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PROSYN®

Artificial Intelligence in Process Engineering

Description of the expert system and its functionalities

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1 INTRODUCTION

In Conceptual Process Design (CPD) a first design of a petrochemical or biochemical plant is made based on preliminary research data and ideas. The outcome is a selection and combination of process steps, which determines the overall technical and economic feasibility. Generally, CPD efforts are relatively small while the impact on the final plant design and costs are significant. PDC has a track record showing that when structured conceptual process design or process synthesis (PROSYN®) is successfully applied at an early R&D stage, cost and energy savings of 20 to 50% can be realized and development time can be shortened considerably.

PROSYN® (**Pro**cess **Syn**thesis) is a heuristic-numeric knowledge-based system assisting the structured conceptual design of (chemical) processes. The software uses rules of thumb (heuristics), numerical routines, and databases to propose appropriate flowsheet alternatives. PROSYN® considers a large number of unit operations commonly encountered in the (chemical) industry.

1.1 History

The development of PROSYN® started in the 1980s, when Prof. Simmrock of the Technical University of Dortmund established a consortium with the key players in the German chemical industry (BASF, Bayer, Degussa, Hoechst, Hüls). The basic idea behind the development of PROSYN® was to establish a computer-aided strategy tool which copies the industrial practice of inventing chemical processes. This is why the tool can take different types of information (quantitative as well as quantitative) at multiple working levels (management, specialist, service).

Initially the PROSYN® development was conducted with PhD students from the Technical University Dortmund (TUDO), Hamburg (TUHH), Berlin, Bochum and RWTH Aachen. They worked closely together with the specialists from the German chemical industry to extract specific knowledge and engineering rules of thumb, which they translated in heuristic rules and numerical methods. From the second half of the 1990s PROSYN® was exclusively used by Process Design Center (PDC) for industrial consultancy.

Since the 1980s more than 300 man years have been spent by chemical engineers and IT specialists to develop the program. In total the program comprises 800,000 lines of code, which represents an estimated rebuild value of 60 million US$. Continuous effort is spent not only on the development of new expert systems, like crystallization, reactive distillation, membrane and membrane reactors, but also to transfer the system to new platforms (web-based). From 2010 to 2017 a major IT effort was made to turn the academic software into commercially licensable software.

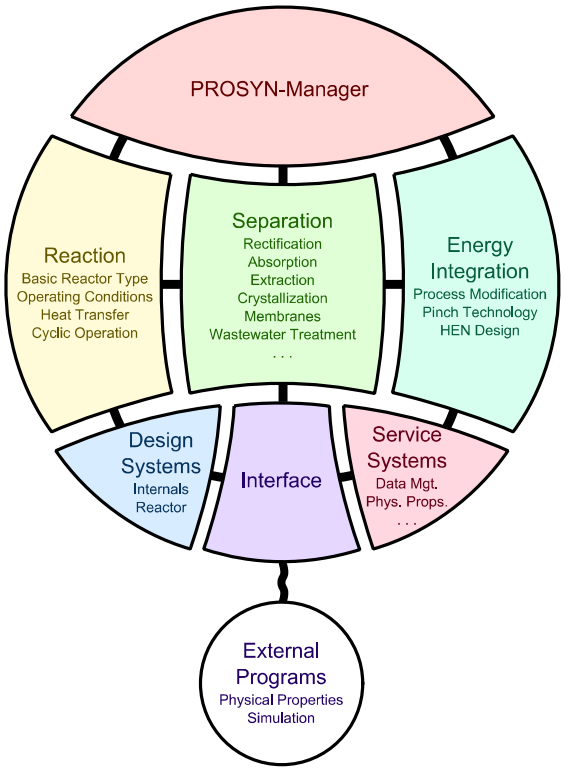

Figure 1: Basic structure of PROSYN®

1.2 Application areas

PROSYN® is a unique tool, which helps process development engineers, experts and multi-disciplinary development teams to generate and validated conceptual ideas, check alternative options that initially may have been overlooked, and to structure the conceptual design process.

PROSYN® can be applied in virtually all sectors of the processing industry dealing with reaction, separation and purification steps. Product areas include organic and inorganic chemicals, polymers, biochemicals, food & health care products, pharmaceuticals, (bio)fuels and more. PROSYN® has been successfully applied to redesign existing processing plants, but also for new and next-generation feedstock, catalysts, processing routes and plant environments. The applicability is not limited to large production scales and covers the range from single unit operation to integrated production plants.

