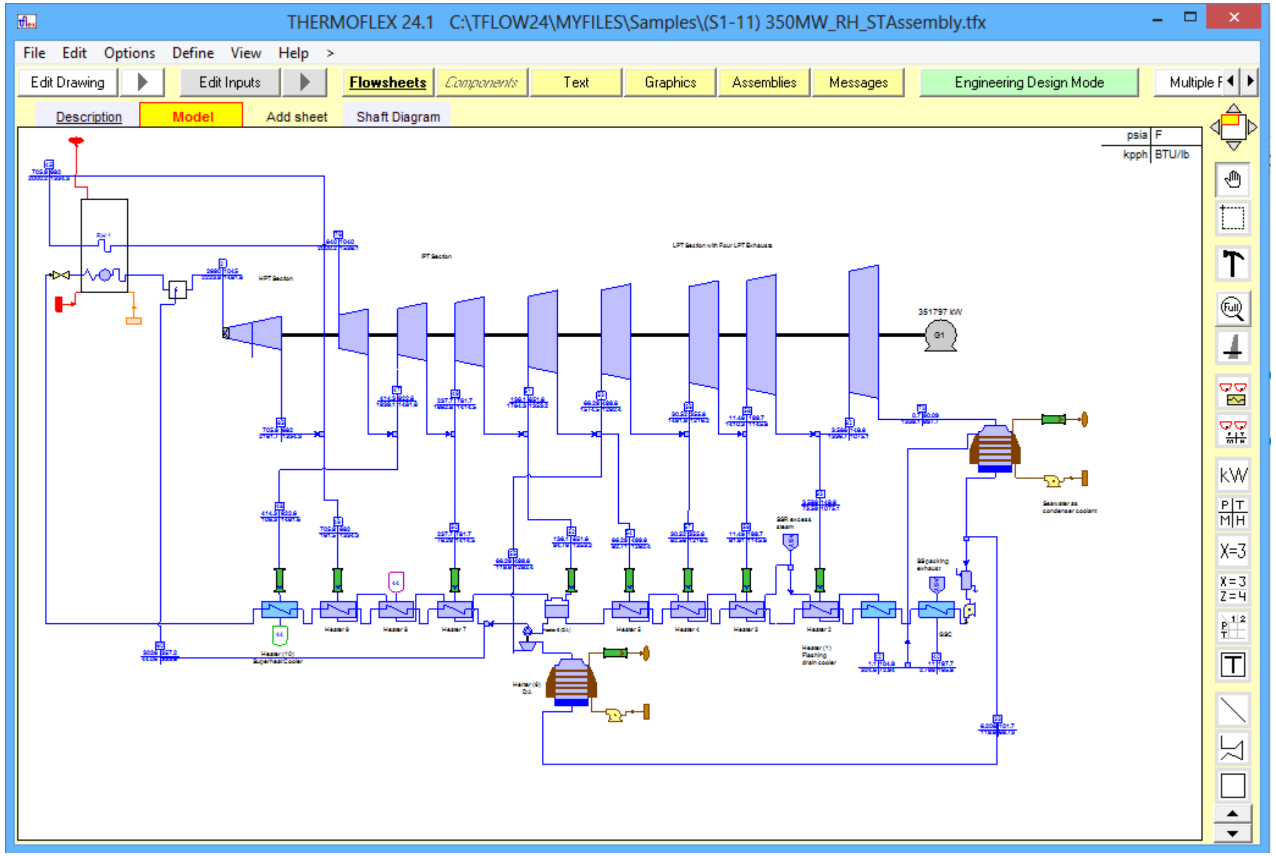
- placed in the category that engineers commonly refer to as "**heat balance software**";
- graphic user interface in which the user creates a thermal system network by selecting, dragging, dropping and connecting icons representing **over two hundred different components**;
- covers both **design and off-design simulation**, and models all types of power plants;
- model general thermal power systems and networks, and fulfills the need of some customers for a single, "**jack-of-all-trades**" program;
- a **default hierarchy of pressure and flow dictators will automatically be create**, by default, a solution for a new design of any common type of power or cogeneration plant.

Source: https://www.thermoflow.com/products_generalpurpose.html

THERMOFLEX® (2)



Example showing gas turbine combined cycle modelled with THERMOFLEX



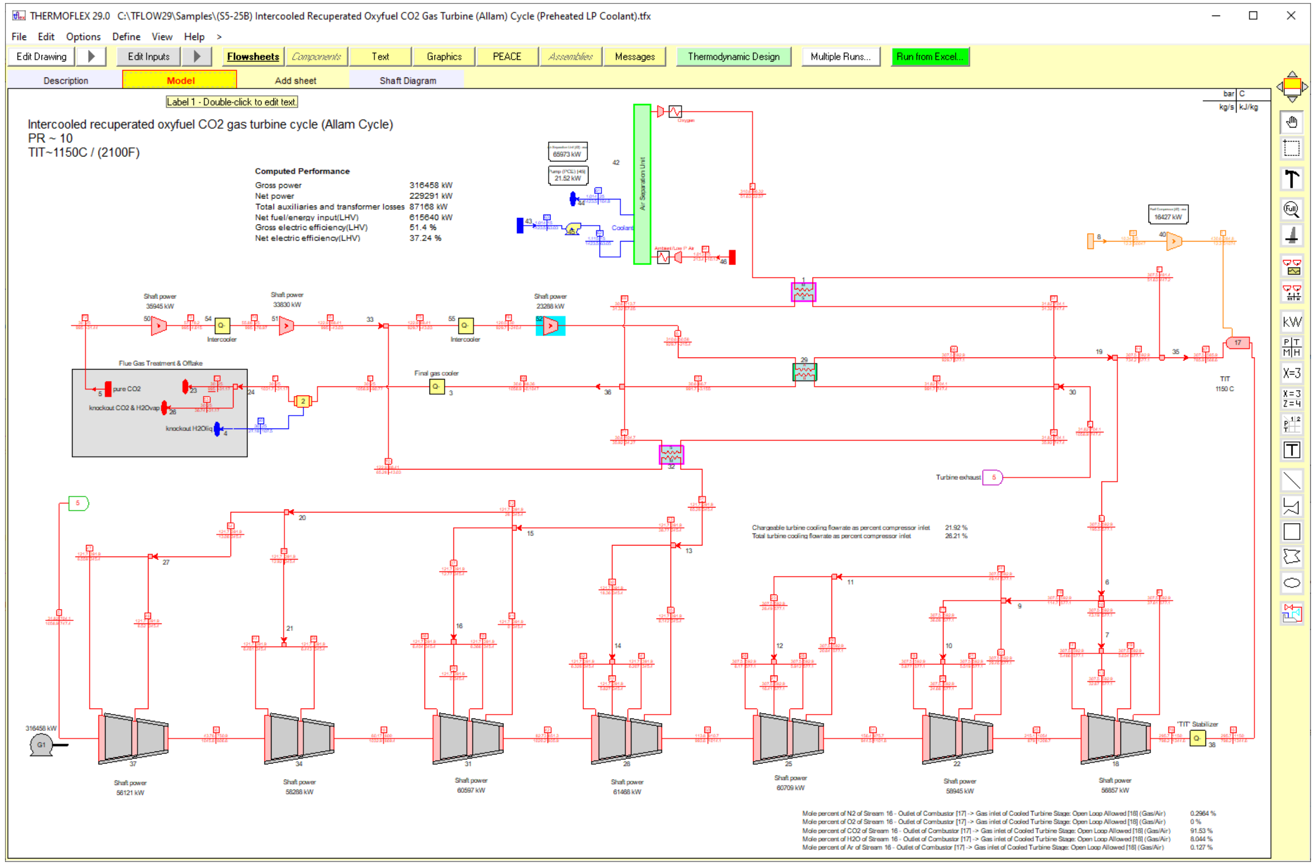
Example showing conventional steam plant modelled with THERMOFLEX

Source: https://www.thermoflow.com/products_generalpurpose.html

THERMOFLEX® (3)

Personal opinions and conclusions:

- straightforward flowsheet process modelling tool,
- great database of components,
- suited for power plants,
- easy and intuitive to setup the model,
- widely used in industry for design and case studies (in Poland),
- additional features – cost estimation, thermodynamic design mode, …



Example showing Allam Cycle modelled with THERMOFLEX

Source: https://www.thermoflow.com/products_generalpurpose.html

EBSILON® Professional (1)

STEAG - **EBSILON® Professional**:

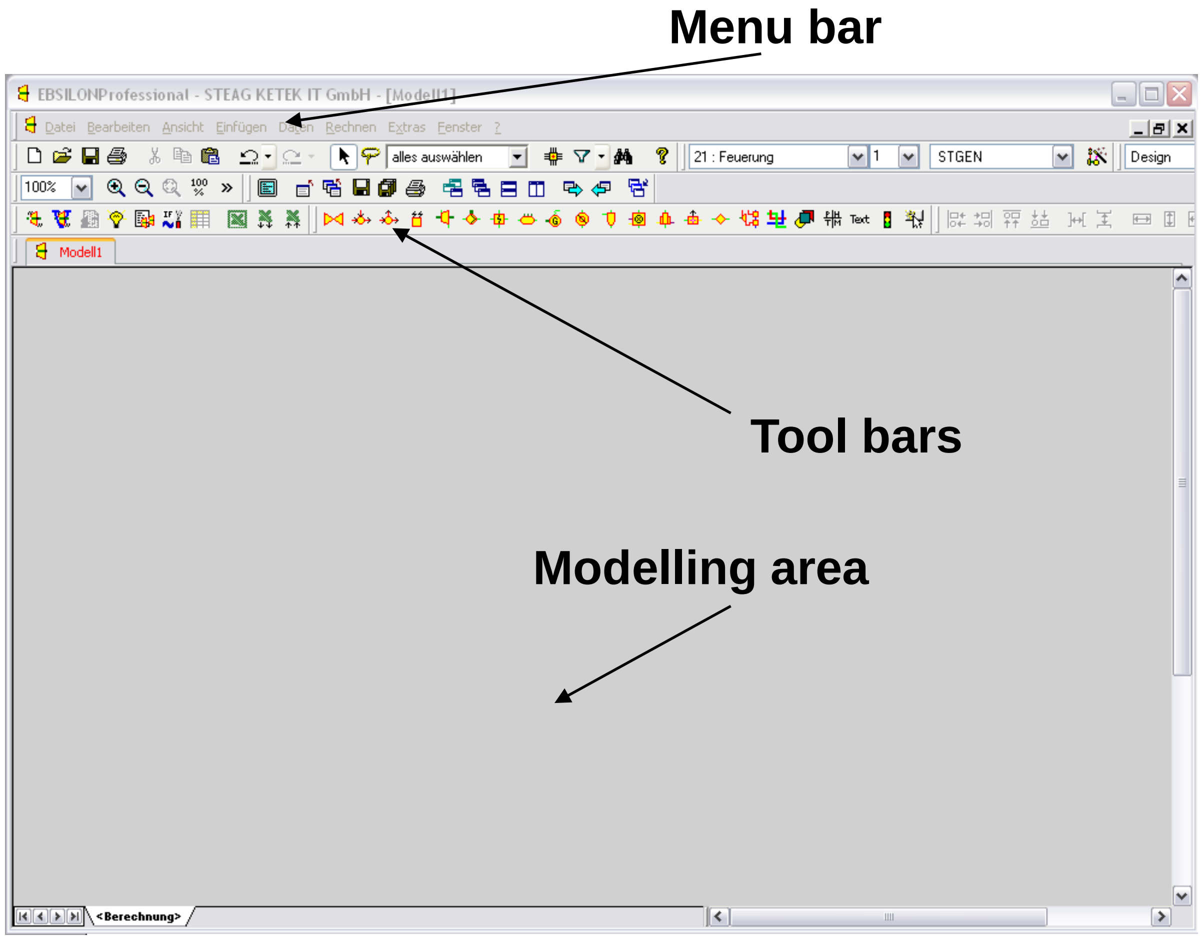
- simulation system for **thermodynamic cycle processes** that is used for plant planning, design and optimization;
- **powerful calculation kernel** and solution algorithm;
- comprehensive **component library** for different energy systems and **material data libraries** for working fluids and fuels;
- intelligent **error analysis** and online help;
- expansion of the functionality by means of **add-on modules**, as well as open software architecture and powerful interfaces.

Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (2)

STEAG - **EBSILON® Professional**:

- parallel display of models in tabs;
- user-defined macros;
- tools for selecting, zooming as well as manipulating components like resize, rotate, mirror;
- customizable display and design of components;
- user-defined keyboard shortcuts;
- graphical elements for improving the clear arrangement of the model.



Build topology → Schematic ready to use in publications.

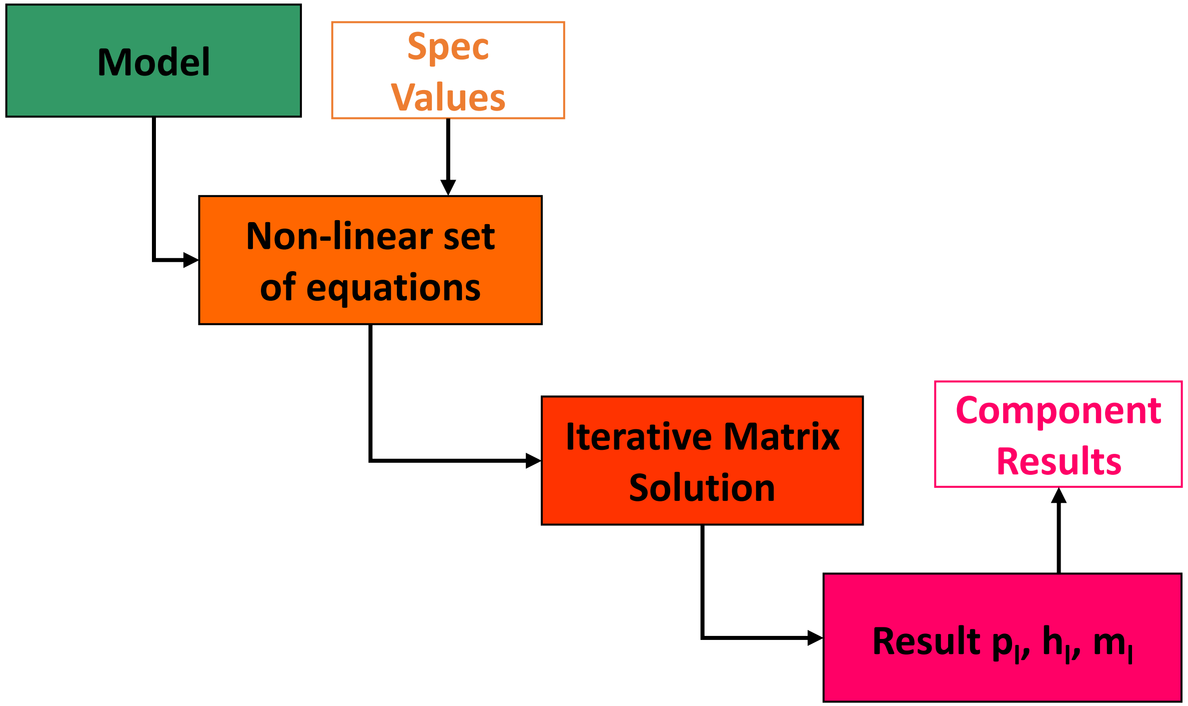
EBSILON® Professional (3)

Powerful calculation kernel and solution algorithm:

- detailed simulation of complex applications;
- exceptional speed and convergence reliability of the algorithm:
  - calculate a model with 1,100 components and 1,400 lines in only 2.5 seconds;
- possibility of transient calculations:
  - useful for heat storage technologies;
- **convergence analysis tools**:
  - convergence and controller diagrams.

Variables: p_l, h_l, m_l on all lines

Equations: components define the relations $f_k = (p_l, h_l, m_l)$ between the lines depending on spec values



Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (3)

Comprehensive component library

Physical components
- turbines
- steam generators
- heat exchangers
- cooling towers
- filters
- etc.

Logic components
- controllers
- signal transformers
- calculation modules
- efficiency meters
- etc.

User-defined components
- kernel scripting
- DLL-programmable component

All of the components in ONE library (with application examples).

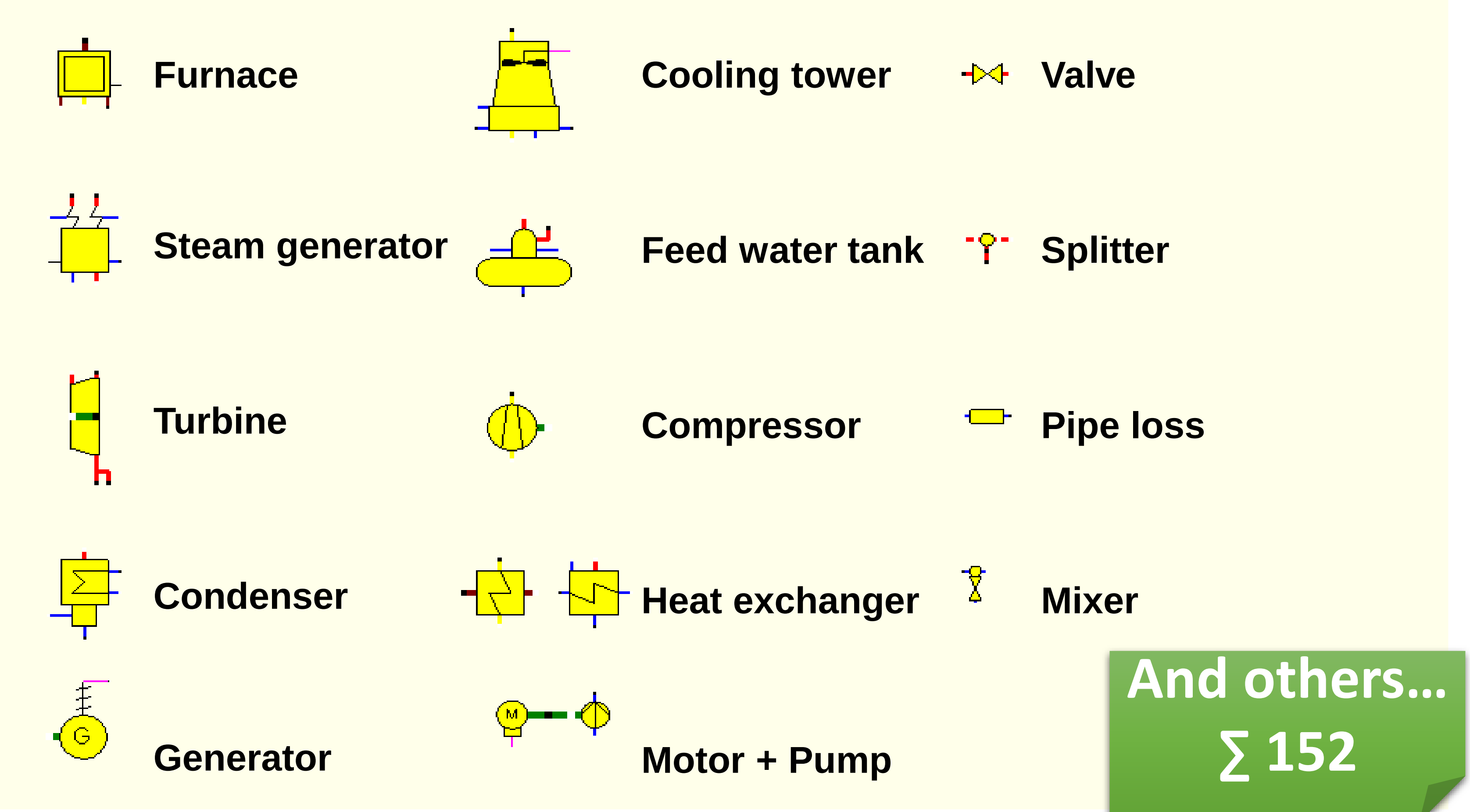
Availability of components depending on add-on modules (without add-on modules – **around 120 components**).

Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (4)

In addition to the physical components (pumps, turbines, heat exchangers…), Ebsilon also possesses numerous **logic elements**. The most important ones are:

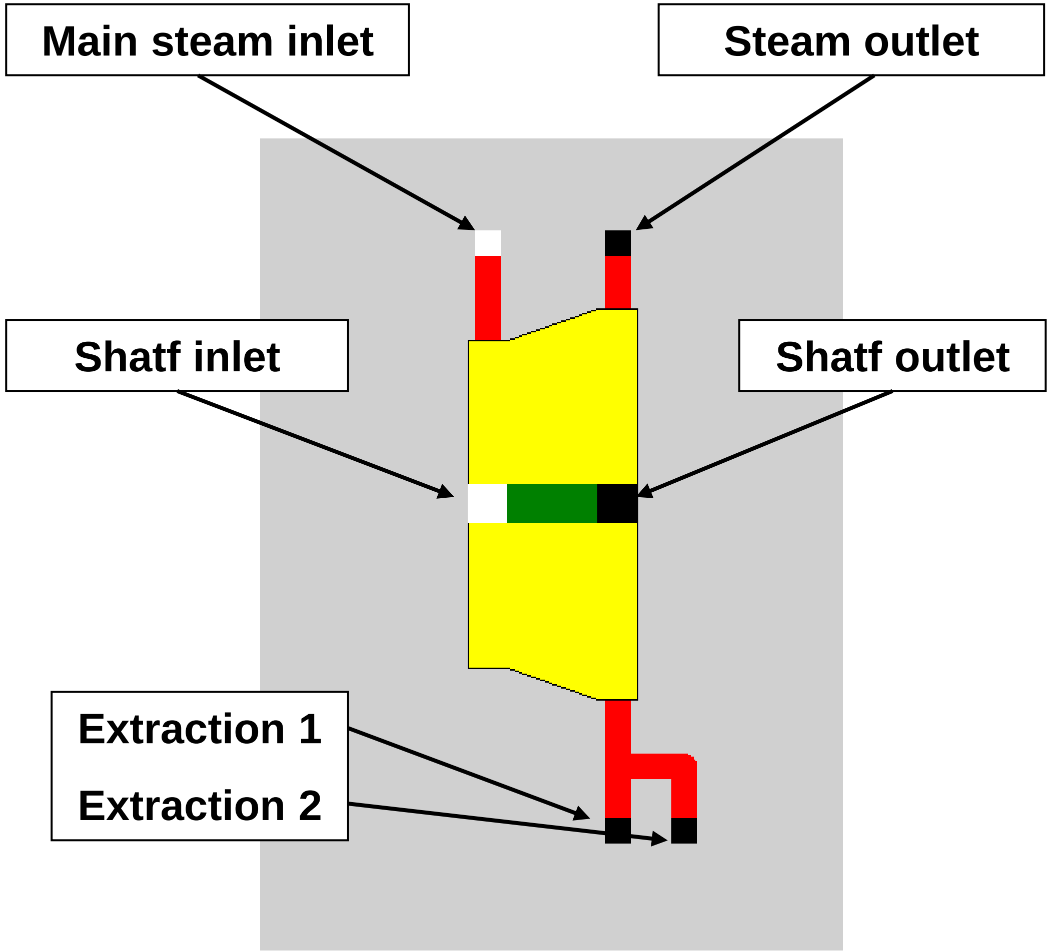
- **controllers (Components 12, 39, and 69),**
- signal transmitter (Component 36),
- calculation modules (Component 77),
- **display of values (Component 45).**



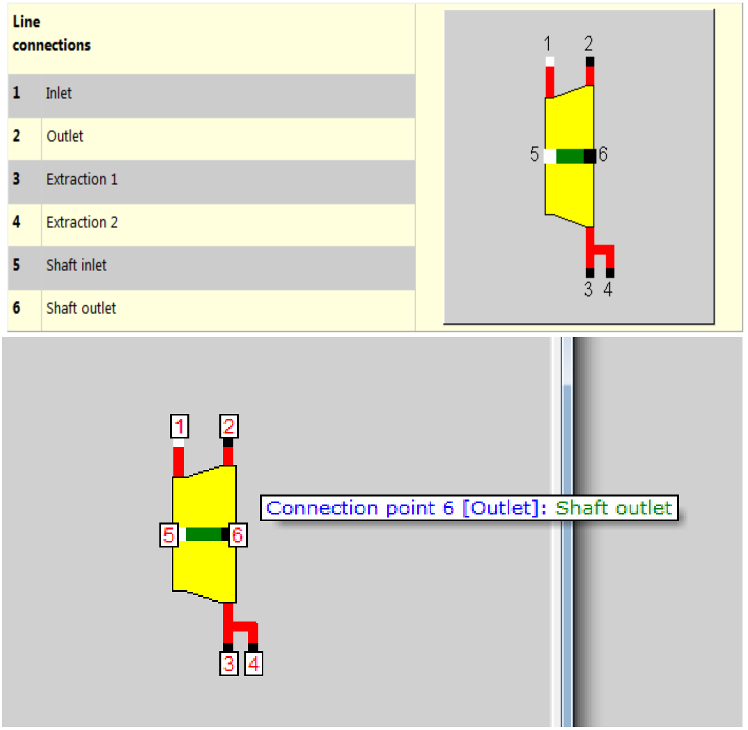
And others…
∑ 152

Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (5)



Component 6:
Steam turbine / General expander

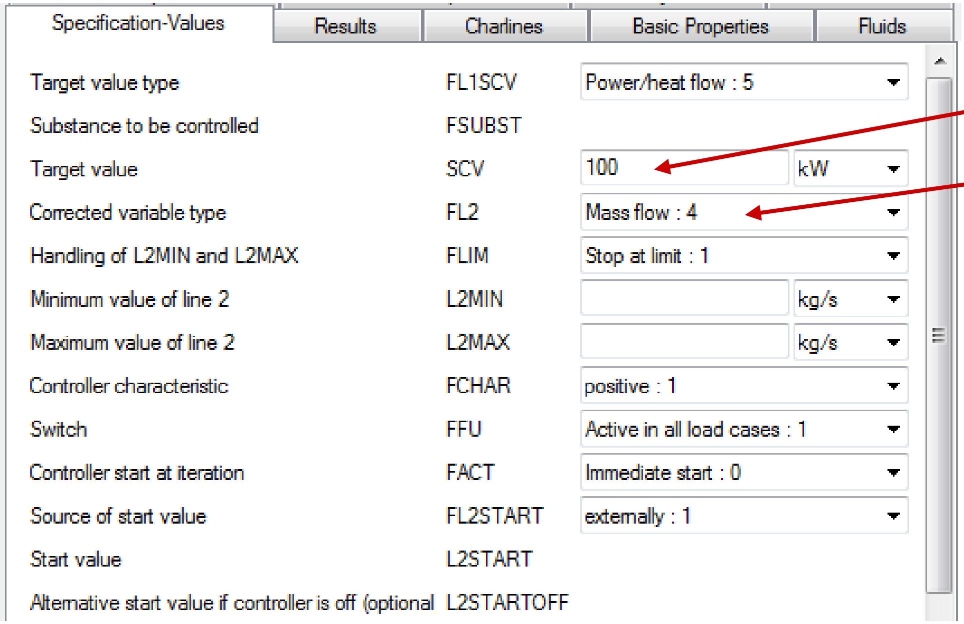


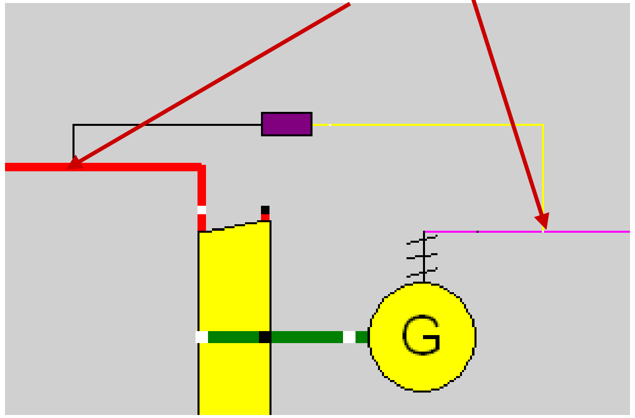
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (6)

A controller changes a specification value in order to achieve a certain result value.

Actual value is compared to setpoint value. Actuating variable is adjusted.





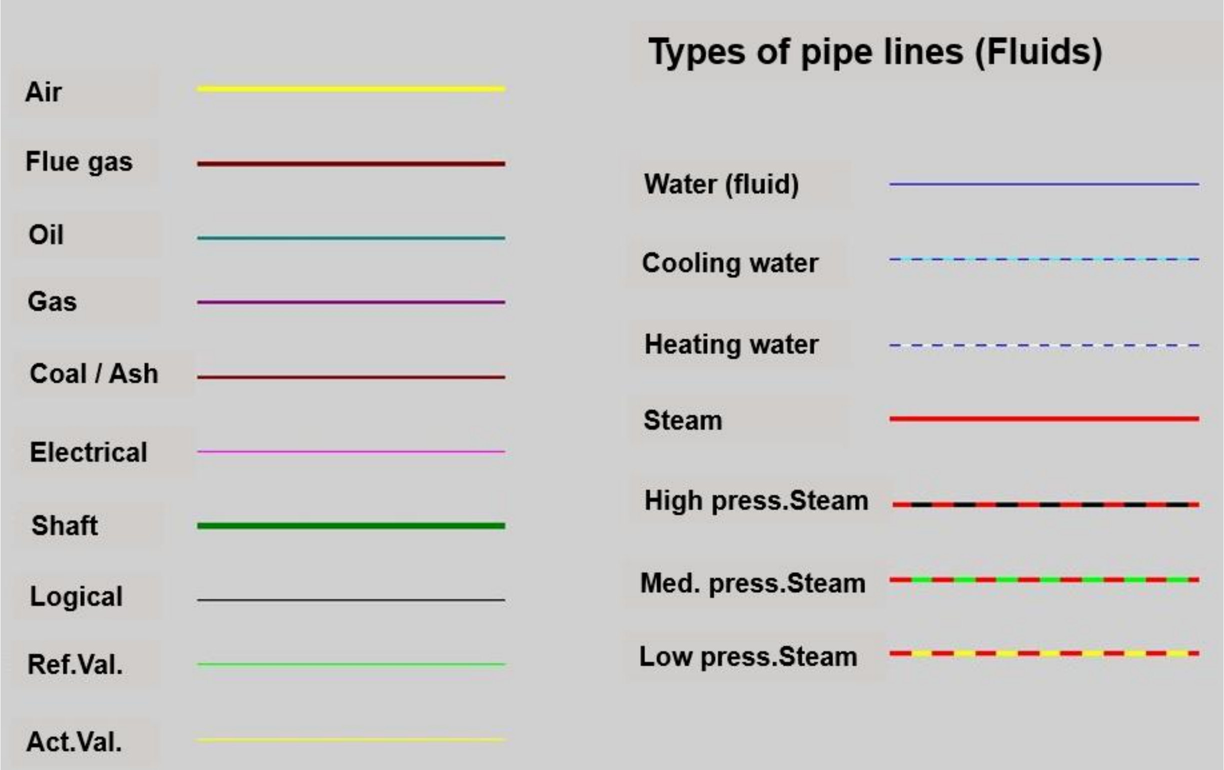
EBSILON® Professional (7)

Fluids:
- water and steam
- brine
- humid air
- salt water
- REFPROP library (NIST): 90 fluids from acetone to xenon
- thermal oils and molten salts
- binary mixes: ammonia / water, water / lithium bromide
- ideal and real gases
- two-phase fluids
- **user-defined fluids**

Fuels:
- coal
- oil
- gas
- **user-defined by composition**

Connections:
- logical
- reference values
- actual values
- etc.

Material data libraries for working fluids and fuels



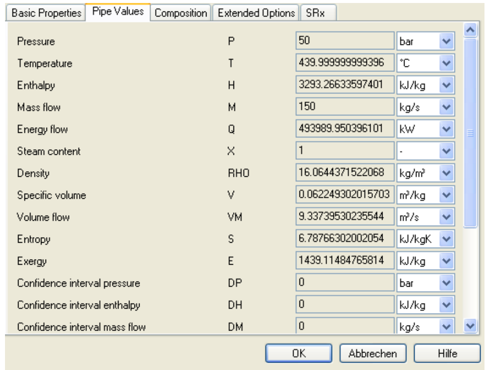
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

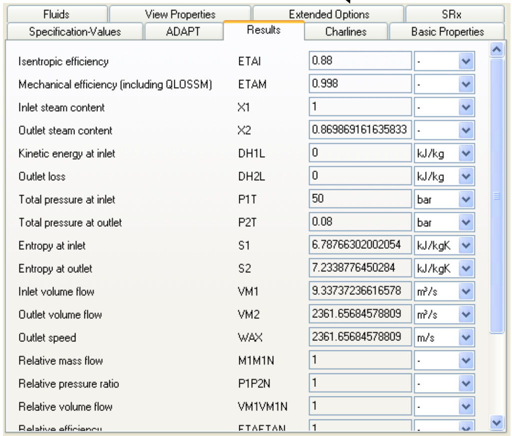
EBSILON® Professional (8)

Comfortable analysis and presentation of results:

- **value crosses, text and alarm fields in the model**;
- simulation reports in MS Excel.
- **State diagrams: Q-T, h-s, h-xi, T-s, log(p)-h**;
- convergence and controller diagrams.
- user defined diagrams in MS Excel.

After the simulation you‘ll find the results in the pipes and the components properties menu.





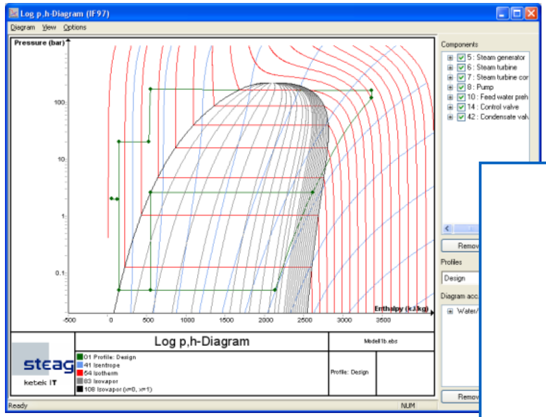
And more:

- export to MS Excel allows to further process the simulation results easily,
- customizable component display and structure.

Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (7)

Diagrams



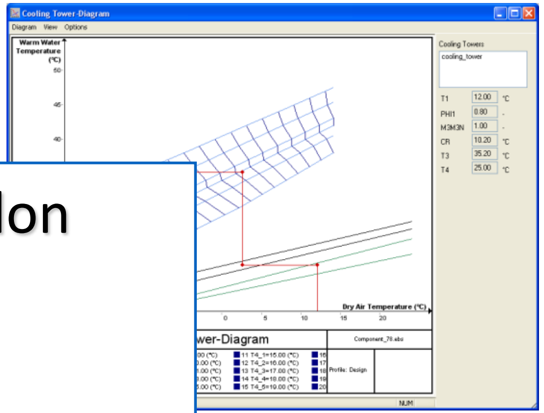
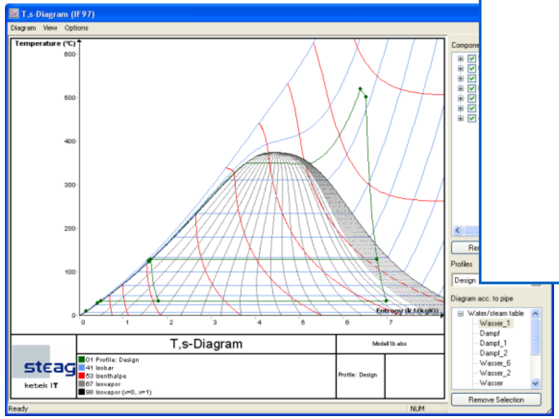
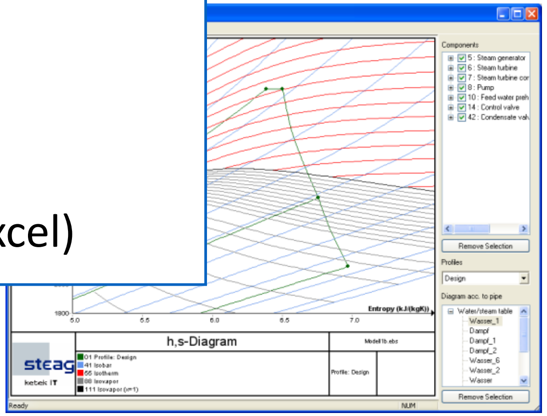


Diagram types in Ebsilon

H,s-diagrams
T,s-diagrams
log p,H-diagrams
Q,T-diagrams
Cooling tower diagram
General X,Y-diagram (via Excel)

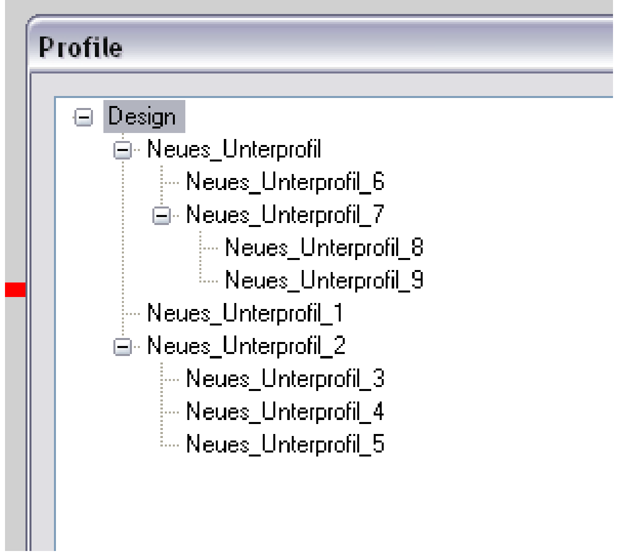




Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (8)

Powerful calculation kernel and solution algorithm:



Design mode („Full load“)

- Design equations are used.
- These equations are based exclusively on „black“ values (e.g. terminal temperature differences).
- Characteristic lines and adaptational polynomials are not used.
- As a result of the design calculation, the „blue“ partload reference values are calculated (e.g. KAN).

Off-design mode („Part load“)

- Off-design equations are used.
- These equations are based on some black and all blue values.
- Usage of characteristic lines and adaptational polynomials and physical models.
- It is helpful to create subprofiles for off-design calculations.

Identification mode (only component specific)

- Outlet values are not calculated via the physics of the component but are specified by a measurement point or a start value.
- The characteristic quantity for the component is calculated (e.g. KA, ETAI).
- Implemented for usage in off-design, but also available in design (beware: as „black“ values are not overwritten it has to be done manually or by EbsScript).

EBSILON® Professional (9)

Powerful calculation kernel and solution algorithm:

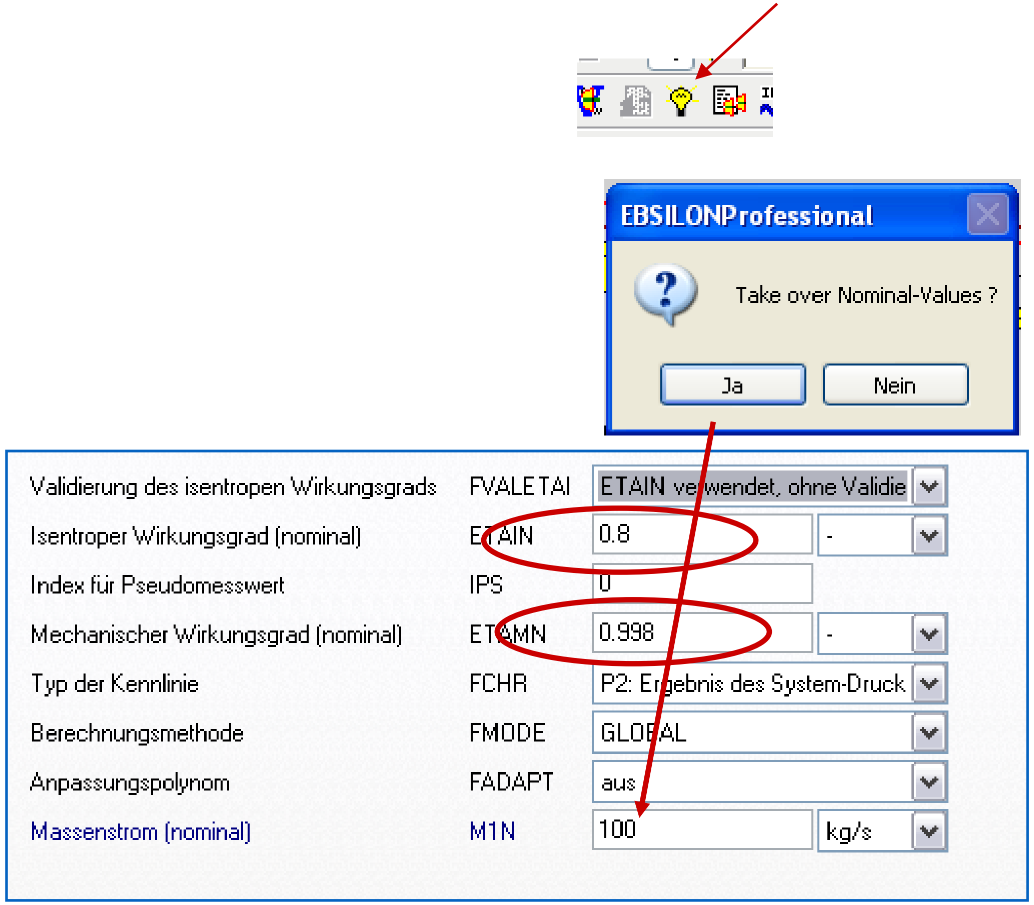
Design mode („Full load“)

- Design equations are used.
- These equations are based exclusively on „black“ values (e.g. terminal temperature differences).
- Characteristic lines and adaptational polynomials are not used.
- As a result of the design calculation, the „blue“ partload reference values are calculated (e.g. KAN).

