

A Hybrid Expert-Procedural System for the Design of Reverse-Osmosis Desalination Plants

D. Voivontas¹, K. Papafotiou¹, D. Assimacopoulos^{1*} and E. Mitsoulis²

¹ Department of Chemical Engineering, Section II, National Technical University of Athens 157-73, Athens, Greece

² Department of Chemical Engineering, University of Ottawa, Ottawa, Ontario, K1N 6N5 Canada

*Author to whom correspondence may be addressed. E-mail. assim@chemeng.ntua.gr

Abstract

The problem of computer-aided design and synthesis of a reverse-osmosis desalination plant is presented. A hybrid expert-procedural system has been developed that deal with the synthesis problem at two levels of abstraction. The expert part of the system uses qualitative data, and through heuristics, makes decisions about the structure of the plant. The procedural part of the system uses the decisions of the expert part as a basis for detailed design and optimisation. The heuristics used in the expert part come from experienced designers and from proposals of membrane manufacturers. The detailed calculations are based on mass balance equations and correlations for the permeators. The system developed can be used to propose a reverse-osmosis plant structure and to perform detailed calculations for possible design scenarios envisaged by the user. A case study on such a plant is also given and shows how the expert system handles the design problem of a reverse osmosis desalination plant.

Keywords: expert systems, computer-aided design, reverse osmosis desalination, plant design.

1 Introduction

Computer-aided process synthesis is an iterative procedure of transforming abstract ideas into industrial applications through: (i) the analysis of requirements, (ii) the design of the structure, and (iii) the implementation and testing of the application (Coad and Yourdon, 1991a,b; Douglas, 1985, 1988). A large number of methods have been used to tackle the procedure of computer-aided synthesis but in most cases missed to incorporate the basic idea of iterative approach. In traditional computer-aided methods, the iterative approach to the synthesis problem is not an easy task because analysis and design are considered as two different, sequential development stages. Object-oriented analysis and design methods come to bridge the gap between analysis and design. Object-oriented methods, in contrast to traditional methods, offer a unified approach to deal with all the stages of the synthesis based on the abstract model that is the result of the analysis.

A review of methods for computer-aided process design can be found in various references. Venkatasubramanian (1987) presented in his CACHE monograph the principles of artificial intelligence and knowledge-based systems. He developed the basic concepts for building an expert system and introduced some examples. Lien et al. (1987) adjusted the basic principles of expert systems in process design methodologies. Stephanopoulos (1990), and Muratet and Bourseau (1993) explored the applicability of artificial intelligence and expert systems in different aspects of engineering, presenting the current state of the art. Clive and Raymond (1991) presented the basic principles of expert systems development and introduced examples for a large range of

problems. Expert systems for process design or model selection have also been studied. Gani and O'Connell (1989) developed an expert system for the selection of an appropriate model, for physical property calculations in mixtures. Paranjape and Kudchadker (1993) built an expert system for the selection of the correct correlation, for the evaluation of physical properties of mixtures. Fujiwara et al. (1994) introduced an expert system for the synthesis of chemical reaction cycles. Bikos and Flower (1991) presented the basic layout of an expert system for the preliminary design and energy analysis of evaporative desalination cascades. Serra et al. (1997) presented a knowledge-based system for the on-line supervision of activated sludge processes. Coad and Yourdon (1991a,b) presented an object-oriented methodology for software development that can be used to build an expert system. Renard et al. (1993) presented an algorithm for the control of completeness of a knowledge base.

Strategies for the synthesis of reverse-osmosis desalination plants have been presented by Evangelista (1986), who proposed a graphical analytical method, by El-Halwagi (1992), who introduced an analytical procedure for reverse-osmosis synthesis for waste reduction. Papafotiou et al. (1992) developed an expert system for the synthesis of a reverse-osmosis desalination plant. Voros et al. (1996) used a superstructure in order to identify the optimum reverse osmosis network structure and predict the performance of the units employed in the plant.

A fundamental weakness of the expert systems presented above is that the researchers concentrated on the representation and handling of the domain knowledge in order to use it for decision-making. In most cases the dynamic interaction between qualitative decisions and detailed calculations is very

restricted. When quantitative data are used, these are in the form of indices, and therefore the knowledge base contains only qualitative information. However, it is the constant interaction between general decisions and analytical calculations which provides the only way to tackle the process synthesis problem.

In this study, an object-oriented analysis and design method is used, incorporated into an object-oriented programming environment, in an attempt to investigate its applicability to the problem of basic design of a reverse-osmosis desalination plant. The basic ideas presented by Papafotiou et al. (1992) are extended and the methodology for software development presented by Coad and Yourdon (1992a) is adjusted in order to incorporate the principles for the development of an expert system. The hybrid system developed here aims at the dynamic linking of abstract decisions with detailed computational algorithms. The organisation of basic domain principles, heuristics and technical characteristics into a computer program requires the use of a methodology able to formalise different kinds of information. This methodology is presented in section 2 and the synthesis problem is presented in section 3. Section 4 presents implementation issues about the specific application and section 5 presents a case study.

2 The hybrid expert-procedural design system

A fully object-oriented development methodology is employed, which enables the application developer to create an abstract model of the problem, and use it consistently throughout requirements analysis, system design, and

software implementation and testing. This approach seems to be able to provide the strong coupling between qualitative and quantitative knowledge, providing a recycling procedure of adding details to the model, until it meets the specified requirements. Furthermore, implementation of case studies at any point of detail allows the testing of each feature of the system along with the correctness of the heuristics used by the system.