While PROSYN® is designed to work optimally in the phase between research & development and basic engineering, the tool has also proven its added value in the appraisal or screening phase as well as in revamp, retrofitting, and debottlenecking projects.

1.3 PROSYN® software

PROSYN® is configured as an integrated structure of software components (Figure 1), comprising expert systems for reaction, separation and integration, a management system, and supporting tools. Furthermore, the system connects to external databases and tools for physical properties and process simulation.

The bulk of the software is coded in a general purpose logic programming language (PROLOG). This language provides an effective way to set up a conceptual design methodology based on heuristics and to make it readily accessible. For this purpose it is shorter, easier, and better maintainable than an imperative programming language (if-then-else).

PROSYN® runs on a web-based platform, accessible via a user interface. Each expert system can be operated individually, but also through access via another PROSYN® expert system as needed. For example, PROSYN® Azeotropes may call PROSYN® Solvents to identify suitable extraction solvents or entrainers for extractive distillation.

The interaction via the user interface proceeds by successive questions, inputs and recommendations by PROSYN®. The user is in full control and can decide about the source of information (internal/external databases, user input, estimation methods) as well as acceptance of proposals by the system. Depending on the input and choices by the user, PROSYN® guides the conceptual design process and provides feedback through specific proposals and recommendations concerning the selection, design and operation of unit operations. One important feature of the system is the so-called ‘Unknown’ button which triggers the expert system to provide hints or recommendations.

Each PROSYN® session is recorded with an automatically generated report. The tool also has a replay function, enabling to repeat a PROSYN® investigation up to a specific point in the program. This makes it possible to investigate alternatives, which is often useful in case it is uncertain whether specific information, which is not always readily available, is essential for the conceptual design.

A typical screen of the PROSYN® user interface is shown in Figure 2.

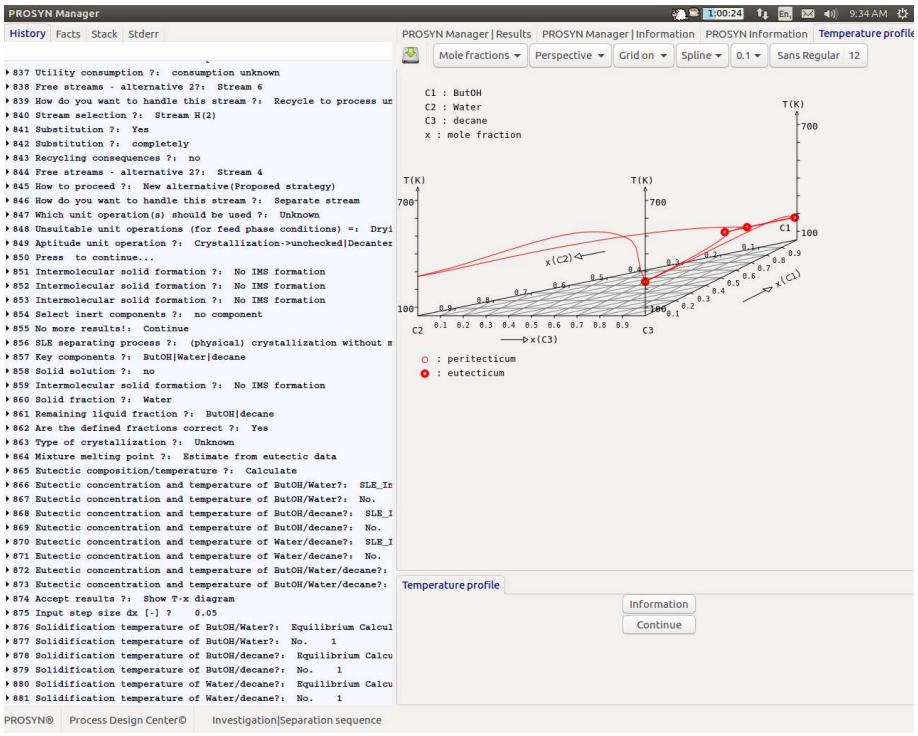

Figure 2: Example of a PROSYN® screenshot

1.4 PROSYN® modules

A list of PROSYN®'s functional modules can be found in Table 1 next to a short description. A further description of each module is provided in Section 2.