Off-Design mode („Part load“)

- On the basis of physical equations.
- By way of characteristic lines.
- By way of user-defined polynomials.
- Always based on the nominal values! (“Blue values“).

Design/Off-Design flag



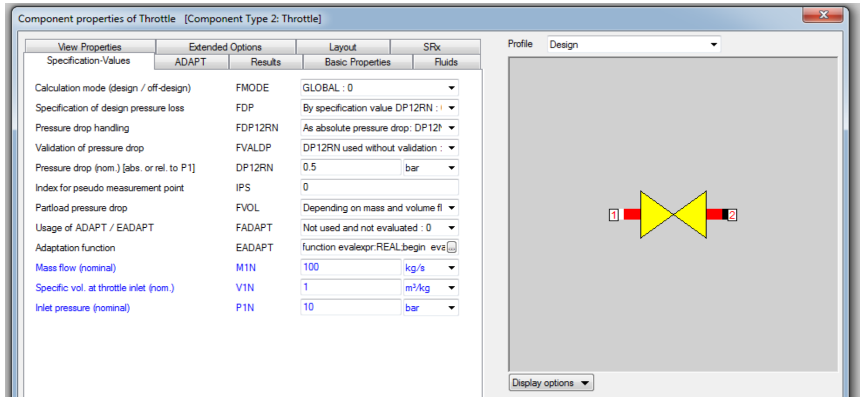
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (10)

Off-design calculation on the basis of physical equations, example: throttle valve (component 2):

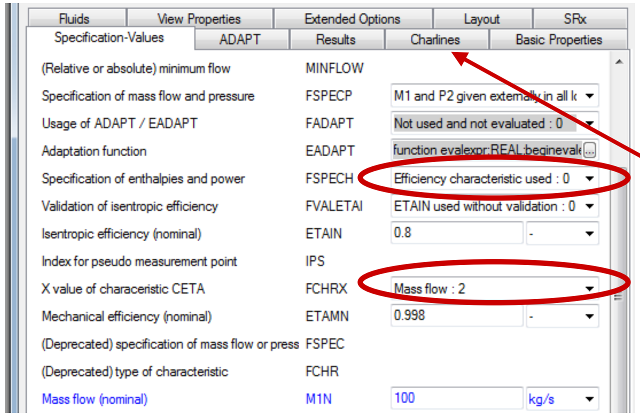
1. In design: DP constantly equals DP12RN (design case).
2. Calculation of M1N and V1N in design.
3. In Off-Design:

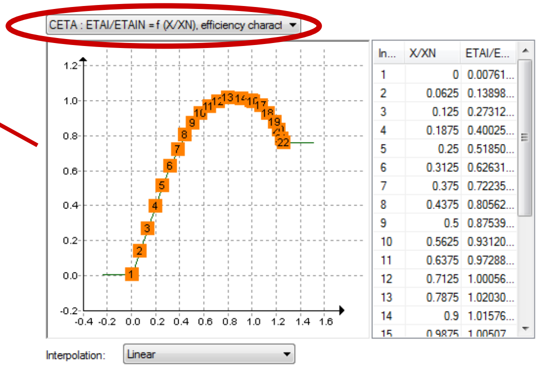
$$DP12 = DP12N \cdot \left(\frac{M1}{M1N}\right)^2 \cdot \frac{V1}{V1N}$$



Off-design calculation on the basis of characteristic lines, example: pump (component 8):

1. In design: ETAI constantly equals ETAIN (design case).
2. Calculation of M1N.
3. In off-design: ETAI calculated from characteristic line, normalized to design condition.

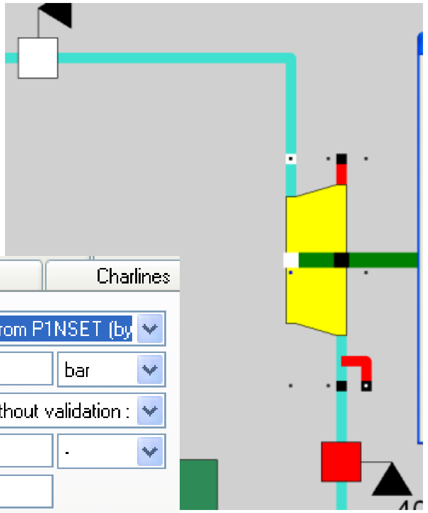




Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (11)

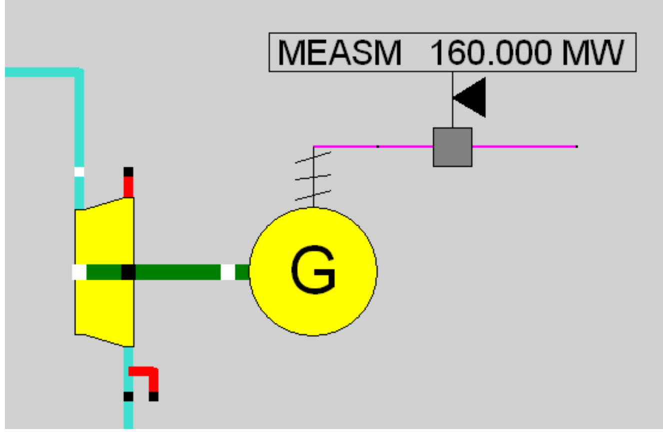
Design / Off design



Specification-Values | Adaptation-Polynomial | Results | Charlines

Inlet pressure handling	FP1N	P1 calculeted from P1NSET (by	
Inlet pressure (nominal)	P1NSET	120	bar
Validation of isentropic efficiency	FVALETAI	ETAIN used without validation :	
Isentropic efficiency (nominal)	ETAIN	0.88	-
Index for pseudo measurement point	IPS	0	
Mechanical efficiency (nominal)	ETAMN	0.998	-
Mechanical loss (constant fraction)	QLOSSM	0	kW
Kinetic energy at inlet	DH1LN	0	kJ/kg
Enthalpy loss at outlet (nominal)	DH2LN	0	kJ/kg
Power flow	FQ	On HP-side with shaft inlet : 0	
Efficiency formalism	FSPEC	Ebsilon standard (CKIN1 and CK	
Type of characteristic	FCHR	ETAI/ETAIN=f(M1/M1N) : 0	
Calculation mode (design / off-design)	FMODE	GLOBAL : 0	

Identification mode



Type of characteristic	FCHR	Power specification : -1
Type of characteristic	FCHR	H2 given : -2

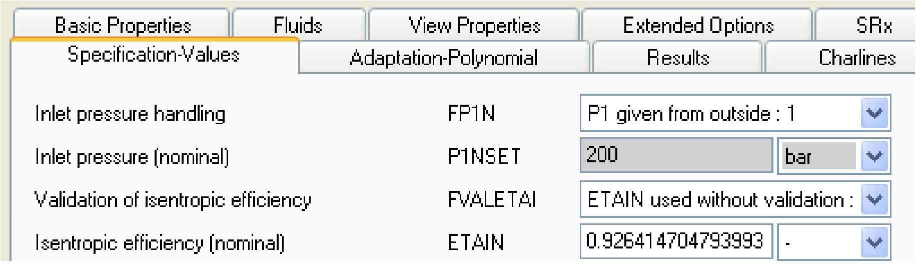
Specification-Values | Adaptation-Polynomial | Results | Charlines

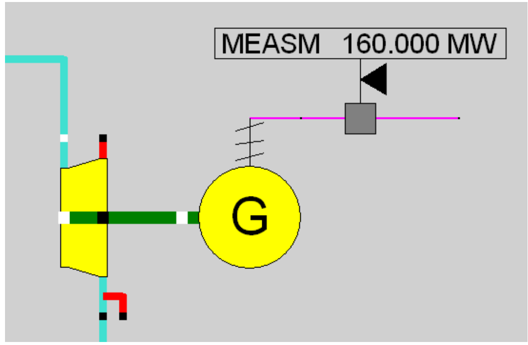
Isentropic efficiency	ETAI	0.871764373909822	-

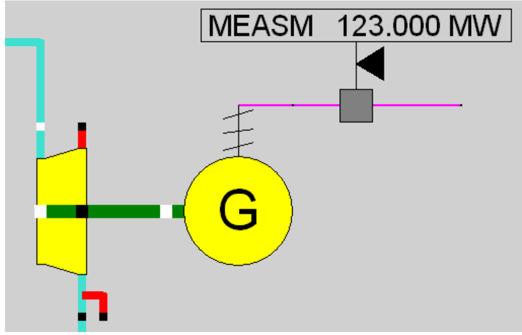
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (11)

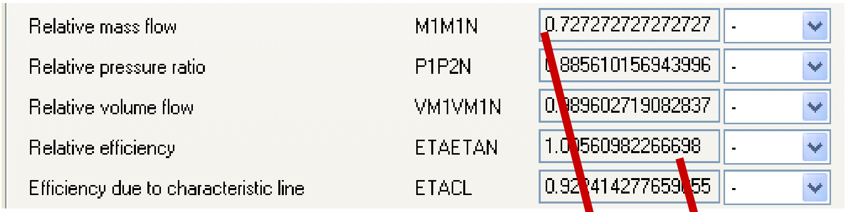
Identification mode

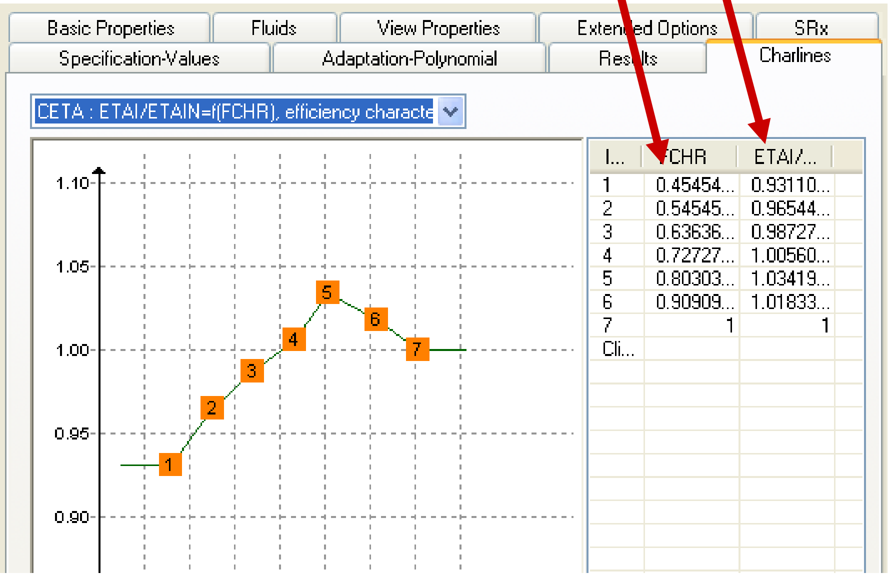






ETAI/ETAIN=f(M1/M1N)





Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (12)

Expansion of the functionality by means of add-on modules:

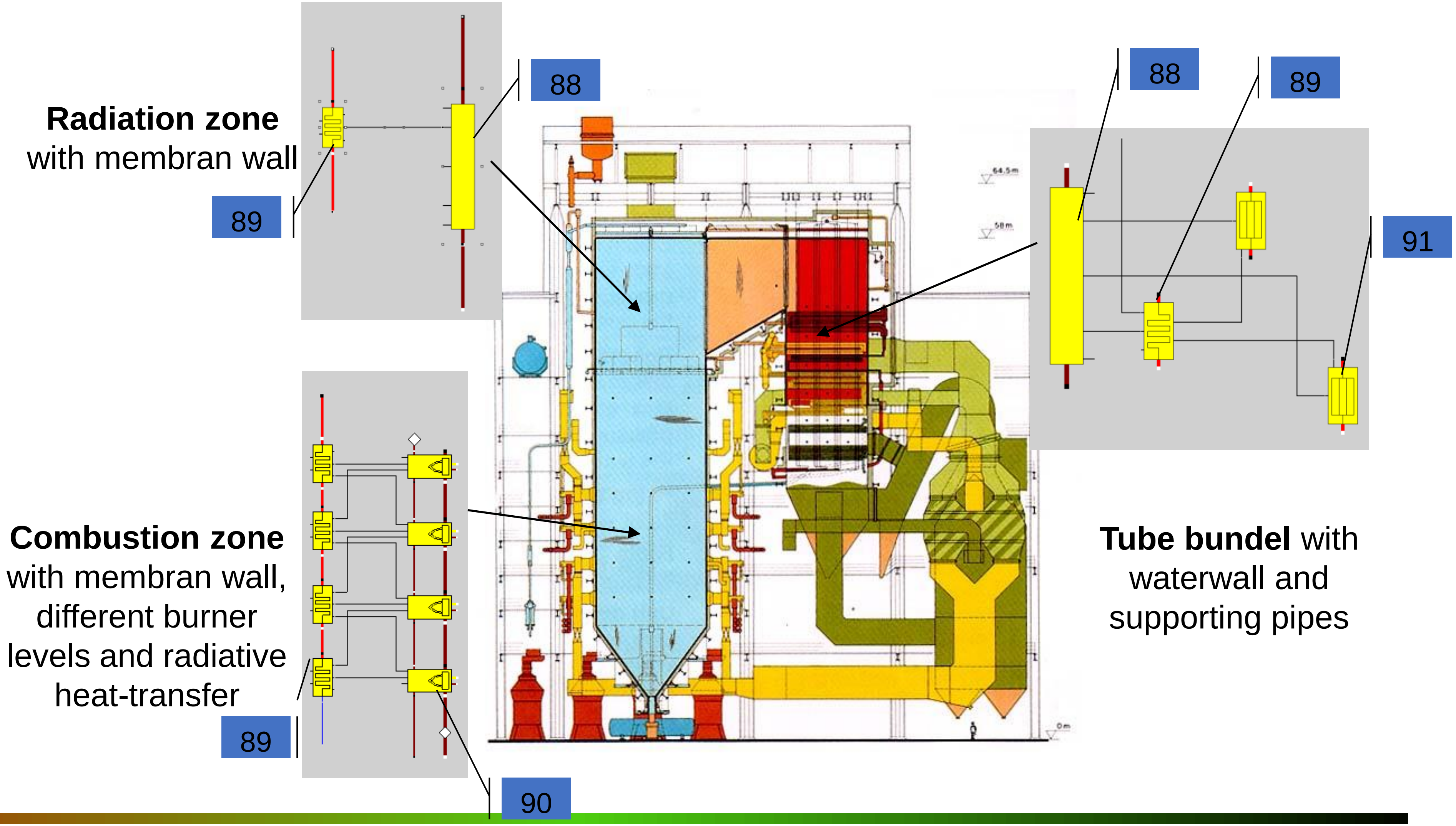
- **EbsBoiler** - components for detailed mapping of the boiler geometry.
- **EbsSolar** - components for detailed mapping of solar fields.
- **OEM-GTLib** - gas turbine library based on manufacturer data.
- **EbsOptimize** - integrated optimizer on the basis of a genetic algorithm.
- **EbsValidate** - data validation according to VDI 2048.
- **EbsHTML** - output of EBSILON® Professional circuits in HTML format.
- **EbsScript** - PASCAL-based script language for EBSILON® Professional.
- **EbsOpen** - integration of EBSILON® Professional into user-specific applications.

Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (12)

Expansion of the functionality by means of add-on modules:

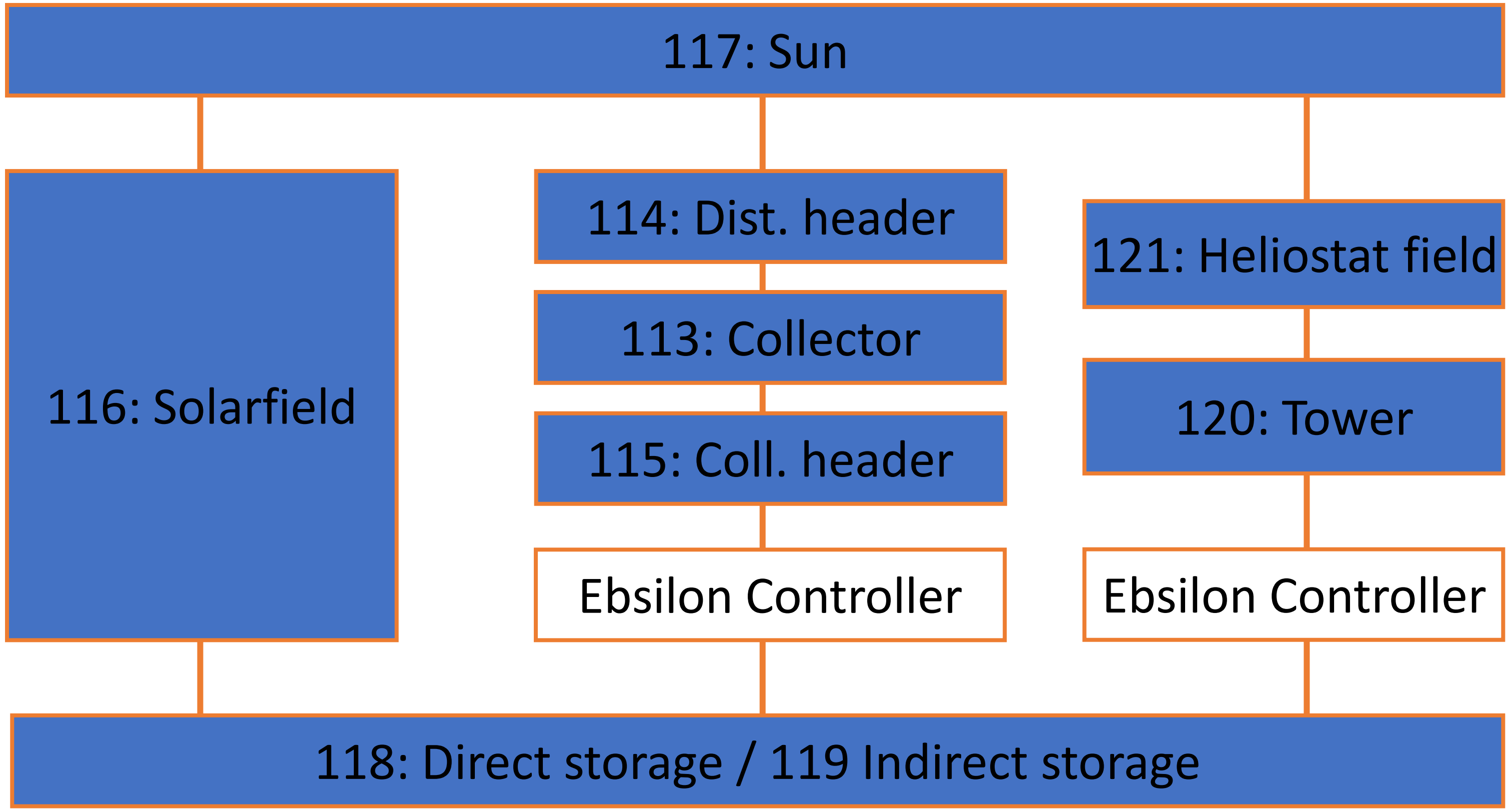
- **EbsBoiler** - components for detailed mapping of the boiler geometry.



