Process Design Center

REPORT

PROSYN® Membranes: Development of a public membrane expert system

Final public report

PROSYN® Membranes

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Summary

Over the past decades, interest in membranes has increased because of their separation performance and generally lower energy requirements. However, with at least 20,000 available membranes around the world, it is virtually impossible to select the most suitable one. Thus, it is complex and time-consuming for most process engineers to assess the feasibility of different types of membranes and systems. Also, it is not straightforward to contact the right membrane suppliers and developers. This contrasts with analyzing the feasibility of distillation applications that can be easily calculated. Therefore, membrane technology is still, to a large extent, unused, and potential energy-saving options remain unrevealed. This can severely affect the environment and the economy of the Netherlands with its world-leading membrane manufacturers and its large process industry as potential users. Therefore, our PROSYN® Membranes system will leverage human and artificial intelligence to address these challenges by providing the fast and structured selection and design of cost-effective membrane processes.

Since membranes can often be used as an energy-efficient alternative to distillation technology, it is expected that this can significantly save on CO_2 emissions. Because the Netherlands is rich in membrane unit suppliers, this leads to the competitive technological position of the Netherlands. The participating suppliers and potential end-users of membrane technology directly benefit from this. In addition PDC and the PROSYN® expert system are promoted. At the same time, the research centers and universities can address remaining knowledge gaps and strengthened their ties with the industry.

Within the PROSYN® Membranes project context, the system was updated and significantly expanded. Heuristics and numerical knowledge rules in the system were verified, adapted, and supplemented by academic partners, research institutes, and PDC/K&K. The system encompasses an extensive set of knowledge rules in the field of reverse osmosis (RO), nano-, ultra- and microfiltration (NF / UF / MF), pervaporation, vapor permeation, electrodialysis, membrane distillation and organic solvent nanofiltration. The updated PROSYN® Membranes is available via a web application. In various iterations, participating suppliers and potential industrial users validated the system with concrete separation cases. The system will be made publicly available after the end of the project.

As a result of the project, the expert system allows interested parties worldwide to check whether membrane technology could potentially be applicable and feasible for a specific separation.

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1 Project details

Project number

TEEI117002 (Program 1b. Energy-efficient process technology)

Project title

PROSYN® Membranes – Development of a public membrane expert system

Secretary and co-applicants

Participant name	Organization type	Role in the project
Process Design Center	*SME*	*Knowledge provider/developer & leader*
Keuken & de Koning	*SME*	*Knowledge provider*
Eindhoven University of Technology	*Research organization (no economic activity)*	*Knowledge provider*
University of Twente	*Research organization (no economic activity)*	*Knowledge provider*
Corbion	*Large scale company*	*End user*
Cosun	*Large scale company*	*End user*
Pentair/X-flow	*Large scale company*	*End user*
SolSep BV	*SME*	*End user*
Pervatech BV	*SME*	*End user*
Wafilin	*SME*	*End user*
NXFiltration	*SME*	*End user*
VITO	*Research organization (no economic activity)*	*End user*

Project period

1 April 2018 – 1 April 2022

Contact person for this project:

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Mohamed A. Mahmoud (mahmoud@process-design-center.com)

2 Background and objectives

Membrane processes are used sporadically in the Dutch and international process industry. In addition to the conservative approach that characterizes the process industry in general, membrane systems do not appear extensively in the normal process manuals or in the practice of comparative system studies by engineering contractors and consultants. One of the causes is the lack of easily accessible comparative tools with sufficient basic data to calculate a membrane process as a variant of existing processes. The main objective of this project is to change that.

The knowledge of membranes and membrane applications is hardly bundled and relatively difficult to access. The expert system PROSYN® Membranes from the 90s comprised an extensive set of knowledge rules in the field of reverse osmosis (RO), nano-, ultra- and microfiltration (NF / UF / MF), pervaporation, vapor permeation. The system also contained an outdated database with nearly 5000 membranes and modules and an additional physical property unit connected with the system.