Table 1. PROSYN® modules and their application.

Module	Application
PROSYN® Reactors	Reactor selection and design
PROSYN® Manager	Process synthesis manager
PROSYN® Absorption	Absorber design
PROSYN® Crystallization	Crystallization
PROSYN® Distillation	Distillation sequences
PROSYN® Azeotropic Distillation	Distillation of azeotropic and close-boiling components
PROSYN® Complex Columns	Complex distillation columns (Petlyuk, dividing wall columns, etc.)
PROSYN® Reactive Separation	Integrated reaction and separation
PROSYN® Reactive Distillation	Reactive distillation
PROSYN® Extraction	Liquid-liquid extraction
PROSYN® Solvents (beta)	Selection of solvents
PROSYN® Membranes (beta)	Separation by membranes
PROSYN® Membrane Reactors	Membrane reactors
Support modules	
PROSYN® Properties	Physical properties
PROSYN® Azeotropes	Investigation of azeotropic systems

2 DESCRIPTION OF PROSYN® MODULES

2.1 PROSYN® Reactors

PROSYN® Reactors is PROSYN®'s reaction engineering module. It is a heuristic-numeric system, which, by applying relevant reactor selection criteria, selects and designs a basic reactor type suited for a certain reaction network/mechanism.

The reactor type, its characteristics and the reaction conditions are choices with far-reaching consequences to the process. They should therefore be made at an early stage of process synthesis, typically before or during design of the separation section of the process. The exact influences of catalyst, reactant concentration and operating conditions can only be understood after many experiments and a careful interpretation of experimental results. Such information is usually not available at an early stage of conceptual process design. PROSYN® Reactors therefore relies on qualitative decision criteria which can be applied with only basic knowledge of the reaction system. This module can also identify knowledge gaps, which should be investigated prior to complete the basic reactor selection and design.

In order to keep the decision path transparent to the user, PROSYN® Reactors applies several sequential selection levels. Each level takes relevant reactor selection decisions which the following levels generally rely on. The target for the investigations is the maximization of the reactor performance (conversion, selectivity, yield or productivity).

1. The **basic reactor conditions** are first studied based on the reaction phase(s), type and qualitative reaction kinetics:
   - concentration level of reactants
   - temperature profile
   - residence time distribution
   - backmixing characteristics of the phases
   - interfacial area between the phases
   - holdup and contacting of phases

   Within this investigation, additional aspects such as the structure of the catalyst particles (pore and particle size) and phase dispersion are analyzed. This step considers characteristic mass transfer phenomena, especially typical for multiphase reaction systems.
2. The possible **operating conditions** of a reactor are explored and recommended on the basis of the results of the preceding investigation step. The following essential reactor operation parameters are investigated:
   - reactant feeding mode (normal, interstage, …)
   - reactants ratio
   - recycle streams
   - product or byproduct removal during reaction
   - conversion level
   - pressure level (in case of gaseous reactants)
   - safety aspects

   Many of these operating conditions are coupled and cannot, in practice, be analyzed separately.
3. For each suitable basic reactor type a list of most favorable **technical reactor** designs and design alternatives is created and then shortened based on appropriate knock-out selection criteria: foam/deposit forming, catalyst regeneration time, dusty feeding, liquid viscosity, catalyst attrition, etc. Possible technical reactor designs are the multi-tubular fixed-bed reactor, the fluidized-bed reactor, etc. In total the system distinguishes more than 120 reactor configurations depending on the reaction phase(s).

4. Different **heat transfer** options are investigated. This is done after the reactor selection phase as it is generally possible to create technical solutions for the heat transfer. Using information about the reaction temperature level, cooling/heating demand, boiling behavior of the mixture, etc. PROSYN® Reactors selects suitable heat transfer equipment (external, internal or combinations), if needed, by employing shortcut methods for a first estimation.

Additional features include the graphical representation of diagrams such as a plausible concentration-time plot.

2.2 PROSYN® Manager

PROSYN® manager allows a scan of the applicability (rating) and suitability (ranking) of separation technologies for a user-specified separation case. Such a scan is based on heuristic rules, physical property information of system components/mixtures and user input information (via a "question & answer" approach). The following separation technologies are considered:

- Drying
- Filtration
- Crystallization
- Decanting
- Extraction
- Liquid phase adsorption
- Pressure flashing
- Stripping
- Absorption
- Condensation
- Distillation
- Gas phase adsorption
- Membrane separation processes

Depending on the outcome of the screening, PROSYN® can guide the user towards the appropriate specialized PROSYN® modules. After running such a PROSYN® module, the user is brought back to the PROSYN® Manager for further guidance.