EBSILON® Professional (12)

- **EbsSolar** - components for detailed mapping of solar fields.

Includes components for the **detailed design of a solar field** and is suitable for site and technology comparisons as well as for **annual yield calculations** including thermal storage.



Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (13)

EbsOptimize automates the tedious search for maximum performance system parameters by optimizing target parameters with variation of multiple input parameters.

- Freely customizable target and input parameters.
- **Genetic algorithm**.
- Non-linear descent methods.

EbsValidate calculates the statistically most probable system condition by improving the **measuring values of redundant measuring stations** in such a way that all component equations are met and the error square sum of measuring values is minimized.

- Usage for acceptance inspections and to identify malfunctions in structural components and the measuring system.
- Integrated quick validation and validation according to **VDI 2048.**

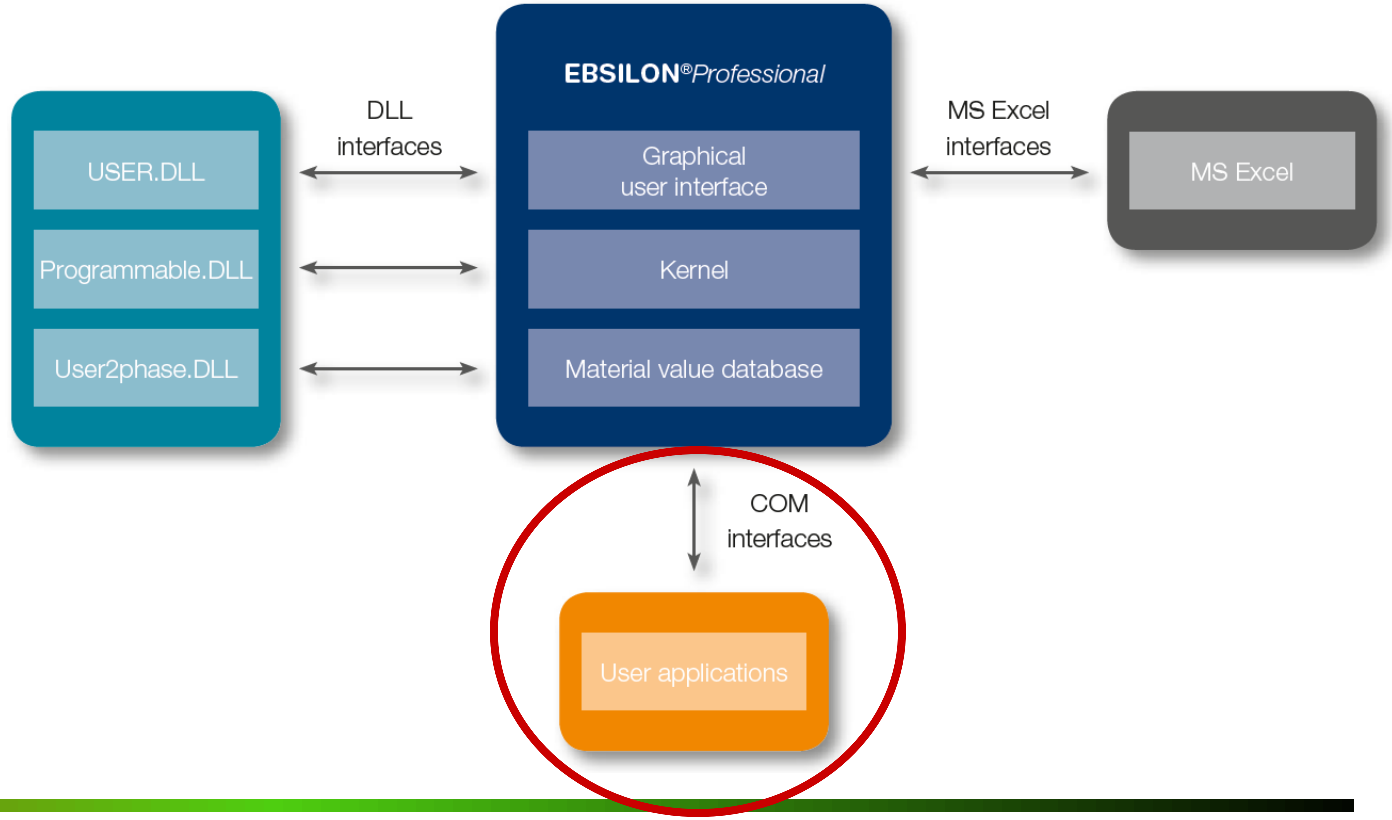
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (14)

Open software architecture and powerful interfaces (EbsScript & EbsOpen)

COM interface EbsOpen

EbsOpen can be integrated into all common automation and programming environments like e.g. Visual Studio .Net for direct programming with Visual Basic or C++ as well as the VBA environments of the MS Office products.



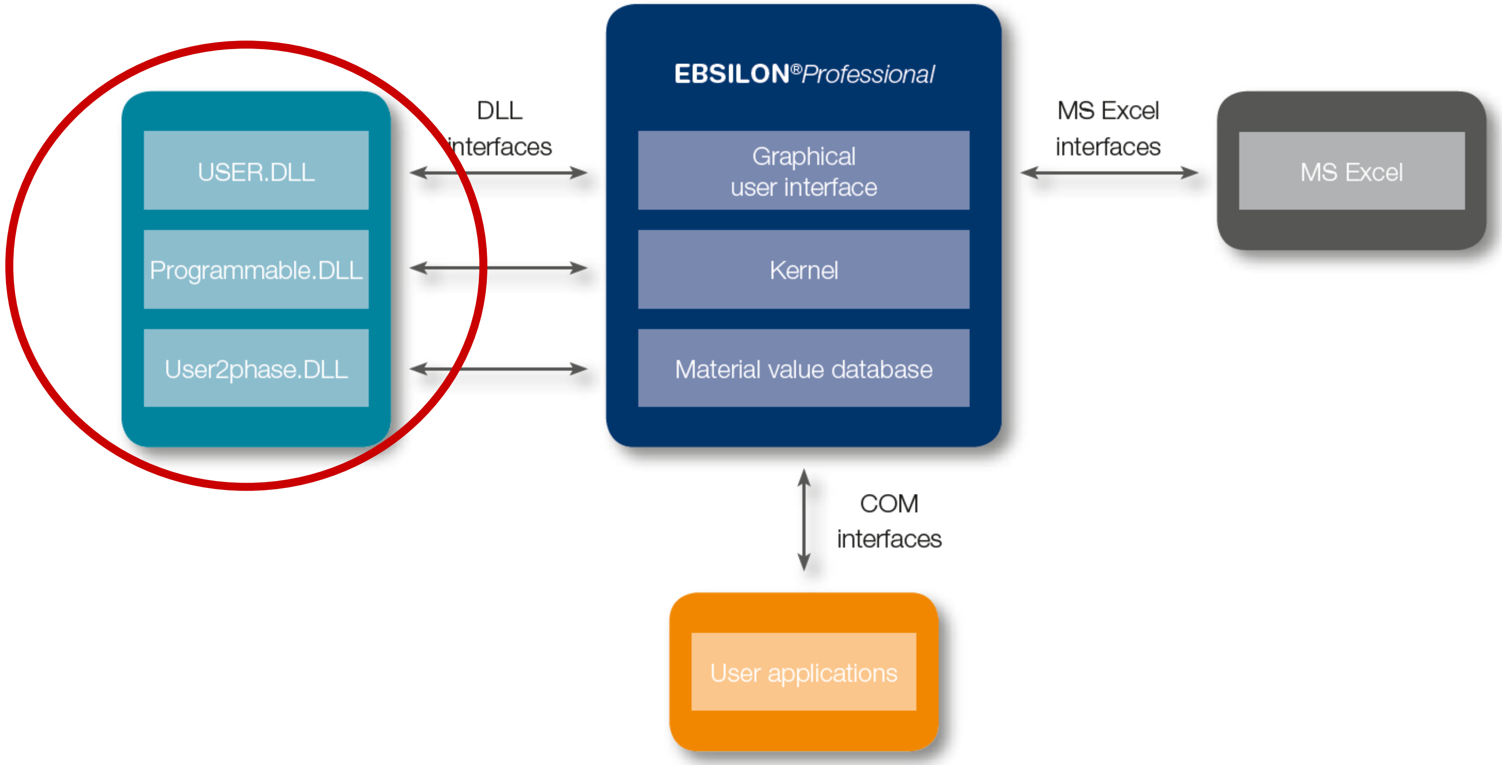
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (14)

Open software architecture and powerful interfaces (EbsScript & EbsOpen)

DLL interfaces

By means of Dynamic Link Libraries (DLL), data can be exchanged between other programs and EBSILON® *Professional*, and the calculation kernel can be expanded by individual components.



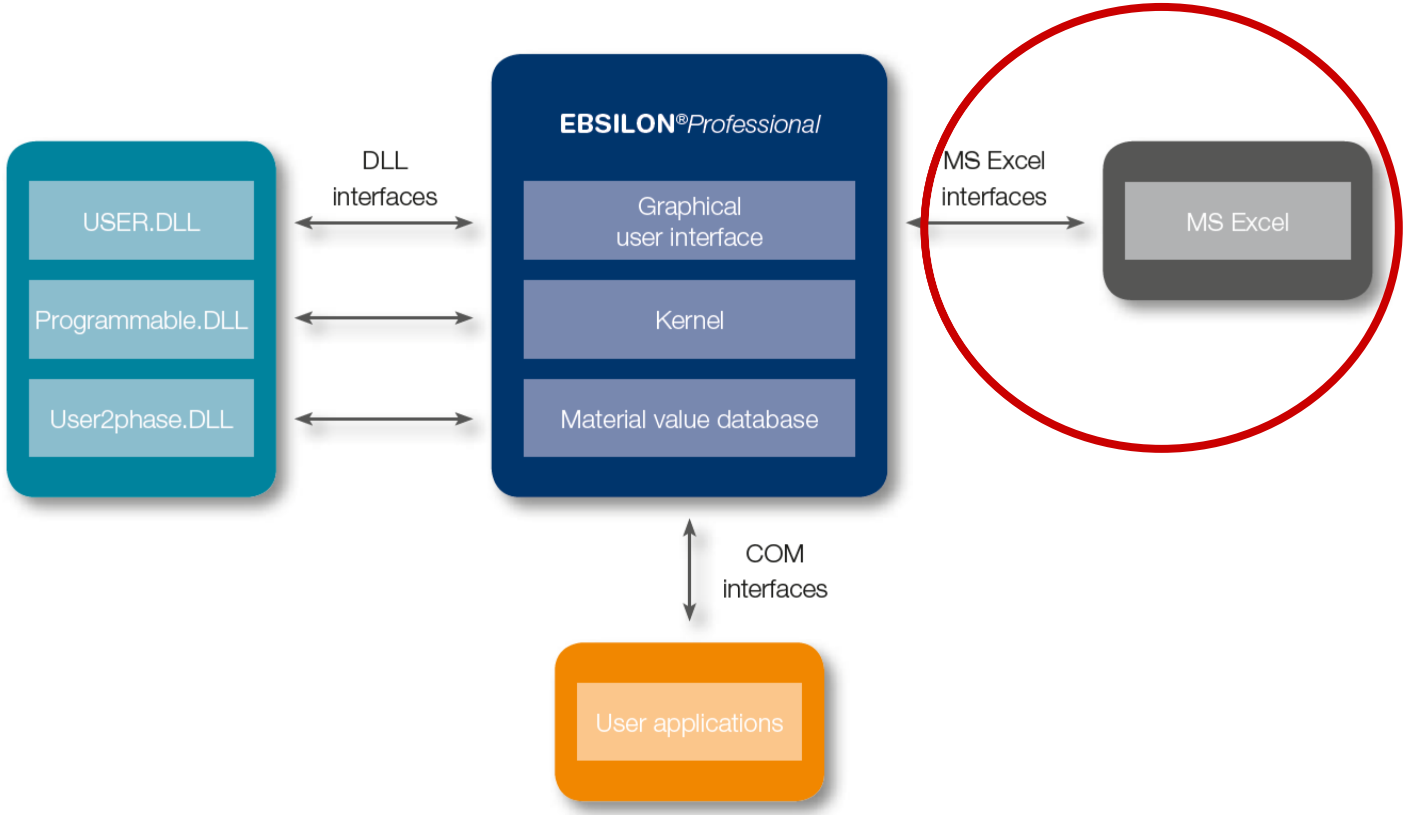
Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (14)

Open software architecture and powerful interfaces (EbsScript & EbsOpen)

MS Excel interfaces

Simulation results as well as parameters and characteristics of individual components and lines can be exported and imported. It is possible to run simulations directly from the Excel worksheet using the MS Excel add-in for EBSILON® *Professional*.



Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

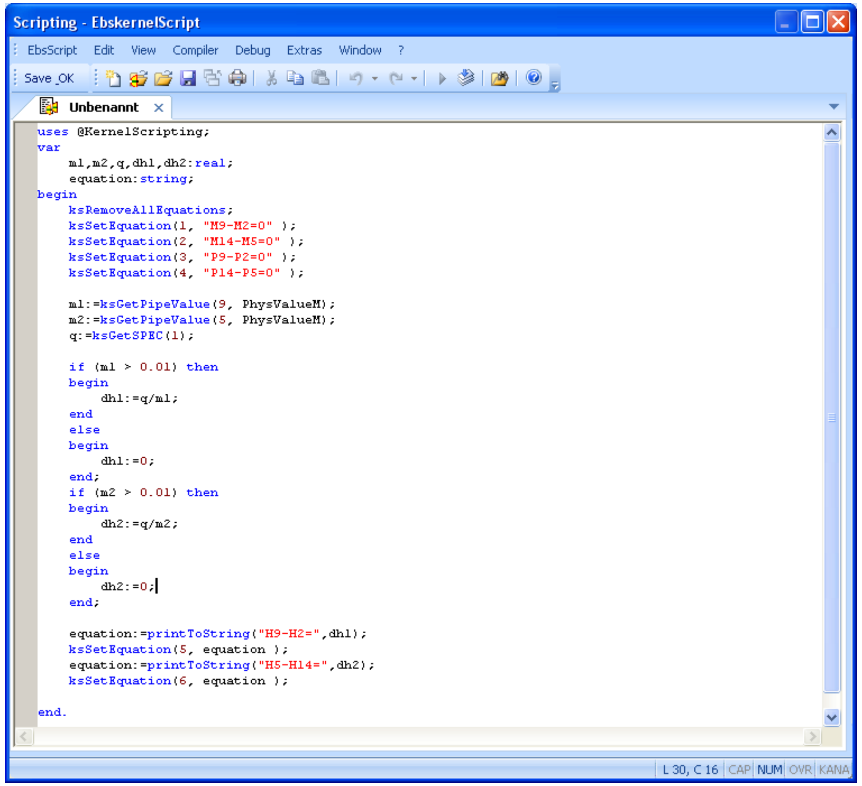
EBSILON® Professional (14)

Open software architecture and powerful interfaces (EbsScript & EbsOpen)

EbsScript – Script language for EBSILON® Professional

The fully integrated **PASCAL-based script language** allows programming of all processes and individual components within EBSILON®- Professional, with full access to all model data, external text, MS Excel files and all interfaces.

- User-friendly editor with browser-supported data entry.
- Compiler with syntax check.
- Integrated script administration.
- Console window for sequence control and output.
- **Programming options for user-specific components** (component: kernel scripting).
- Usage for automated processing of case studies, optimizations etc.

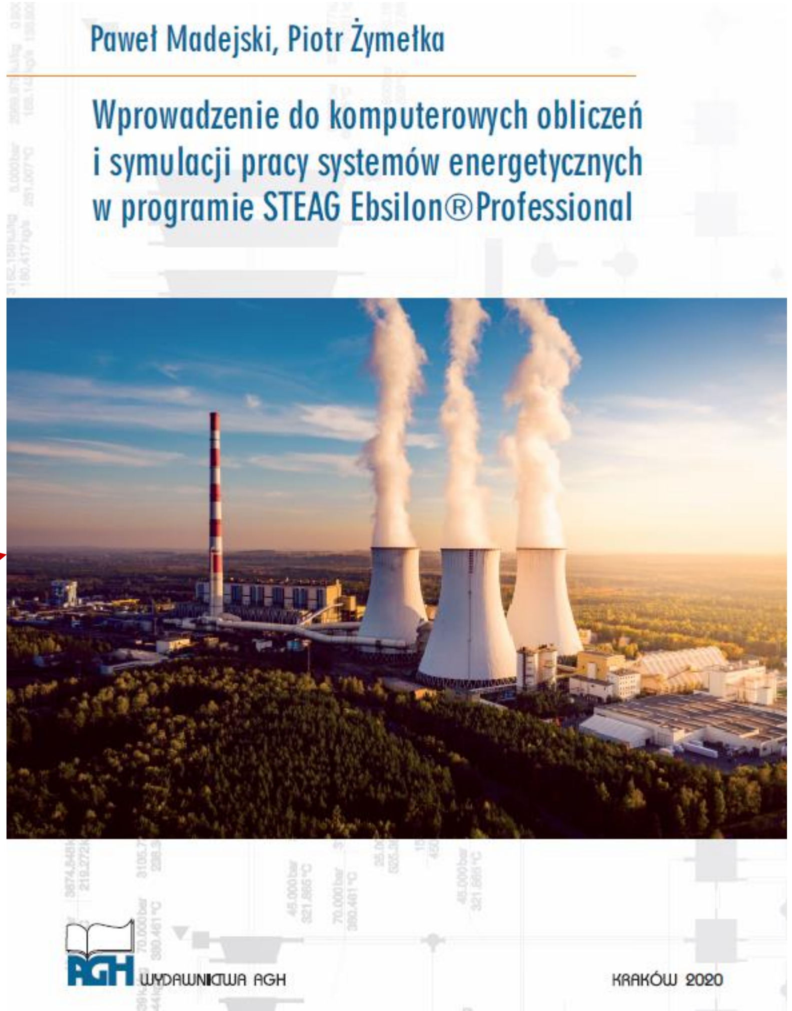


Source: Sergej Pulyaev: EBSILON®Professional. Training at AGH Krakow. Kraków, 15.09-17.09.2015, STEAG Energy Services

EBSILON® Professional (15)

Personal opinions and conclusions:

- straightforward flowsheet process modelling tool;
- great database of components (inlcuding the specific add-ons);
- suited for conventional power plants, renewable energy systems, diagnostic systems;
- easy and intuitive to setup the model, great for teaching activities;
- widely used in German power industry for maintaince control and optimisation.



IPSEpro (1)

SimTech GmbH - **IPSEpro**:

- software system for **calculating heat balances and simulating processes**;
- set of **software modules** for creating process models for a wide range of applications and for utilizing these models throughout the lifecycle of process plants;
- **quick process assessments**, **detailed engineering**, **design**, retrofitting, repowering, and acceptance testing;
- **component-level flexibility** and **component-by-component approach** allows to model virtually any type of system;
- **ready-to-use model libraries** are available, but can be adapted to specific needs through a unique level of flexibility by allowing to **create new component models** or create completely new model libraries.