In the meantime, new membranes and membrane applications emerged, and potential user of membranes are lacking concrete tools to make their way through this membrane forest. In fact, because a new potential user of a membrane application cannot master this domain, the chance that he or she will reach the right membrane, or the right supplier is extremely small. Of course, membrane suppliers are often willing to test certain separations, but if one has not first made a good membrane selection and preliminary design, one runs the risk of not being involved with the right type of membrane, supplier, or developer. This results in significant risk factors, not only for the membrane and the supplier in question but also for membranes as a solution for separations in general. Therefore, the end-user (industry), process developers, engineering contractors, membrane suppliers, and membrane developers need to update and develop a tool for better initial selection and preliminary design.

Goals

The project aims were as follows;

1. Revise the existing expert system PROSYN® Membranes,
2. Work on outdated matters,
3. Expand with the current membranes,
4. Make it publicly accessible to all possible users via the internet.

The effort within this project was to make at least an update until 2020 with the membrane community, suitable for internet-based deployment and a central platform for additional membranes and suppliers for the future.

The result is a public operational membrane expert system that is accessible worldwide free of charge and physically runs on a server under the management of PDC in Breda. The important learning process in this project was that we got a very detailed overview of almost the entire membrane domain and the application possibilities, which were made directly accessible to all users and for educational purposes (E-learning). In addition, users would come into contact with PROSYN® expert system and PDC's (AI based) conceptual design methodology.

Users and developers can also experience that there are gaps in their fundamental knowledge (substance properties and the like) to be able to continue within the expert system. For example, PROSYN® also provides additional support when estimating physical properties. Furthermore, a collective membrane expert system strengthens the synergy and promotes process innovation using membranes in general. For PDC, this project is an important marketing tool to enable with the industry to utilize PROSYN® expert system. PROSYN® has a monumental importance in the road towards creating a better industry and achieving sustainable and clean industry as it is considered the largest knowledge-based artificial intelligence system for process design in the world. PDC applies PROSYN® to provide feasible breakthrough process designs and road maps to more sustainable production. The Dutch process industry, the large engineering contractors in the Netherlands that operate worldwide, and the Dutch membrane and system suppliers can thus explore energy-saving options for well-balanced projects and improve their market opportunities.

3 Working method

The different work packages and tasks are shown below with timing and implementers (with work package managers underlined). The table below shows the summary of the working method.

WP	Short Description	Executors (with name)	Results	Start date and end date
1	Preparation of expert system for adjustment and expansion	PDC, K&K, TU/e, UT	Summary analysis existing expert system, List of needs for adjustment and expansion, IT development environment operational	1/9/2017-30/6/2018
2	Development and implementation of the expert system	TU/e, PDC, K&K, UT, producers	Extensive expert system operational with web-based access within the consortium, User manual	1/7/2018-31/8/2020
3	Validation of the expert system	PDC, K&K, TU/e, UT, End-users, producers, VITO	Expert system is operational with universal access	1/9/2020-31/8/2021
4	Knowledge dissemination	TU/e, PDC, K&K, UT	Two presentations at NL-GUTS member meetings (at the latest M48) Reporting on NL-GUTS website Two scientific publications and / or conference contributions	1/9/2017-31/8/2021
5	Coordination	PDC, K&K, TU/e	Results are achieved on time	1/9/2017-31/8/2021

4 Project results

4.1 Preparatory work

During the first phase of the project, an analysis of the existing PROSYN® Membranes system was performed to prepare the list of the needs for adjustment and expansion. Additionally, the new system's architecture with minimum required features was completed and confirmed with the project partners. Also, a significant amount of time was spent on converting all the documentation from German to English to make the system ready for an international audience. On the software engineering side, the environment for developing the web application was prepared and tested before the project's development phase.