2.3 PROSYN® Absorption

This module handles the selection and design of absorption as a way to clean or separate gases. It can be applied on a stand-alone basis or as part of the design of a full process.
A run of the module proceeds in 8 steps:

1. Definition of the feed stream.
2. High-level evaluation of the applicability of absorption based on knock-out criteria.
3. Generation of suitable separating cuts on the basis of process-technical requirements.
4. Assessment of absorption for the generated separating cuts. Evaluation on several criteria (e.g., suitability for low gas pressures) for the kind of application envisaged (e.g., exhaust air, flue gas). Comparison with other technologies, e.g., partial condensation.
5. Selection of absorbents for chemisorption (e.g. NaOH) and physisorption (e.g. Rectisol).
6. Determination of suitable operating conditions.
7. Preliminary design and validation.
8. Selection of units (e.g., packed bed column, Venturi scrubber) and internals.

2.4 PROSYN® Crystallization

PROSYN® Crystallization is a heuristic-numeric system for the determination of possible and suitable separating cuts, operating conditions, mass- and energy balancing and the selection of suited crystallizer types. In the current PROSYN® module, only physical crystallization is covered while the functionalities of chemical and antisolvent crystallization are work in progress.

A run of PROSYN® Crystallization proceeds as follows:

1. User input of the feed data. The characterization of the feed stream includes temperature, pressure, flow rate and composition.
2. Proposed separating cuts. Based on SLE information, potential separating cuts are determined. The crystal product is not necessarily the component with the highest melting point. By changing the liquid composition inside the crystallizer, e.g., by partial evaporation of the feed, crystallization boundaries can be crossed, allowing obtaining a different crystalline product.
3. Rating of potential separating cuts on criteria such as maximum crystal yield, expected temperature level, expected crystal shape or required product quality.
4. Type of crystallization. The most suitable type of crystallization and heat removal or supply will be proposed, including proposals about direct or indirect cooling/heating or adiabatic operation by feed flashing as well as general distinctions such as the classification as melt crystallization or crystallization from solution.
5. Operating mode. Batch or continuous operation will be proposed together with suitable operating temperature and pressure. Also, the expected crystal yield is estimated.
6. Type of crystallizer. Suitable apparatuses are selected for an optimal performance of the crystallization and to obtain the required separating cut. At present, PROSYN® Crystallization considers 13 different crystallizer types plus add-on equipment. Examples of add-on equipment are an elutriation leg, a clear-liquor advance or a fines removal loop.
7. Mass and Energy Balance. A mass and energy balance is estimated around the crystallization unit as a basis for economic evaluation.

Besides these mainly heuristics-based investigations PROSYN® Crystallization offers a set of tools for mixture analysis of potential crystallizer feeds. For example, crystallization boundaries can be calculated, indicating whether crystallization is expected for a given composition.

2.5 PROSYN® Distillation

This module is a heuristic-numeric system for the synthesis of distillation sequences. The application of this module is limited to those mixtures with a separation/boiling behavior which can be described by separation coefficients and by pure components' boiling points. Complete distillation sequences or single separating cuts can be investigated. It is not applicable to azeotropic and/or close-boiling systems, which are covered by the PROSYN® Azeotropic Distillation module.

Heuristics contained in PROSYN® Distillation are based on technical as well as economic considerations. The module can also refer the user to PROSYN® Complex Columns.

PROSYN® Distillation can provide a tentative mass balance for a distillation sequence, which may serve as a starting point for process simulations with process simulation software.

The general strategy of this module is as follows:

1. Definition of the separation task
2. Basic data (physical properties to calculate boiling points and separation coefficients). Based on physical properties, the possible separating cuts are grouped according to their degrees of 'difficulty'

3. Exclusion of separating cuts (which components may not end up in one product fraction?)
4. Proposal of suitable separating cuts
5. Tentative mass balance and product stream temperatures. An infinite number of stages is assumed here.
6.