Source: https://www.simtechnology.com/CMS/index.php/ipsepro

IPSEpro (2)

IPSEpro's modules are used to:

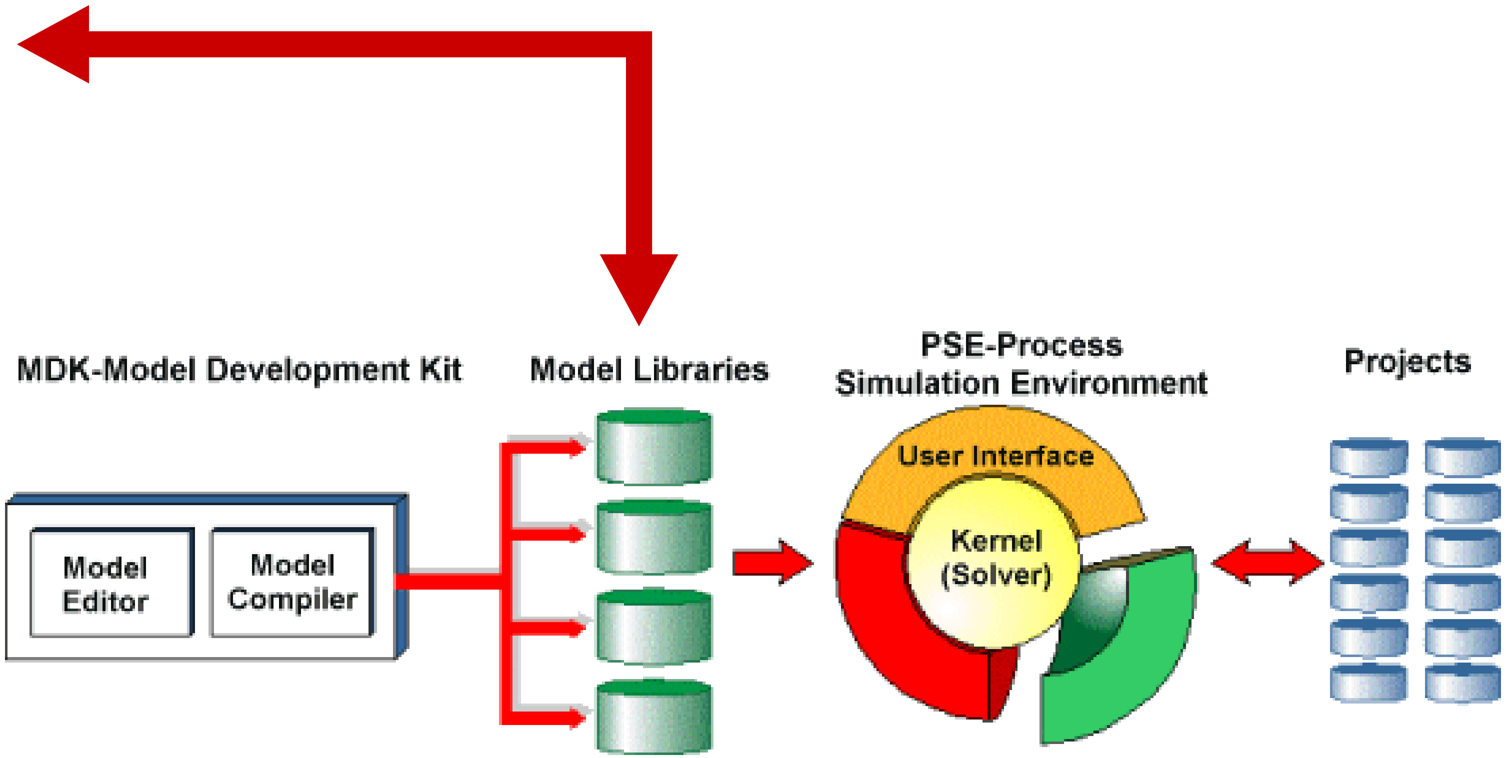
- calculate heat balances and predict design and off-design performance;
- verify and validate measurements during acceptance tests;
- monitor and optimize plant performance on-line;
- plan modifications and upgrades of existing plants.

Source: https://www.simtechnology.com/CMS/index.php/ipsepro

IPSEpro (3)

Ready-to-use solutions are available for a wide range of applications:

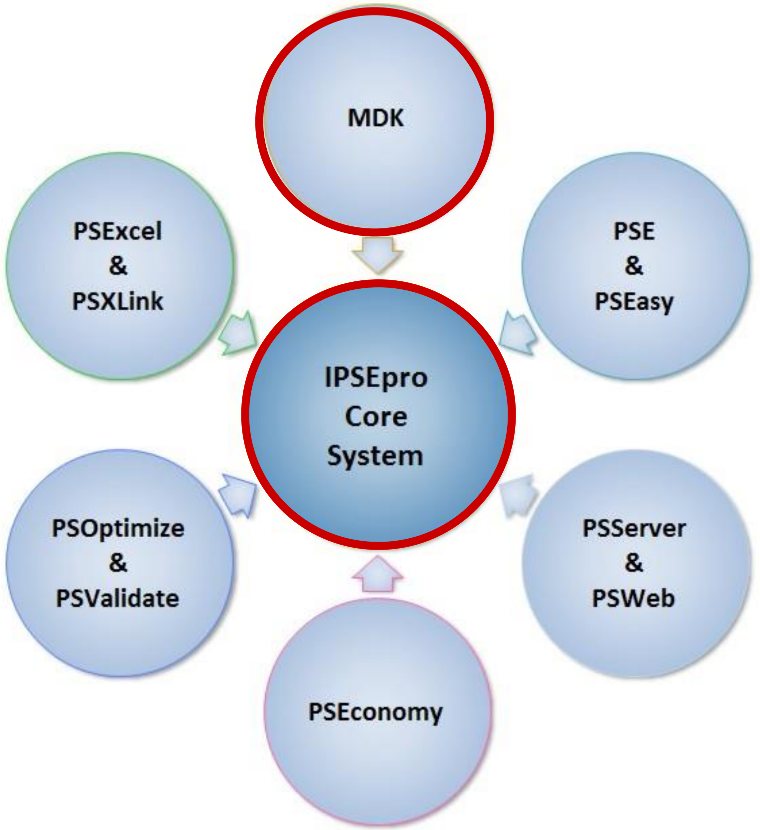
- thermal power;
- geothermal energy;
- concentrating solar power;
- desalination;
- refrigeration;
- flue gas cleaning;
- biomass gasification.



IPSEpro (4)

IPSEpro's modules are used to:

- calculate heat balances and predict design and off-design performance (**Design Suite Configurations**);
- estimate costs during conceptual design (Design Suite Configuration with **PSEconomy**);
- verify and validate measurements during acceptance tests (**Design Suite Configuration** with **PSValidate**);
- integrate PSE projects with Microsoft Excel worksheets (**Design Suite Configuration** with **PSXLink**);
- define and build new component models and to translate them into a form that can be used by IPSEpro's Process Simulation Environment (**Design Suite Configuration** with **MDK**);
- monitor and optimize plant performance on-line (**Plant Operation Suite** with **PSOptimize**);
- plan modifications and repowering of existing plants (**Design Suite Configurations**).



Source: https://www.simtechnology.com/CMS/index.php/ipsepro

IPSEpro (5)

APP_Lib: Advanced Power Plant Library

Advanced Power Plant Library for modeling of a wide range of thermal power systems

GT_Lib: Gas Turbines Library

Commercial gas turbines library

Desal_Lib: Desalination Process Library

Desalination plant modeling, supports all major desalination technologies

Frigo_Lib: Refrigeration Process Library

Compression and absorption refrigeration and heat pump process modeling

LTP_Lib: Low Temperature Process Library

Organic Rankine Cycles (ORC) and Kalina Cycles

CSP_Lib: Concentrating Solar Power Library

Concentrating solar power process modeling

FGC_Lib: Flue Gas Cleaning Library

Modeling of flue gas cleaning systems

PGP_Lib: Pyrolysis and Gasification Process Library

Library for modeling biomass gasification systems

+ Third Party Model Libraries:

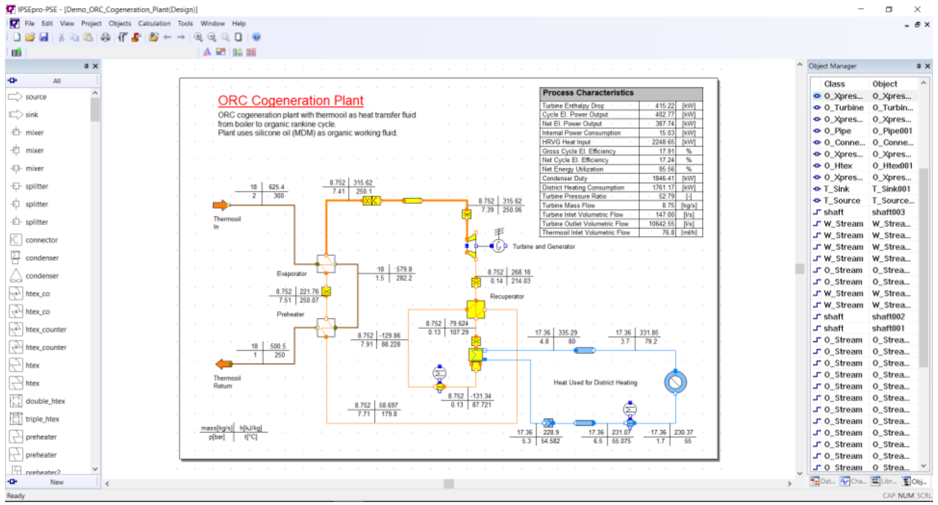
- EPP_S_Lib (for advanced, detailed modelling of biomass, coal and other solid-fuel technologies);
- EPP_B_Lib (for geothermal systems);
- EPP_IGCC_Lib (for IGCC systems).

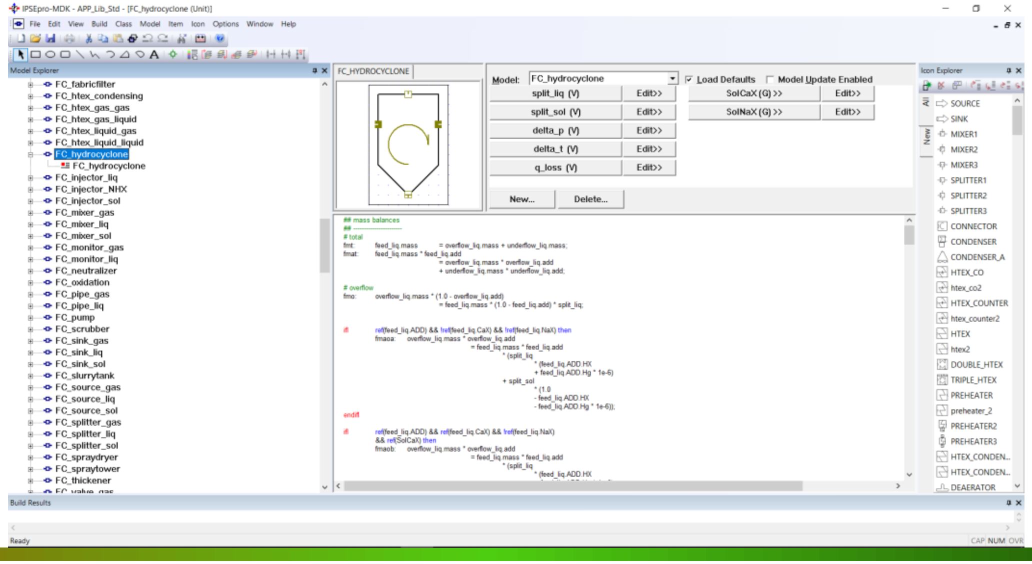
Source: https://www.simtechnology.com/CMS/index.php/ipsepro

IPSEpro (6)

Hands-on presentation:

- Process Simulation Environment
- Model Development Kit





IPSEpro (7)

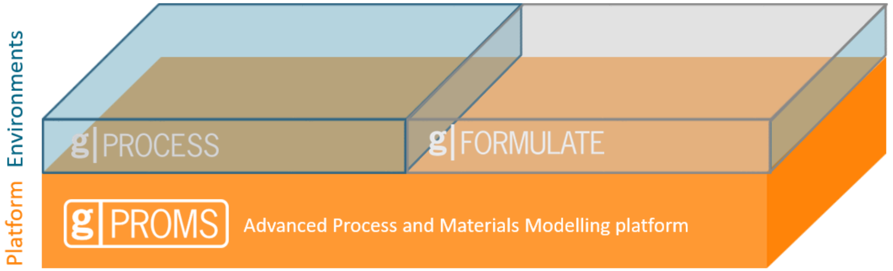
Personal opinions and conclusions:

- straightforward flowsheet process modelling tool;
- great **database of components** (including the specific libraries) that are **open to adapt and modify**;
- fairly easy programming language for own models development and making them flowsheet ready;
- suited for conventional power plants and renewable energy systems;
- easy and intuitive to setup the model and develop own models;
- **great for teaching activities**;
- **upcoming online platform**.

gPROMS (1)

Siemens Process Systems Engineering - **gPROMS**:

- advanced **process modelling platform** is the powerful equation-oriented modelling and optimization framework;
- a **single software platform** that provides all core capabilities **for digital process design and operations applications**, from formulation and R&D through **engineering design** and manufacture to product performance, for **diverse process industry sectors**;
- a feature-rich, next-generation **equation-oriented modelling** and solution environment that brings many major advantages over traditional process simulation software.



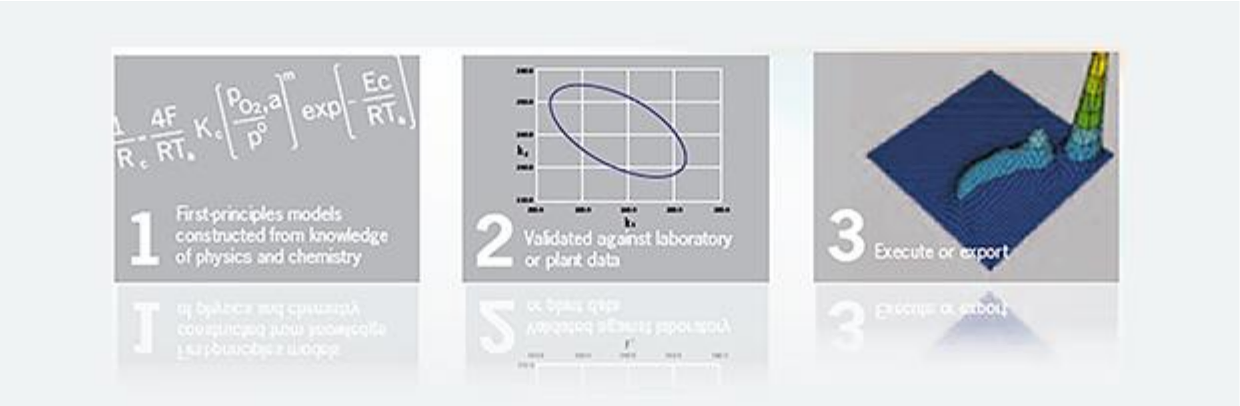
Source: https://www.psenterprise.com/products/gproms

gPROMS (2)

Siemens Process Systems Engineering – **gPROMS Process**:

- next-generation Advanced Process Modelling environment **for design and operation of high-performance process plants**;
- combines industry-leading **steady-state and dynamic models** with all the power of the **gPROMS equation-oriented modelling**, analysis and optimization platform in an easy-to-use **process flowsheeting environment**;
- gPROMS Process can:
  - **model;**
  - **analyse;**
  - **validate;**
  - **optimize.**

Advanced process modelling is a combination of three elements:



Source: https://www.psenterprise.com/products/gproms

gPROMS (3)
pPROMS Process

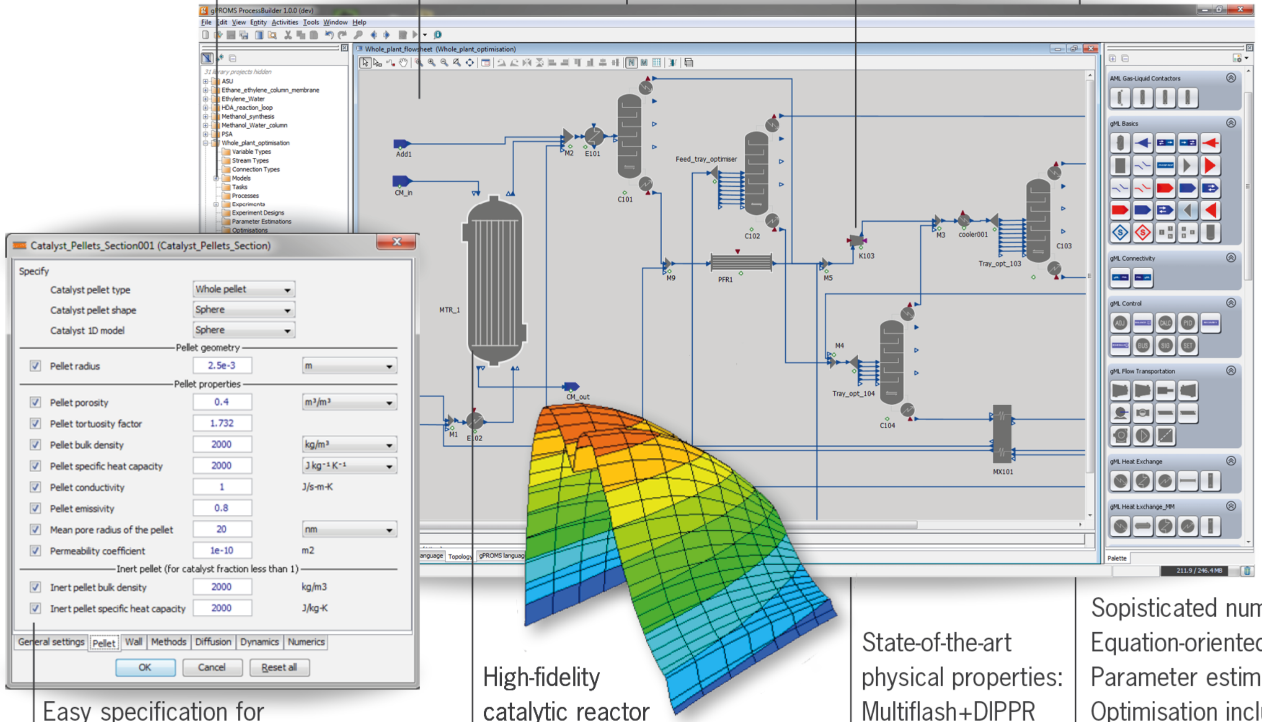
Project tree
for easy control

Graphical
drag & drop
flowsheeting

Steady-state
and dynamic
models

Easy custom
modelling
– add own
libraries

Library models:
gPROMS Model Library
Advanced Model Libraries



Easy specification for
complex units

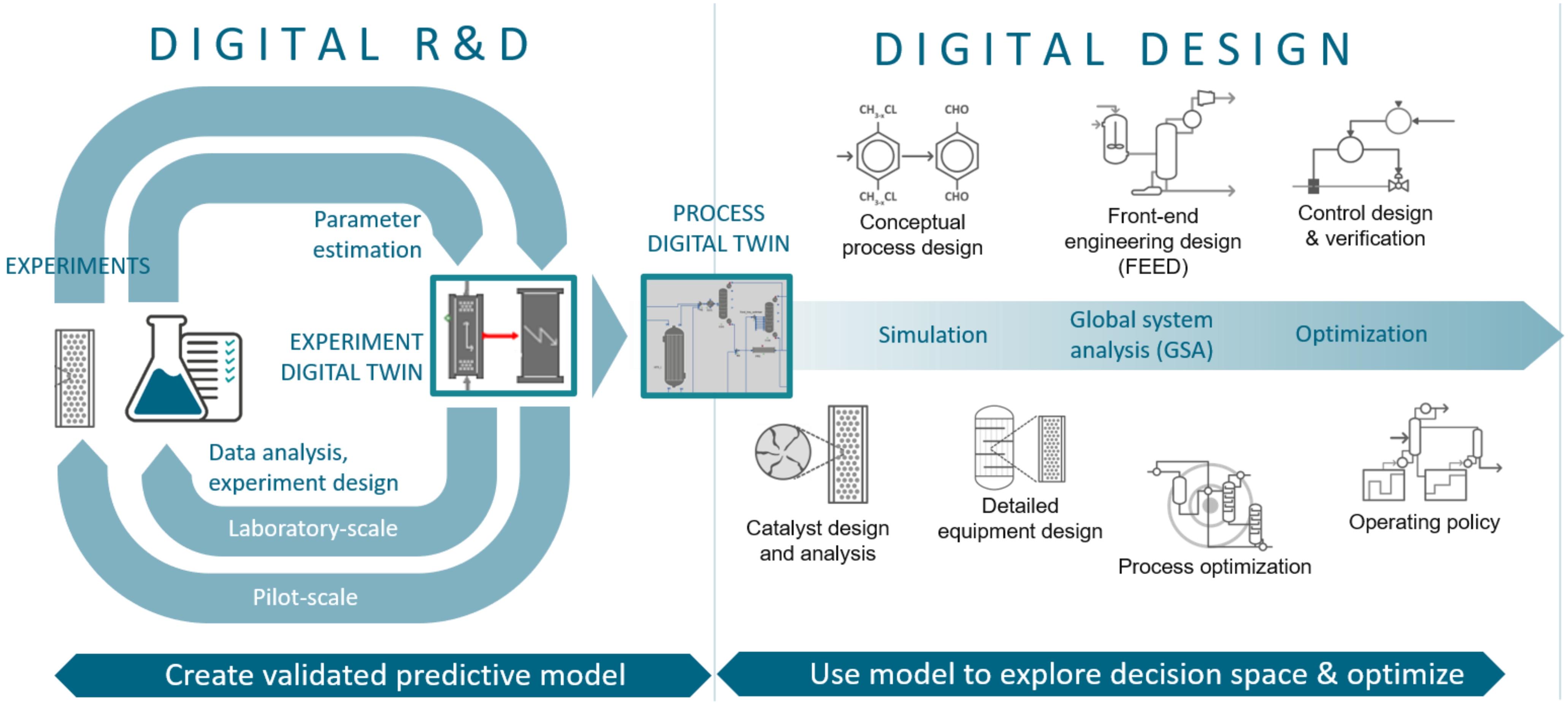
High-fidelity
catalytic reactor
models

State-of-the-art
physical properties:
Multiflash+DIPPR
gSAFT

Sopisticated numerics:
Equation-oriented solution
Parameter estimation
Optimisation including MIO
Global System Analysis