4.2 Development

An incremental methodology (scrum agile) was adopted to update and further expand the existing expert system. In this method, updating the old system was divided into sprints of two weeks of work. At the end of each sprint, an incremental change to the existing system was tested and released. Using this method, and in the period of two years, the existing system was totally renewed and further expanded with the minimum number of generated bugs and consistent with the rest of the more extensive PROSYN® system.

Initially, and based on the expert knowledge obtained through interviews, a new algorithm for the applicability analysis of membrane processes was prototyped and validated through several case studies. After validation, the developed prototype was implemented in SWI-Prolog and GCC (the underlying PROSYN® development tools). The updated algorithm allows a dedicated applicability analysis over a complete range of membrane processes and offers a separate analysis for gas and liquid separation processes. Also, the list of applicable processes was expanded from seven basic processes to ten. Electrodialysis, membrane distillation, and organic solvent nanofiltration were added to the existing list of processes.

The newly developed applicability analysis, like the old algorithm, requires a specific set of physical properties that should be calculated based on the feed mixture and process specification. PROSYN® offers a dedicated physical property system with an extensive list of methods for pure substances and mixtures. However, to enhance the user-friendliness of the system, the method selection was automated using a proper algorithm and based on the applicable criteria of different methods. This minimizes the time and effort by the user to arrive at a first applicability analysis in a short frame of time.

Based on the analysis phase of the project, it was concluded that most data stored in the existing membrane database were outdated, and a new membrane and module database with an updated structure was required. The database structure was initially developed through several interviews with membrane experts and several internal discussions among the development team members. Accordingly, an updated membrane and module database was developed, tested, and implemented in the PROSYN® environment. Such a database was implemented in MySQL, a widely used open-source relational database management

system. Also, the existing PROSYN® databases were expanded to enhance the system's performance, and the Wikidata database was added to the system.

Another part of the project's development phase was dedicated to the development of rigorous design models for a wide range of membrane processes. Initially, a sophisticated design model was developed for the gas permeation process, followed by reverse osmosis and nanofiltration processes. Also, a simplified model was developed for pervaporation and vapor permeation processes. Next to that, a shortcut model was developed for the electrodialysis process specifically designed for the desalination of brackish water. Due to the extremely complex nature of ultrafiltration and microfiltration separation processes, the design models for these processes were left out after several trials together with the project partners.

Furthermore, a dedicated costing module was developed, prototyped, and implemented in the PROSYN® system. The expanded costing modules includes several costing methods with different precision level for each similar set of membrane processes. For calculation of CAPEX of membrane processes, the costing module requires information from the design models (i.e., total area of membrane needed for the desired separation), where OPEX calculation relies on the energy consumption of the process and energy cost, which the user should provide.

Next to that, the existing fouling analysis module of the PROSYN® system was analyzed, and its heuristics were updated and re-implemented in the PROSYN® environment. According to the feed stream specification, the fouling module enables the user to predict the chance of fouling (i.e., biofouling, organic fouling, and colloidal fouling). Also, the occurrence of scaling (inorganic fouling) can be evaluated by the existing PROSYN® system using its design rules and solubility databases. The existing databases were further expanded and validated using data from the available literature.

In parallel with the technical development of different modules of the system, significant work was dedicated to developing an operational web-based interface in which the user can access the developed system using a normal Internet browser. Regarding the user interface, it was implemented using a modern framework like jQuery, and Bootstrap for the graphical design, which will facilitate further extension and improvement.

To facilitate further deployment and scalability, it supports multi-user execution, meaning that several web users can access the same application at the same time without interfering with each other. Since the database resides in a different platform, MySQL, in case of future heavy load it is possible to deploy it on a different server. It will also be possible to launch several instances of the web application if we need to distribute the load among different web servers.

Due to the requirements of some potential users, a framework for the conversion between units, the metric system and imperial system was implemented from scratch. Now users can choose the system and currencies and specify different units for input values. It is worth mentioning that due to the complexities of the imperial system, the unit conversion

subsystem is quite complex, since it is not only about conversion factors, but also whether a given unit applies for a given situation or physical property, but also, since the number of basic properties in the system is big, around 660, it takes time to implement any change that affect all of them in this part of the system.