Usually more than one distillation sequence will be proposed. Rejected alternatives will not be shown. Suitable alternatives, however, are listed without ranking.

2.6 PROSYN® Azeotropic Distillation

This module investigates the possibilities of separating a close-boiling and/or azeotropic component mixture by means of distillation technology.

The module covers 6 alternatives for the separation of azeotropic and/or close-boiling multi-component systems:

1. Simple distillation of non-ideal mixtures
   - Azeotropic cut
   - Pre-concentration followed by azeotropic cut
2. Extractive distillation with (user specified) mass agent
3. Hetero-azeotropic distillation without mass agent
   - Pre-defined multi-column (2 column) systems with recycles between the columns are embedded and checked integrally by PROSYN® in one run.
4. Hetero-azeotropic distillation with (user specified) mass agent
   - Here, also 2-column systems with recycles are embedded and checked in one run.
5. Pressure swing distillation without mass agent
   - PROSYN® performs a sensitivity study in order to find the best minimum and/or maximum pressure.
6. Homoazeotropic distillation with recycle

With proper VL(L)E thermodynamic models and appropriate parameters (e.g., NRTL parameters estimated via the UNIFAC method), PROSYN® Azeotropic Distillation predicts the occurrence of binary and ternary (homogeneous/heterogeneous) azeotropes and determines close-boiling system. It assists in arriving at an appropriate separation flowsheet (employing one or a combination of the above 6 alternatives) to obtain the products in a user-defined purity class and at a user-defined recovery level.

During flowsheet development, PROSYN® provides ternary diagrams showing distillation boundaries and positions of azeotropes.

In most cases, a separation flowsheet will not be finished in one run. A run starts with the original feed and usually results in two product streams that need to be further purified/separated, thus requiring additional PROSYN® runs. Per run, a 'tree of possible alternatives' is obtained; each of the alternatives is called a 'branch'. No rating of branches is given by PROSYN® Azeotropic Distillation as this would require rigorous simulation (and cost estimation). However, per branch, tentative mass balance information is provided based on maximum achievable component splits (azeotrope compositions). Furthermore, underlying heuristic rules also capture cost criteria. Hence, the economically unattractive alternatives will not appear as PROSYN® proposals. This information may serve as a starting point for rigorous simulation.

2.7 PROSYN® Complex Columns

This module checks the possibility of applying complex column configurations instead of the following two basic configurations:

1. Direct distillation sequence, i.e., start by distilling off the lowest boiling component
2. Indirect distillation sequence, i.e., start by distilling off all components except the highest boiling one.

The main complex column design types embedded in this PROSYN® module are:

1. Side rectifier + its dividing wall column equivalent
2. Side stripper + its dividing wall column equivalent
3. Petlyuk types of column configurations + dividing wall column equivalents

Depending on the user-specified component purity requirements, this module can also propose a direct side draw-off from simple distillation columns.

Embedded complex column heuristics follow a method based on a graphical representation of operating spaces for a number of different column design types. In triangle diagrams, the suitability regions of specific design types are indicated based on heuristics.

As these triangle diagrams do not result from calculations, a number of different diagrams proposed by several research groups have been embedded in PROSYN® Complex Columns. The operating spaces of the different design types depend on the following parameters: purity specifications and Ease-of-Separation Index (ESI). The ESI is the ratio of the volatility of the low- and medium-boiling components to the volatility of the medium- and high-boiling components.

PROSYN® Complex Columns comprises 9 primary complex column design types and 15 primary and sub-design types in total. The work of several research groups on complex column application has been covered and their heuristics are evaluated in parallel. PROSYN® Complex eventually presents an overall conclusion on suitability.

2.8 PROSYN® Reactive Separation

This module was built for the selection and design of reactive separation technologies. The technologies considered include reactive distillation, reactive stripping, membrane reactor technology, reactive adsorption (true moving-bed reactor, simulated moving-bed reactor) and reactive extraction. Execution of this module proceeds through the following, mostly heuristic steps:

1. Definition of the purpose, e.g., increasing overall yield, selectivity.
2. Analysis of the reaction system through rules which are also contained in PROSYN® Reactors.
3. High-level evaluation of whether integrating reaction and separation presents a real advantage. This evaluation is based on knock-out criteria.
4. Establishment of the motivation for reactive separation. Is the expected advantage worth the higher complexity?
5. Definition of the separation task, e.g. increase conversion and/or selectivity by a selective removal of a product (extraction mode) or an accumulation of a reactant (accumulation mode).
6. Determination of the window of operating conditions of the reaction and the physical separation. Verification whether there is an overlap of these windows allowing physical integration of both functions.
7. Comparison of alternative technologies. Less economical alternatives are excluded. This last step contains the largest rule base of all steps of the module.