Source: https://www.psenterprise.com/products/gproms

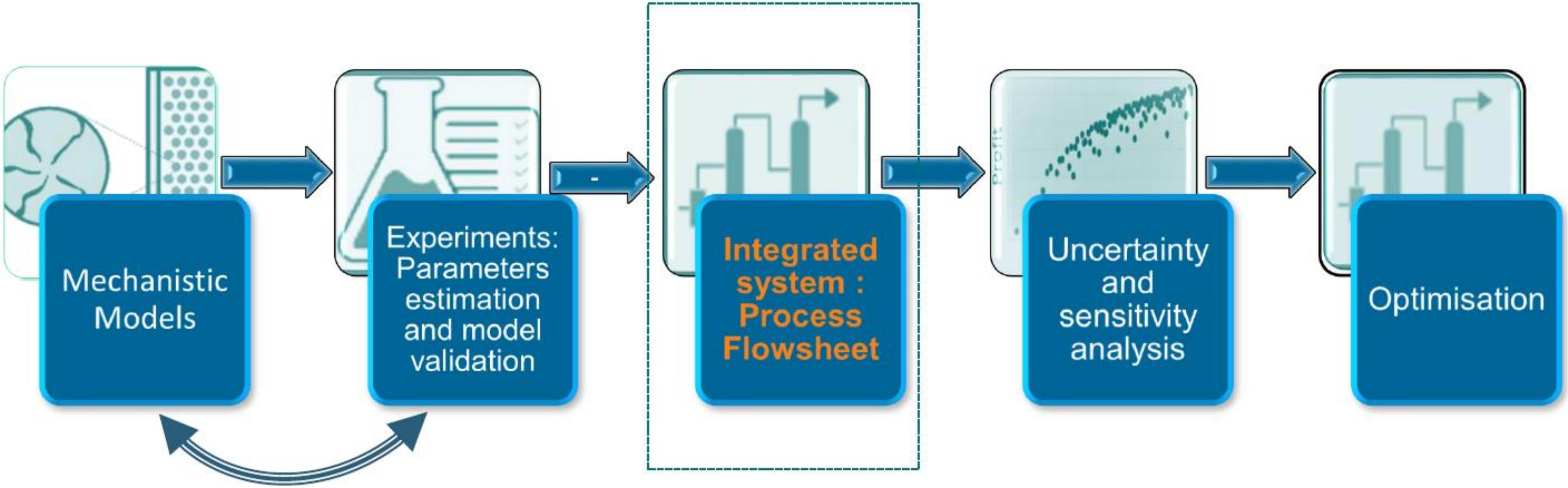
gPROMS (4)
gPROMS Process



Source: https://www.psenterprise.com/products/gproms

gPROMS (5)
gPROMS Process

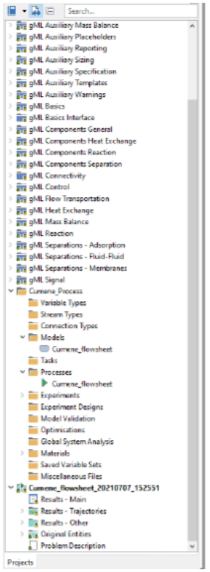
Siemens Process Systems Engineering – **gPROMS Process**:



Source: https://www.psenterprise.com/products/gproms

gPROMS (6)
gPROMS Process

Siemens Process Systems Engineering – **gPROMS Process**:



Library projects

gMLs

Re-usable components

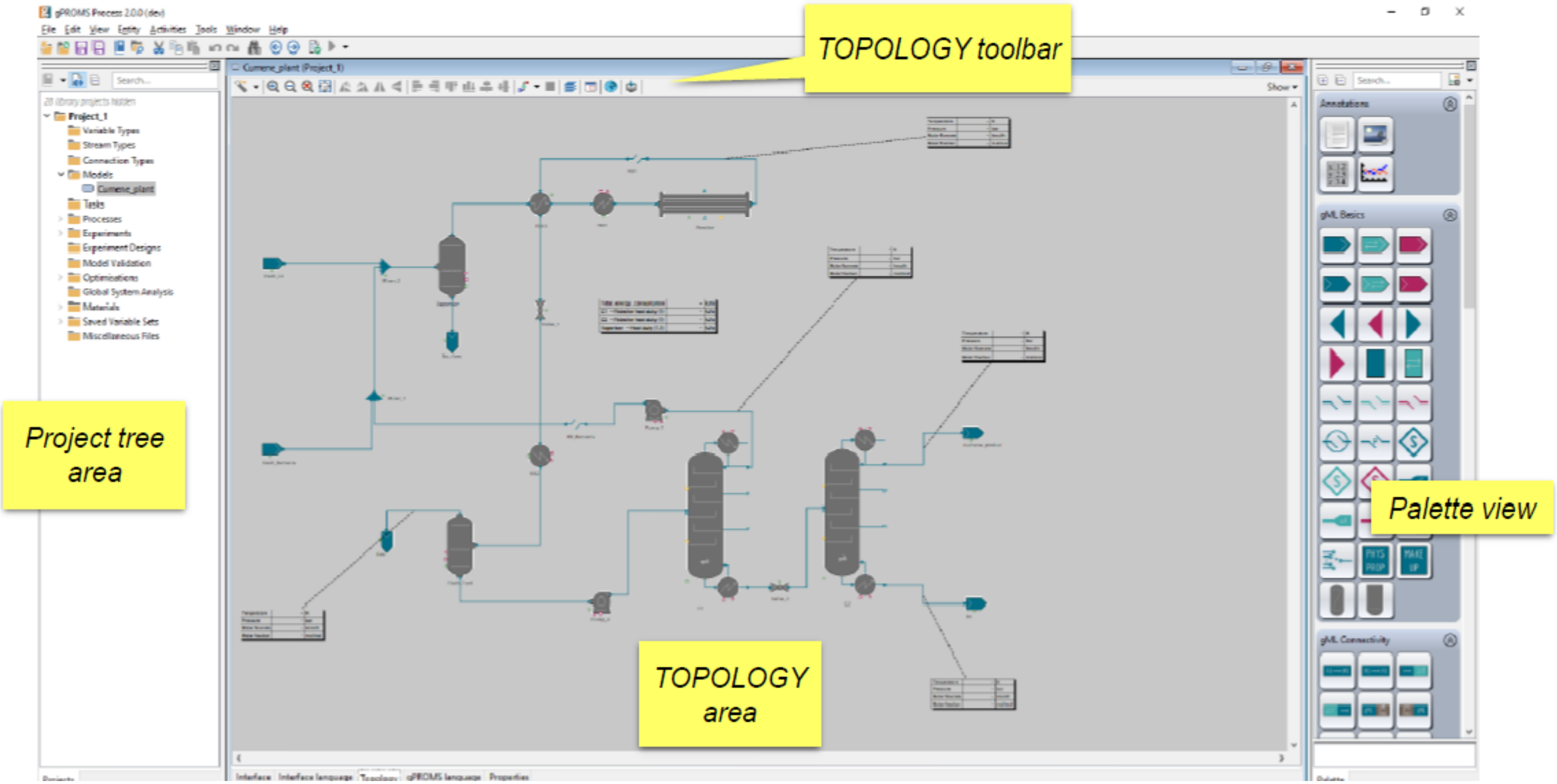
Read-only/protected

Projects

- Developed by the user
- Several sub-folders
- Each sub-folder: model-based entities

Cases

- Input and output information
- Complete record of a model-based activity



gPROMS (7)
ModelBuilder

Siemens Process Systems Engineering – **gPROMS ModelBuilder**:

- environment for expert modellers to build, validate and execute steady-state and dynamic process models;
- for creating and managing custom models, from single units such as novel reactors to entire corporate process simulation and optimization environments;
- gPROMS ModelBuilder can:
  - **build;**
  - **validate;**
  - **execute;**
  - **deploy.**

The gPROMS language:

Equations on paper | Equations in gPROMS language

$$\frac{dM}{dt} = F_{in} - F_{out}$$

```
$M = F_in - F_out;
```

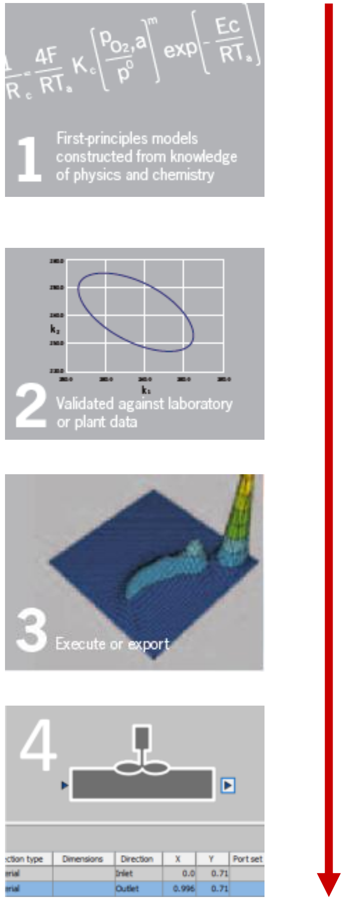
$$\frac{\partial C_i}{\partial t} = -v\frac{\partial C_i}{\partial z} + D_z\frac{\partial^2 C_i}{\partial z^2} + \sum_{j=1}^{NR} v_{ij} r_j$$

```
$C(I,z) = -v*PARTIAL(C(i,z), Axial)
  + D*PARTIAL(C(i,z), Axial, Axial)
  + SIGMA(Nu(I, )*R( ,z)) ;
```

gPROMS (8)
ModelBuilder

gPROMS ModelBuilder - a step-by-step approach to creating custom models:

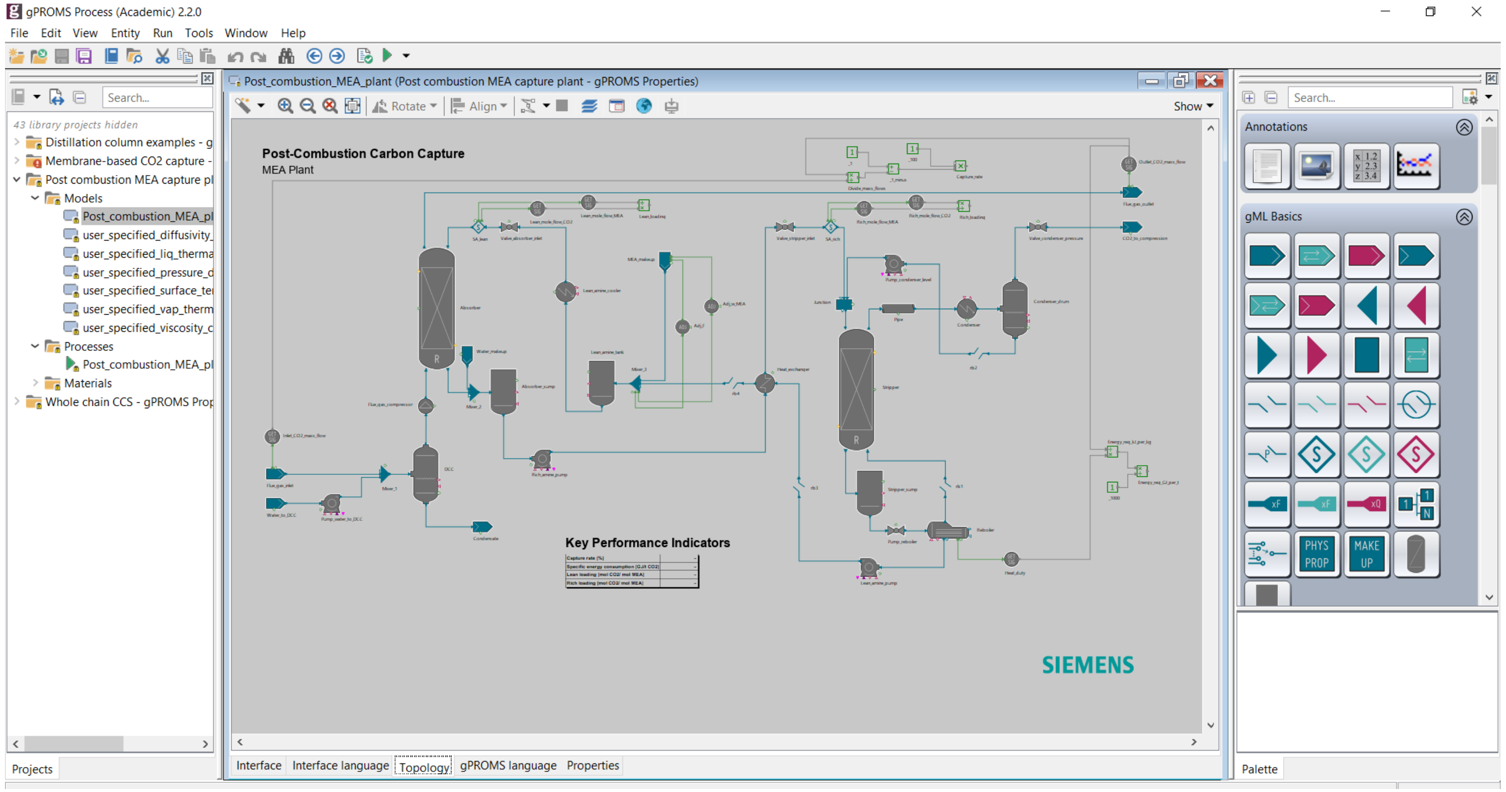
1. Create a first-principles mathematical model that embodies the physics, chemistry and chemicals engineering relationships governing the process and phenomena that occur within it.
2. Where necessary, fit any empirical constants within the first-principles model to experimental data.
3. Test the model standalone to verify results and ensure that it works under all anticipated conditions.
4. Optionally, provide various interface attributes (icon, port definition and placing, specification dialogues, results reports) and add the model to a custom library.



gPROMS (9)
gPROMS Process

Hands-on presentation:

- gPROMS Process



gPROMS (10)

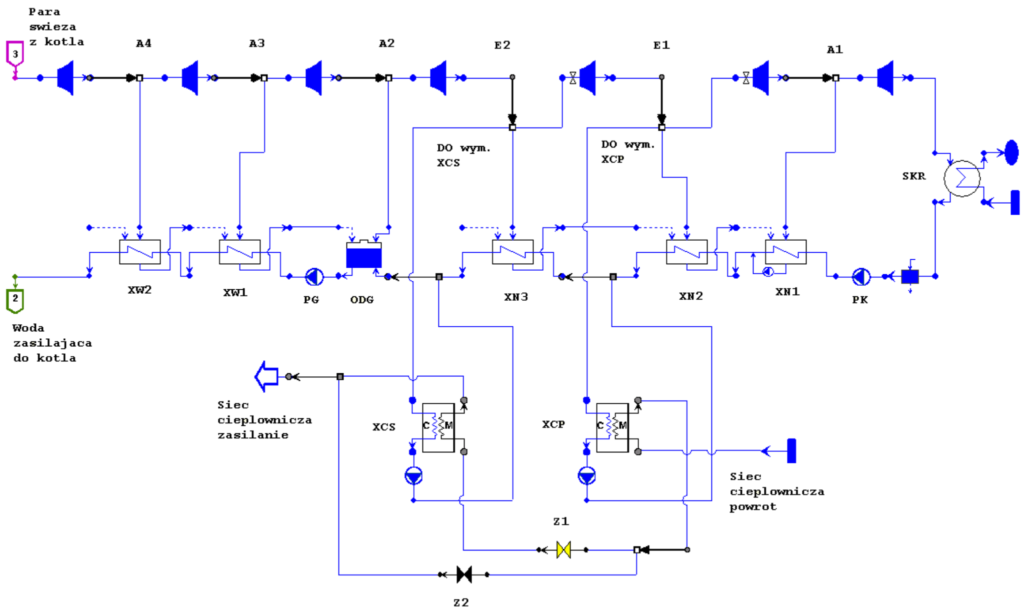
Personal opinions and conclusions:

- straightforward flowsheet process modelling tool;
- great **database of components** (including the specific libraries);
- fairly easy **programming language** for own models development and making them flowsheet ready;
- suited for conventional power plants, **chemical plants, industrial processes**, …;
- easy and intuitive to setup the model and develop own models;
- great support, trainings and help from the software provider.