4.3 Validation

The validation part of the project was initially started with the RO and NF processes. For that, and using several case studies from the project partners, the quality of the system predictions was analyzed, and necessary changes in the system were implemented. Also, several extra features were added to the system based on the recommendation of the project partners.

For validation of the UF and MF, the project partners provided several case studies. Although the applicability analysis's validity was confirmed using the case studies, the system design models could not be validated to the complexity of these processes in practice. Typically, empirical correlations are required for such processes, which should be derived from pilot-scale experiments.

For validation of the PV and VP design models, data from industrial case studies were collected from open literature and compared with the models' predictions for identical cases. The results obtained showed that a good agreement between the implemented models and reported cases studies could be found.

4.4 Dissemination

During the lifetime of the project, two articles were published [1, 2]. In addition, the development team participated in eight workshops[3]. Also, during the last three months of the project, a workshop on the application of the PROSYN® Membrane systems was offered to the PDEng students at TU/e. In this workshop, the students were trained on how to use the developed system for the design of potential membrane processes in their electrochemical process design task.

4.5 Coordination

For coordination of the project and development of the expert system, a scrum-agile methodology was adopted. In this method, the development work was divided into several subtasks with different priority levels. Every two weeks (so-called one sprint), and according to the project's priorities and following the desired features of the system, several tasks could be covered. In total, more than 850 tasks (issues) were resolved within over 78 sprints of work. Also, to keep the project partners updated about the project's progress, project meetings were organized every six months.

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[1] Helmi, A. PROSYN Membranes - das freie, spezialisierte Auslegungs-Programmpaket fur Membranverfahren Teil 1: Struktur und Funktionalitat des Programms, F&S Filtrieren und Separieren, Jahrgang 33 (2019) Nr.4
[2] Helmi, A.; Gallucci, F. Latest Developments in Membrane (Bio)Reactors. Processes 2020, 8, 1239. https://doi.org/10.3390/pr8101239
[3] A. Helmi, E. Mera Menendez, M. Van Sint Annaland, F. Gallucci, PROSYN® MEMBRANES – knowledge based examination of membrane processes, ICCMR14 conference, Eindhoven 8-11 July 2019, (poster presentation)

5 Future work and challenges

The goal of the project was to develop an expert system that allows users to check whether membrane technology is applicable and feasible for a specific separation. This is important because membranes are one of the key technologies to make the process industry more sustainable. The next steps are the deployment and promotion of the developed PROSYN® Membranes expert system publicly. In this respect the user-friendliness is still far from ideal, and this is extremely important to get PROSYN® Membranes publicly accepted by the targeted audience. We also noticed during the development that the costing model would be extremely difficult to maintain, due to the dynamic nature of the membrane market which leads to uncertainty of the parameters and the results. Therefore, we decided to exclude the costing module from PROSYN® Membranes and to leave this to specialized vendors and consultancies like EMI. We also decided to exclude the fouling analysis and design models because they are either unpredictable in case of fouling or complex and require too much knowledge and data in case of the design models. Specialized vendors and consultancies are far better placed to address those detailed issues on a case by case basis.

To address the remaining above-mentioned challenges, PDC is currently in the process of hiring an expert in the field of user interface & user experience design to tackle them. The developed PROSYN® Membranes expert system in the framework of this collaborative project is meeting the main objectives as initially defined. The new expert system will allow the user to check the applicability of membranes and select the appropriate membrane module, which is a unique feature because comparative tools are lacking.

6 Implementation of the project

The implementation of the project was done with no significant problems (technical and organizational) despite the Corona period. No changes compared with the initial project plan were introduced. PROSYN® Membranes is now implemented and available on web platform that will be publicly available after upgrading the user-interface.

Acknowledgement

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