2.9 PROSYN® Reactive Distillation

This module tells whether reactive distillation is suitable for a given chemical reaction system as compared to conventional sequential reaction and distillation. If this is the case, the module indicates attainable separating cuts and column designs. Application of PROSYN® Reactive Distillation proceeds as follows:

1. Evaluation of the reaction system (components, reactants, reaction type, products and co-products, reaction rate and reaction enthalpy of the main reaction, type of side reactions and the separation of inerts, catalyst presence, equilibrium position, feed streams, reactant ratios…).
2. High-level evaluation of applicability of reactive distillation technology based on basic knock-out criteria. For example, reactive distillation is not applicable to a reaction with a high exothermic/endotherm effect.
3. Investigation of the distillation area (boiling points of singular components, possible binary and ternary mixtures…)
4. Establishment of reactive distillation areas after estimation of chemical equilibrium coefficients and determination of the presence of a reactive azeotrope.
5. Generation of a number of attainable separating cuts for several alternative column designs (number of feeds, number of reaction and distillation zones, with/without decanter…).
6. Proposal of column design parameters (qualitative): number of theoretical stages of each zone, reflux ratio...

The module is linked with a rate-based numeric simulation for reactive distillation.

2.10 PROSYN® Extraction

This module evaluates the suitability of extraction as a means of separating a given process stream into user-defined fractions. PROSYN® Extraction supplies a suitable design for the extraction process, aiding important choices for process synthesis, e.g., amount of solvent needed, composition of the outlet streams, number of theoretical transfer stages, and mode of operation (flow regime, type of reflux). In addition to the design, PROSYN® indicates which phase should be dispersed and which kind of extractor may be the most suitable.

The application of the module occurs by the following steps:

1. High-level evaluation of the applicability of extraction, including comparison with other technologies, e.g., distillation. The evaluation is based on phase behavior, solution behavior, etc.
2. Solvent selection based on criteria such as distribution coefficient, ease of distillation of the extract stream, difference in density between extract and raffinate. Solvents are assessed before the selection is carried out. Four alternatives are offered to determine the solvent: user input, a database of public domain extraction processes and patents, solvent screening (miscibility gap method), and application of the PROSYN® Solvents module.
3. Determination of operating conditions: pressure and temperature.
4. Selection of the mode of operation: flow regime (counter-current, cross-current), recycling of extract.
5. Preliminary dimensioning: e.g., number of theoretical stages, solvent-feed ratio, recycle ratio (if applicable).
6. Choice of dispersed phase based on direction of mass transfer, required interfacial surface area, volumetric flow ratio, …
7. Selection of extractor type (e.g., rotating disk contactor, centrifugal extractor) based on density difference, viscosity, …

A number of results in PROSYN® Extraction are displayed graphically, e.g., as a triangle diagram.

In the case that the user wants to design the recovery of the solvent (either by back-extraction or distillation) a difference instance of the appropriate PROSYN® module needs to be open. PROSYN® Extraction is limited to processes with only one feed and one solvent. The module is incapable to handle supercritical extraction processes.

2.11 PROSYN® Solvents

PROSYN® Solvents selects a suitable solvent from a database of commonly used solvents based on properties like polarity, hydrogen bonding, dispersion and size. This selection can be used to find a replacement for a solvent or a suitable extractant for liquid-liquid extraction. This module is under development.

2.12 PROSYN® Membranes

This module offers help in the selection and design of membranes and membranes units. A project is conducted in collaboration with TU Eindhoven and University of Twente to develop an up-to-date version of this module.

2.13 PROSYN® Membrane Reactors

PROSYN® Membrane Reactors is a recently built module for the selection of membrane reactor technology. It considers a number of different membrane reactor geometries. As membrane reactor technology is relatively new, not all of these geometries are technologically mature. PROSYN® Membrane Reactors verifies whether any membrane reactor geometry would fit an envisaged application. For this, the module asks the user for relevant input (e.g., expected flux through the membrane) and applies a set of heuristic-numeric rules. The outcome is a ranking of alternative geometries based on an absolute judgment of their suitability. The module can handle uncertain input, typical at an early stage of development.