Selected past R&D projects (1)

- Research Project (national funds) "***Development of dedicated computer application for creating high-efficiency, large-scale cogeneration strategy, taking into account economic and environmental criteria, including CO_2 emissions***" (SUT, 2010 – 2012)

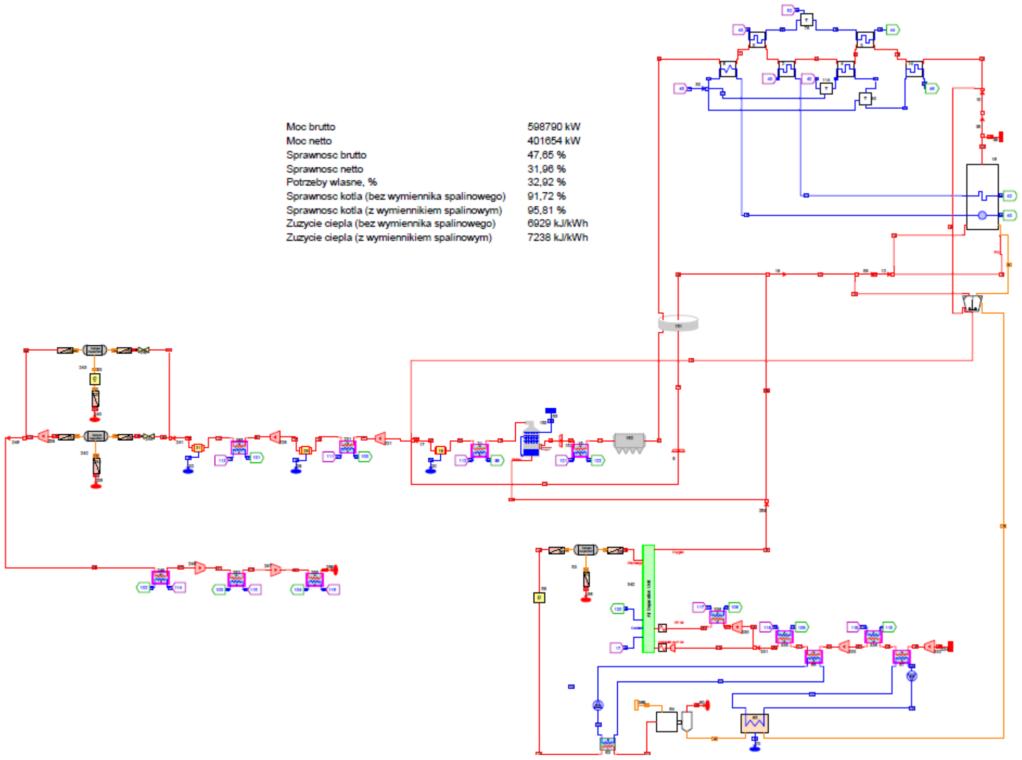
  - **THERMOFLEX®** (process models of different combined heat and power plants)
  - **GateCycle** (combined cycle power plants)
  - **EES** (process models of different combined heat and power plants)
  - **MATLAB** (neutral networks)



Selected past R&D projects (2)

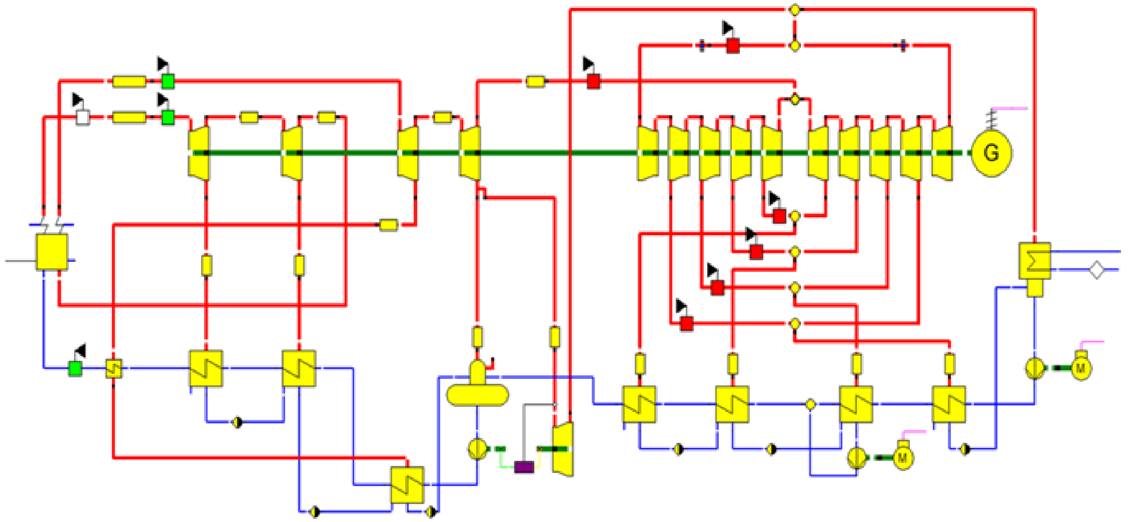
- Strategic Program (national and private funds) “***Advanced Technologies of Energy Generation. Project no 2: Oxy-combustion technology for pulverized-coal and fluidized-bed boilers with CO_2 capture***” (SUT, 2010 – 2015)

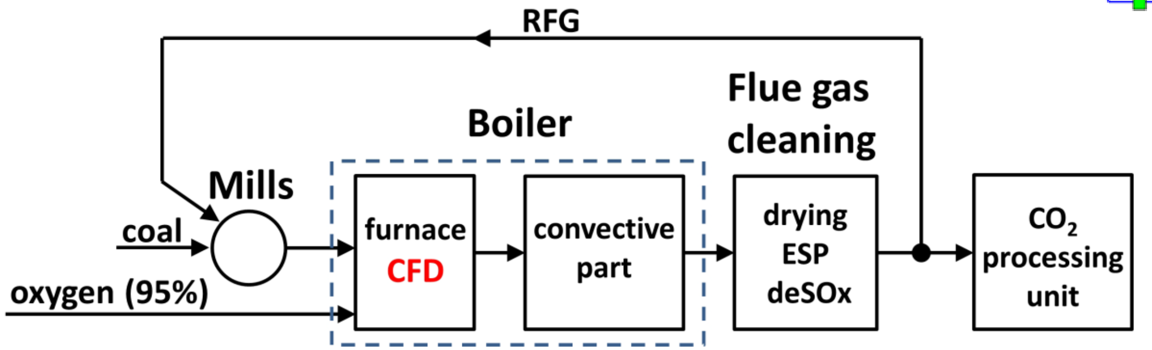
  - **THERMOFLEX®** (process models of different desings of oxyfuel combustion power plants)
  - **EES** (input-output analysis)



Selected past R&D projects (3.1)

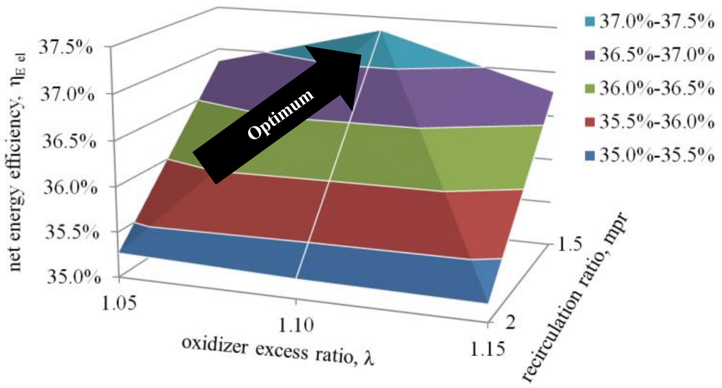
- Research Project (Norway grant) “**Mild Oxy Combustion for Climate and Air**” (SUT, 2016 – 2017)
  - **EBSILON® Professional** (process models of different desings of MILD oxyfuel combustion power plants, detailed boiler model)
  - **ANSYS FLUENT** (MILD OFC furnace)

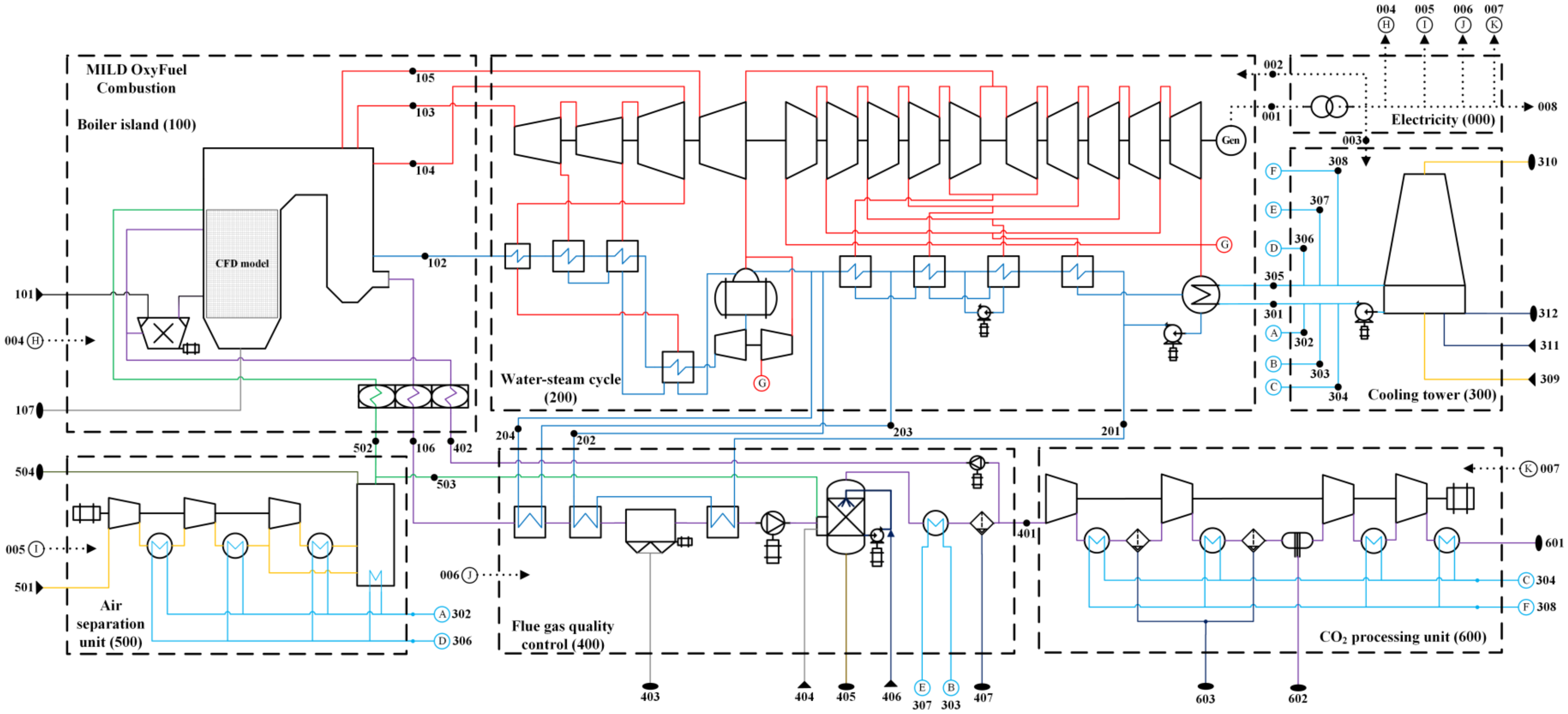




Selected past R&D projects (3.2)

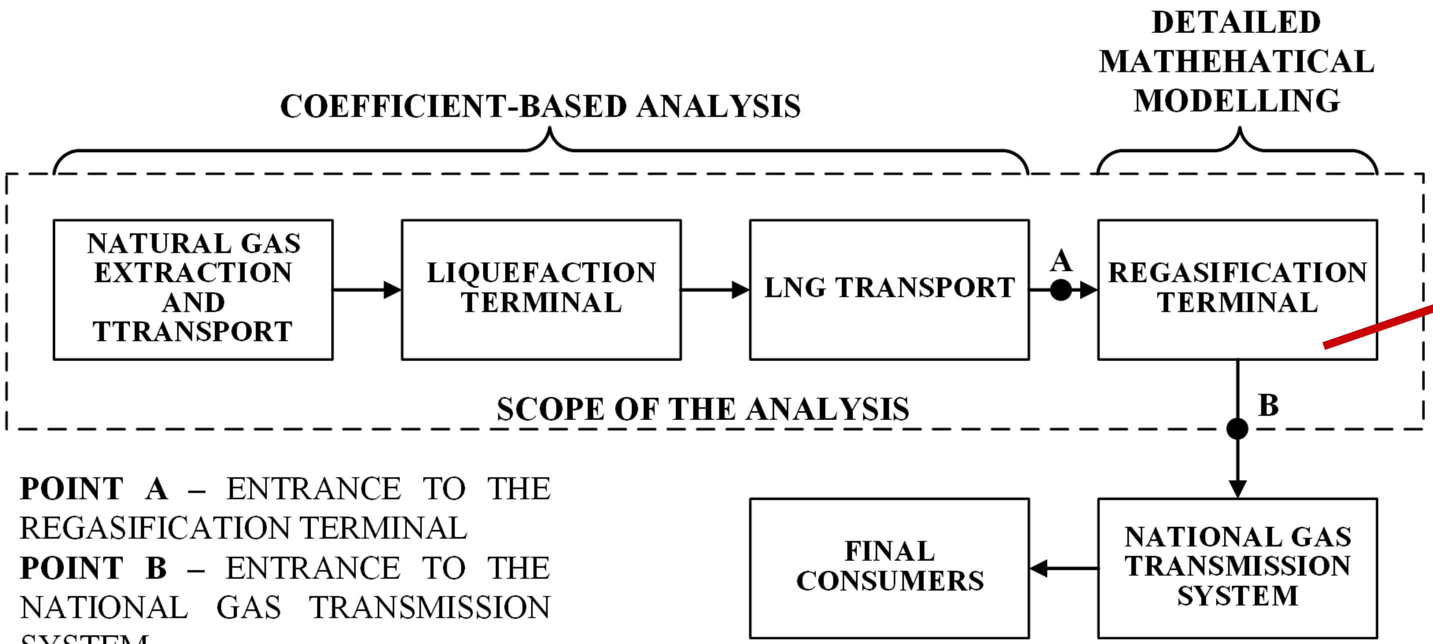
- Research Project (Norway grant) “**Mild Oxy Combustion for Climate and Air**” (SUT, 2016 – 2017)



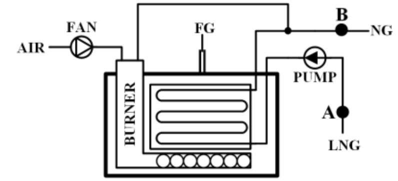


Selected past R&D projects (4.1)

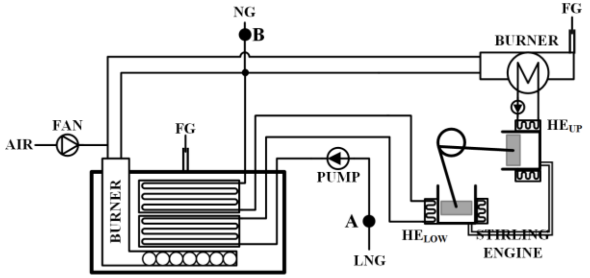
- Research Project (national funds) “***Theoretical and computational investigations of new concepts of power plant with Stirling engine fed with cryogenic exergy***” (SUT, 2016 – 2017)



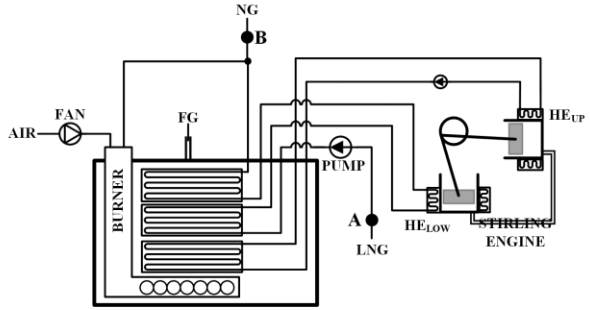
POINT A – ENTRANCE TO THE REGASIFICATION TERMINAL
POINT B – ENTRANCE TO THE NATIONAL GAS TRANSMISSION SYSTEM



LNG SUBMERGED COMBUSTION VAPORIZERS (REFERENCE)



LNG SUBMERGED COMBUSTION VAPORIZERS WITH STIRLING ENGINE (OPTION 1 – WITH ADDITIONAL GAS BURNER)

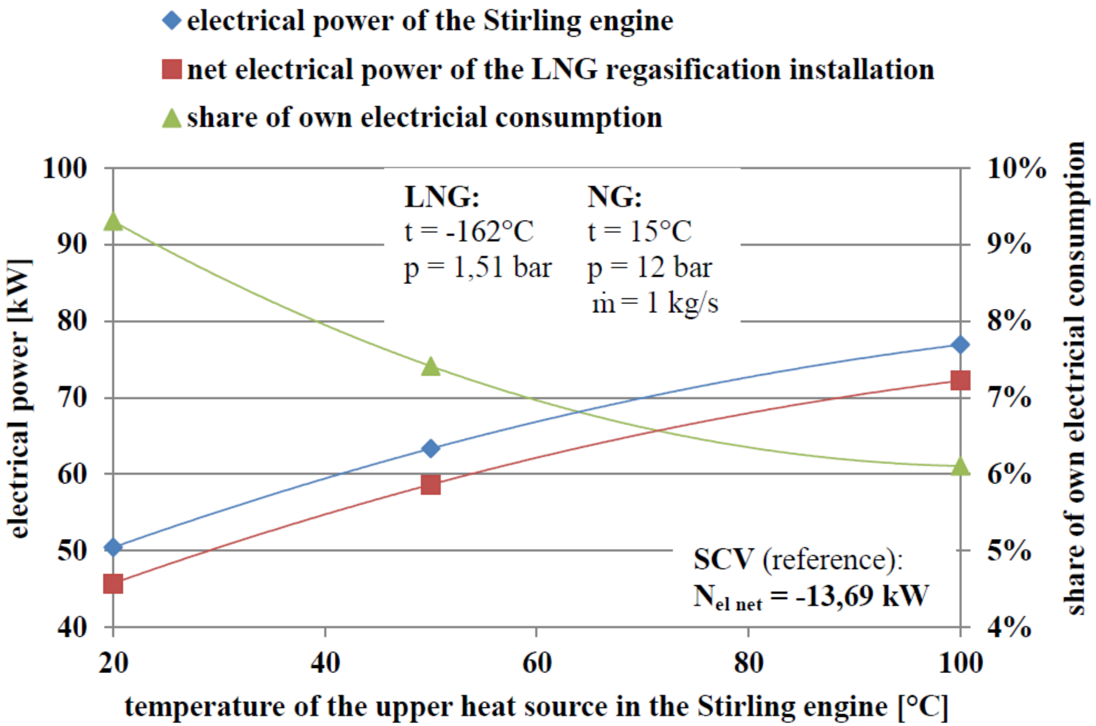


LNG SUBMERGED COMBUSTION VAPORIZERS WITH STIRLING ENGINE (OPTION 2 – WITHOUT ADDITIONAL GAS BURNER)

Selected past R&D projects (4.2)

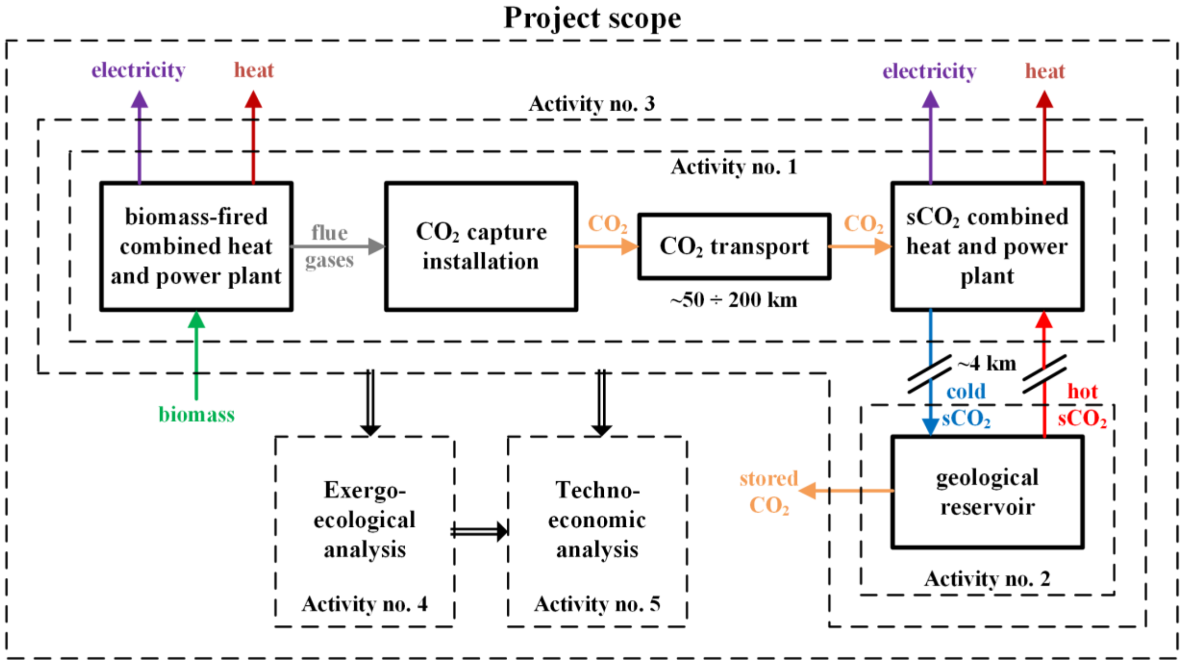
- Research Project (national funds) "***Theoretical and computational investigations of new concepts of power plant with Stirling engine fed with cryogenic exergy***" (SUT, 2016 – 2017)

  - **EBSILON® Professional** (LNG regasification terminal, Stirling engine)
  - **ANSYS FLUENT** (Stirling engine)



Selected past R&D projects (5.1)

- Research Project (national funds) "***Determination of the structure for a biomass-fired combined heat and power plant with CO_2 capture integrated with CO_2 enhanced geothermal system***" (AGH, 2017 – 2021)
  - **IPSEpro** (integrated energy system: biomass-fired combined hea and power plants integrated with CO_2 capture, CO_2 transport and sCO_2 combined heat and power plant)
  - **EES** (steady-state geological reservoir and wells model)
  - **TOUGH3** (detailed geological reservoir model)

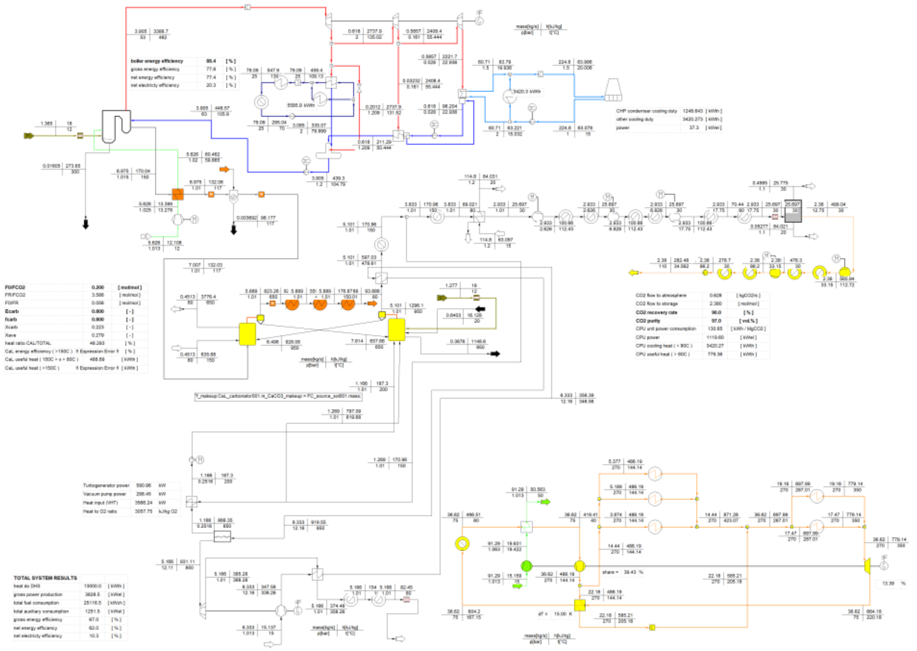


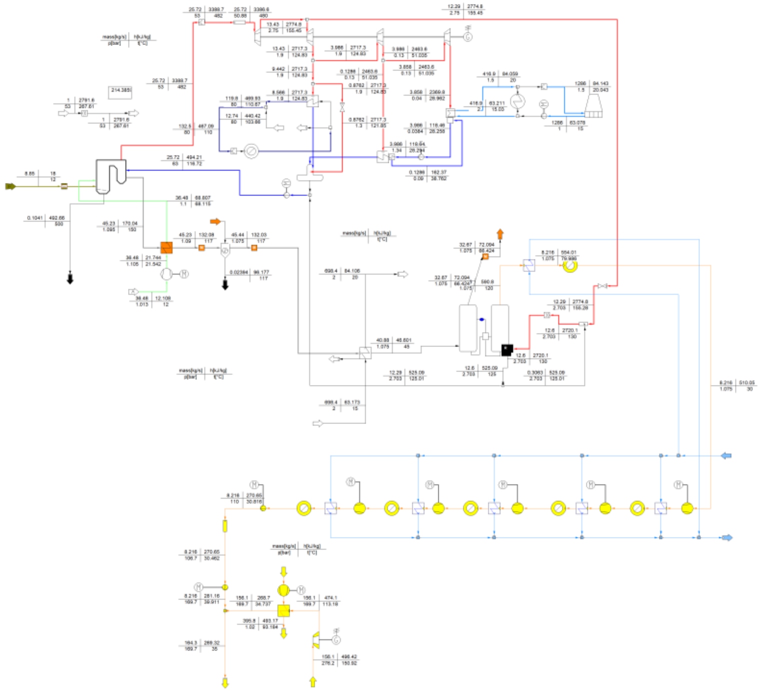
Selected past R&D projects (5.2)

- Research Project (national funds) “***Determination of the structure for a biomass-fired combined heat and power plant with CO_2 capture integrated with CO_2 enhanced geothermal system***” (AGH, 2017 – 2021)

IPSEpro – own models:

- MEA CO_2 capture
- calcium looping CO_2 capture
- HTM O_2 separation installation
- biomass boiler
- …

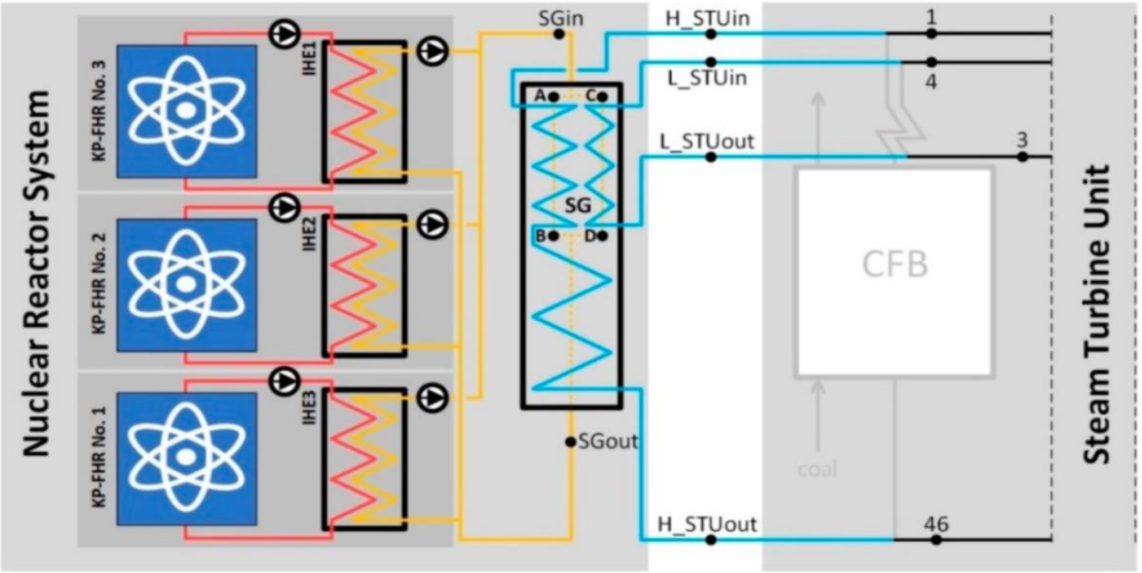




On-going R&D projects (1)

- R&D Research Project (private funds) „***Re-using coal and gas power plant assets in a fully decarbonized Polish power sector***” (2020 – 2022)

  - **EES** (primary and secondary nuclear circuit, new HRSG)
  - **IPSEpro** (primary and secondary nuclear circuit, new HRSG, steam cycles)

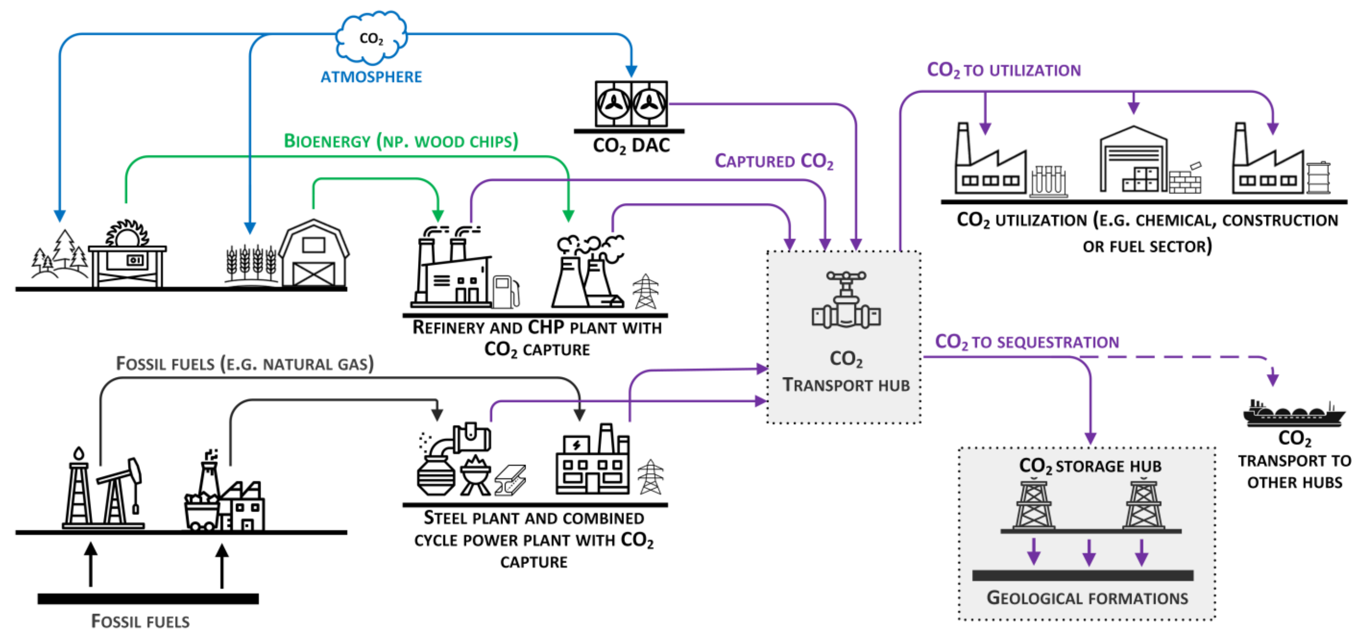


Integration diagram of KP-FHR system with the reference steam turbine unit.

On-going R&D projects (2.1)

- R&D Research Project (national funds) „***Strategy development for CO_2 capture, transport, utilization and storage in Poland, and pilot implementation of Polish CCUS Cluster***” (AGH, 04.2021 – 03.2024)

  - **gPROMS Process** (power plants, CO_2 capture installations, DAC plants, CO_2 utilization, CO_2 transport and storage)
  - **ChemCAD, IPSEpro, …** (existing CCUS models transfer through **gPROMS ModelBuilder**)



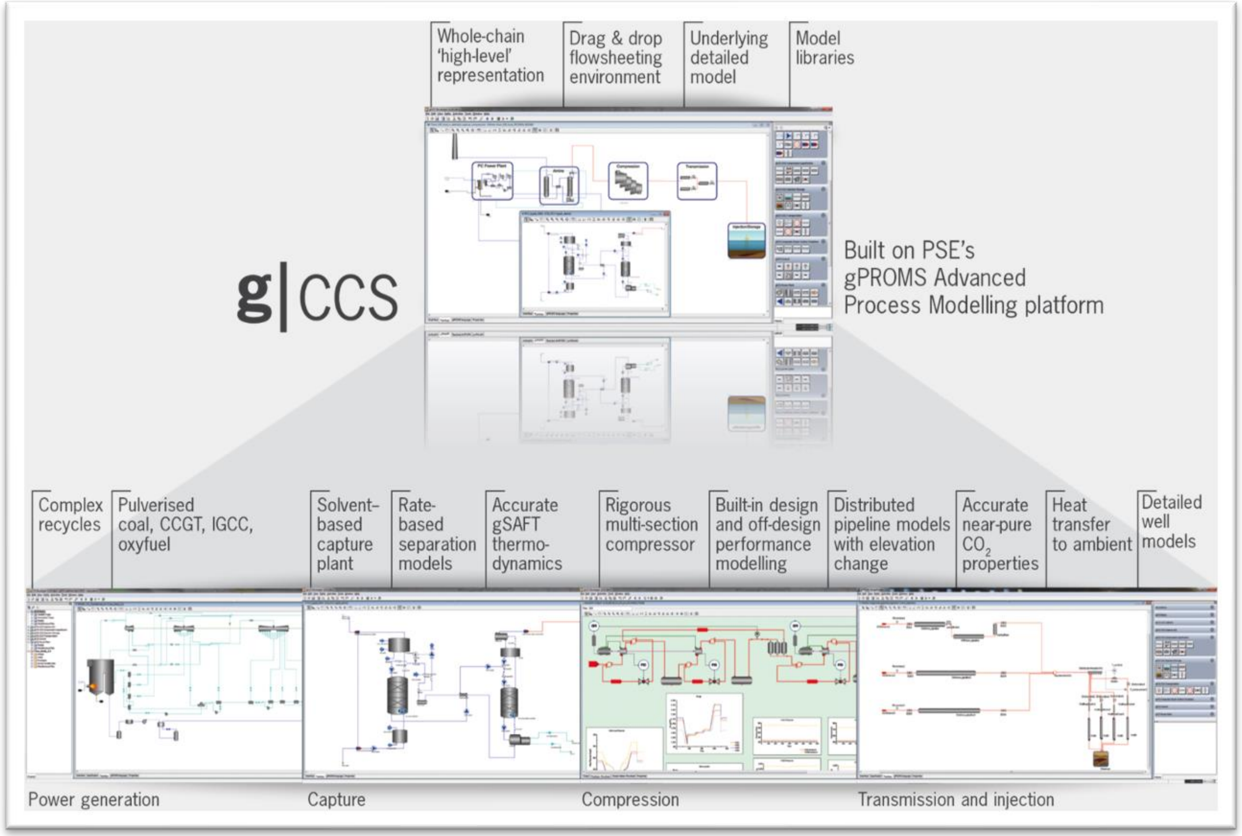
EXAMPLE OF CCUS CLUSTER

On-going R&D projects (2.2)

gPROMS software for the process modelling and optimization of CCUS installations and clusters.

Specialized research team (14 people) at AGH University devoted to the process simulations and optimization of CCUS installations and cluster using gPROMS software.

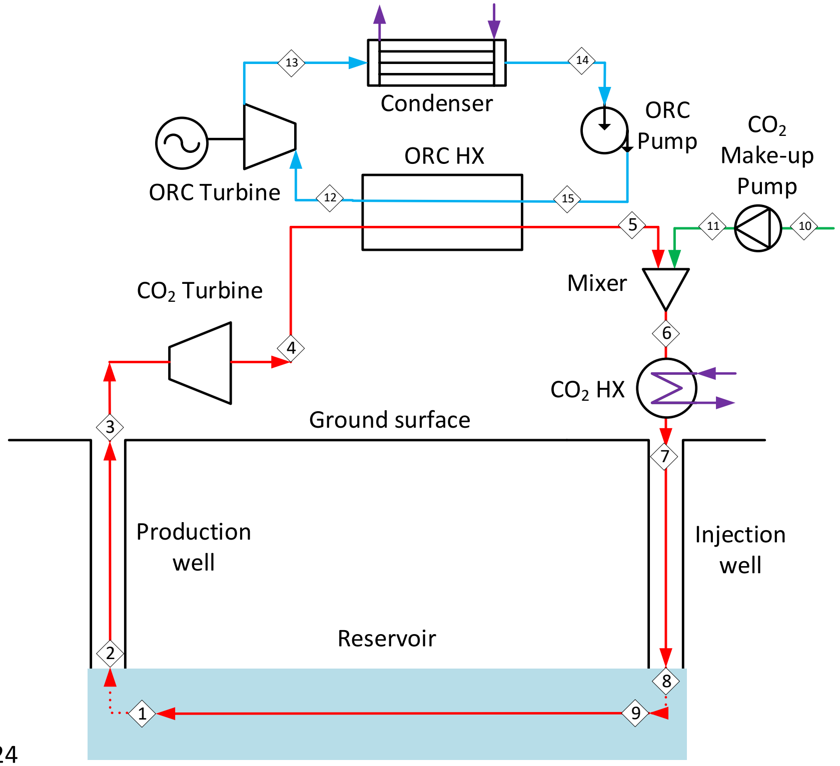
Team experience:
- participation in extensive training by software provider (Siemens PSE Enterprise),
- case studies development for Polish energy sector and industry,
- previous R&D&I projects.



On-going R&D projects (3)

- R&D Research Project (Norway grant) „***CO_2-Enhanced Geothermal Systems for Climate Neutral Energy Supply***” (AGH, 10.2020 – 09.2023)

  - **Excel & CoolProp, EES, TOUGH3, …** (reservoir and well models)
  - **IPSEpro, gPROMS Process, SINTEF own code, MathCad** (sCO_2 and ORC cycles simulation and optimization)

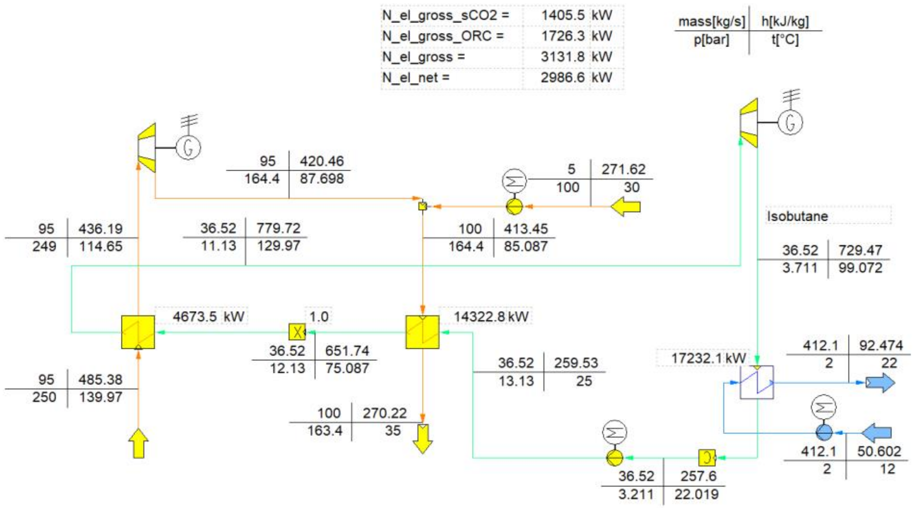


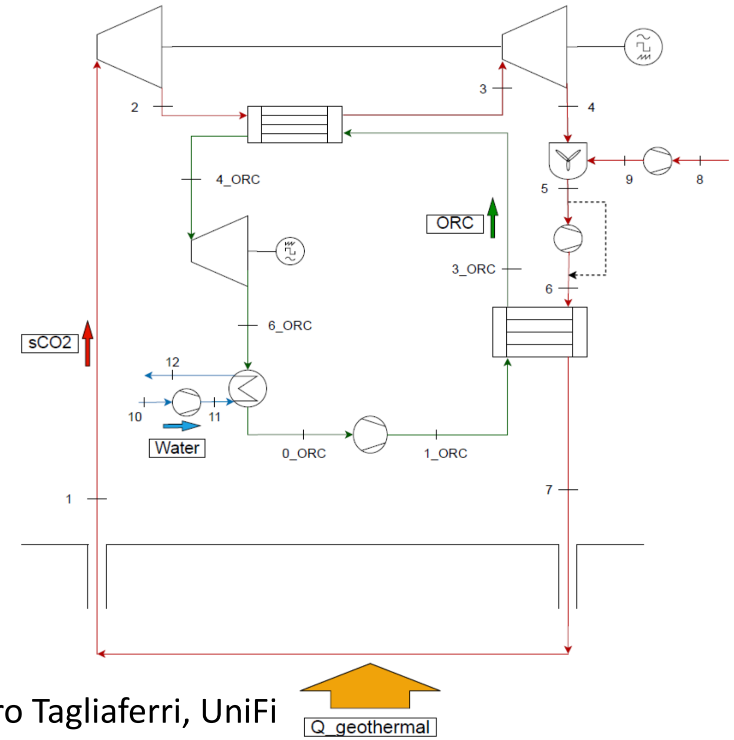
DOI: 10.18462/iir.gl2022.124
Topside cycles for enhanced geothermal systems with CO2 and hydrocarbons as working fluids
Han DENG, Trond ANDRESEN, Geir SKAUGEN, Paweł GŁADYSZ, Leszek PAJĄK, Anna SOWIŻDŻAŁ, Maciej MIECZNIK

On-going R&D projects (4)

- R&D Research Project / Travel Grant (national funds) „*Comparative assessment of enhanced geothermal systems with advanced exergy analysis*” (10.2021 – 03.2022)

  - **EES, Excel & CoolProp** (reservoir and well models)
  - **IPSEpro, EES** (sCO_2 and ORC cycles simulation and optimization)





Mauro Tagliaferri, UniFi

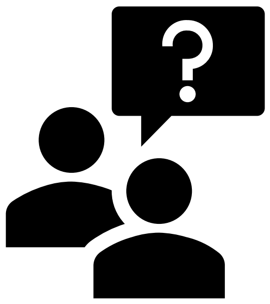
Conclusions

Challenges when choosing adequate process modelling tools:

- own process models development vs libraries (add-ons)
- flowsheet vs equation-oriented approach
- applications: conventional power plants, renewable energy sources, chemical plants, …
- steady-state vs dynamic models
- research vs teaching application
- new designs vs repowering
- maintains models vs optimization algorithms
- …

Discussion

Thank you for you attention.



Next seminars

- **Thermo-ecological cost: an exergy-based lifecycle impact assessment – methods and applications** - 15.03.2022, 10:00 – 12:00, online