The module does not verify whether the application of membrane reactor technology is suitable. As membrane reactors represent a physical integration of reaction and separation, PROSYN Reactive Separation is applied for this purpose. PROSYN® Membrane Reactors also does not assist in the selection of a membrane, for which PROSYN® Membranes can be used.

2.14 PROSYN® Properties

PROSYN® Properties is an interface giving access to physical properties databases and estimation methods. This module can be called by other modules when needed, but can also be executed on a standalone basis.

The functionalities are:

1) The management of physical properties of pure components and mixtures.
2) Providing physical property estimation methods, such as the estimation of NRTL parameters from the group contribution method UNIFAC for VLE and LLE.
3) Controlling access to physical property databases such as Aspen Plus Database or Wikipedia. **Aspen Plus must be licensed by the client before it can be accessed by PROSYN®**. We offer IT support for linking PROSYN® with the aforementioned databases.
   In addition to the above listed databases PROSYN® Properties offers the possibility to retrieve physical property data from Aspen Plus report files.
4) Default settings (e.g., databases, methods for physical properties).

5) PROSYN® Azeotropic Distillation can perform a topological analysis and azeotrope screening to predict the occurrence of binary and ternary (homogeneous/heterogeneous) azeotropes and close-boiling systems.
6) Properties visualization

The general strategy of PROSYN® regarding physical properties is:
1) In case a PROSYN® module needs physical property information, it calls PROSYN Properties.
2) First, PROSYN® Properties checks whether the required information has already been retrieved in the project.
   a) If so, the information is delivered back to the calling PROSYN® module.
   b) If not, PROSYN® Properties starts a search in the connected databases and displays the results.
3) The user may select one of the data sets which are available in the databases (if any), input another value, or start estimation routines to determine the information required. In case estimation methods are applied, PROSYN® Properties shows the results together with the existing database information. PROSYN® Properties offers a large variety of physical property estimation methods for pure components and mixtures. These methods have been selected out of the large amount of existing estimation methods by focusing on the most appropriate and most common ones. Physical property estimation for mixtures containing polymers, solids or electrolytes cannot be performed in the present version of PROSYN® Properties.
4) Once the user confirms the obtained physical property dataset, PROSYN® Properties stores it in the project data base and delivers the information back to the calling PROSYN® module.

2.15 PROSYN® Azeotropes

The PROSYN® module for Azeotropes investigation can handle multi-component mixtures for determining the presence of binary and/or ternary azeotropes. It uses the PROSYN® Properties module for determining the underlying properties needed for a quantitative search for azeotropes. Not only azeotropes can be calculated with this PROSYN® module, but many other physical properties can be selected for calculation, e.g., acid strength, activity coefficients, boiling points.

Results depend on the accuracy of the underlying physical property parameters and methods. Even though PROSYN® has access to a number of physical property databases and physical property calculation methods (e.g., UNIFAC and NRTL), it is recommended to verify any parameters applied when determining the occurrence of azeotropes.

The verification whether azeotropes are present is backed by the option to perform a qualitative search in a database of known binary and ternary azeotropes and to compare results. This database contains over 18500 binary azeotropes and 1000 ternary azeotropes.

PROSYN® Azeotropes is called by PROSYN® Azeotropic Distillation. However, when using the module on a standalone basis, the user has broader access to physical property calculation services and the user is more flexible towards various screening options (e.g., screening of close-boiling areas).

Although this module comprises some heuristic rules, it is largely based on numerical calculations and database data retrieval. Regarding heuristics, this module can predict (without calculations) whether a component mixture may be azeotropic, based on the azeotrope formation tendency between a series of homologues and the azeotropic range concept.

Also, class-oriented heuristic rules are embedded, i.e., azeotrope prediction is performed based on the tendency of forming hydrogen bonds between different classes of organic components along with application of the azeotropic range concept from the regular solution theory. In these ways, PROSYN® may predict azeotropic behavior in a wide variety of mixtures. This is especially useful for underspecified systems.

The Azeotropes module is a strong tool for many chemical engineering activities, especially process synthesis and the selection of a mass agent for azeotropic distillation or a mass agent for extractive distillation or extraction.