The starting point of the development process is the *requirements analysis*. The analysis phase comprises the visualisation and translation of abstract ideas into detailed software requirements by creating an abstract model consisting of *objects*, *attributes*, and *behaviours*. This procedure is implemented by representing the problem domain in five levels of abstraction. *Subjects* are internal independent models used to break down a large problem. *Objects* are abstract models of entities involved in the physical problem used for the knowledge storage and recovery and the communication with other parts of the system. *Structures* represent the connections between objects and subjects in order to simplify a complex problem. The most common structures are *whole-part* connections and *general-special* connections. *Attributes* represent the characteristics of objects and give more detail to the model defining the data to which each model has access. *Methods* are the procedural part of the expert system defining the behaviour of each object.

The next step is the *software design* and the mapping of requirements to implementation procedures. In this phase, more details concerning the implementation in the programming environment enrich the model. The software design procedure focuses in three aspects. Changes that have to be

made in order to implement the *problem domain* model in the programming environment that will be used. The *interface* of the system, and the objects, attributes, and services that have to be created. The *data management* procedures that have to be created in order to implement the expert system's knowledge base.

The final step of the software development is the *implementation* of the system into the programming environment chosen. The programming environment that was used is Smalltalk / V Windows (1992a,b) because its basic concepts of application development are identical to the concepts of the analysis and design methodology that was used. The *whole-part* structures are implemented with attributes and services, for the global object, that represent its part objects. The *general-special* structures are implemented with the inheritance structure that comes with Smalltalk (Savic 1993, Shafer 1993). The result is an easy to use Windows Application.

The objective of the design system, developed in the present work, is to aid the designer to handle efficiently the process design problem by presenting alternative solutions of the process synthesis problem. In order to meet this objective three distinct parts have to be developed. The *expert system* contains the knowledge about the specific process design domain and controls the procedure for taking general decisions based on abstract information. The *procedural system*, which contains the appropriate mathematical models and operates as the solver for specific problems posed by the expert system. The *designer* is the part of the hybrid expert procedural system that is assigned with the linking of the expert and the procedural part providing the algorithm by

which abstract and quantitative information is linked. The methodology for the development of these parts is presented in the next paragraphs.

2.1 The expert system

The basic components of the expert system are the knowledge base and the inference engine. The *knowledge base* contains all the information required to solve the specific design problem. The *inference engine* invokes the sequence in which the knowledge base is handled and guides the search for a path that links initial conditions and final design decisions. The knowledge base contains the expertise necessary to solve the specific problem and the inference engine develops the procedure to approach the problem. The knowledge base and the inference engine are built on the experience of process designers and membrane manufactures. The user of the expert-procedural system developed will have the opportunity to obtain an additional view of the process synthesis problem.

The development of the expert system's knowledge base is the main part of the requirements analysis phase of the system development. As objects of the abstract model are identified the available knowledge of any form (technical characteristics, basic design principles, heuristics, basic mathematical models) about each object is gathered. The knowledge base is then used as the basis to identify the object's interaction with the rest of the entities involved in the model (structures) and the necessary attributes that have to be implemented in order to store the characteristics of the object.

The knowledge base is formed as IF-THEN rules that associate initial and final object states. During the design phase the interrelation of such decisions is identified, the attributes that store the qualitative representations of the input and output of each decision are defined and the methods that trigger each decision are designed. The same base is used to store and handle the quantitative data, such as the technical characteristics of the necessary equipment and the detailed design variables and requirements. The database developed contains technical characteristics of reverse osmosis membrane modules used for water desalination. In addition, the mathematical models and correlations describing the performance of membrane modules and data for their application are stored in the databases.

The inference engine of the expert system determines the order of the decisions to be made and uses the knowledge base and the user's requirements to solve any specific problem that comes forward. The necessary methods are the ones that identify the state of each object, the ones that select the decision that has to be performed and the ones that implement the decisions. This part of the expert system contains the artificial intelligence necessary to solve each problem that comes forward. In other words, it contains the strategy that will be used to tackle the design problem and determines the characteristics of each part of the unit.

2.2 The procedural system

The procedural part of the system uses the decisions of the expert part as the basis for the design of the structure found. The most important calculation is the evaluation of mass balances for each proposed structure. The mass

balance algorithms are implemented in the methods of the relative objects. The structure of the plant and consequently the mathematical model that describes streams and process units are defined from the expert part of the system. All the possible structures are covered by the design and implementation of the appropriate methods and the inference engine of the expert part selects the method to be triggered according to the selected structure.

The mass balances are resolved in two levels of detail. In the first, the system calculates the flowrate of each stream in order to validate the structure proposed by the expert part. In the next level the detailed composition of each stream is evaluated. Each object contains the methods to evaluate the characteristics of the output streams when the input streams are defined.

The mass balances require information that have to be defined either from the user or the expert part of the system. The user's specifications are stored directly into the appropriate attributes of the relevant objects. The data that depend on the expert systems decisions are stored in the knowledge base of the system. In any case, aside of the attributes that store and handle these data the appropriate methods are developed that access the knowledge base.

2.3 The designer

The basic coupling of the qualitative and quantitative calculations is in accordance with the strategy by which a designer approaches a synthesis problem. The designer uses some basic principles, heuristics, and in some cases intuition, to make fast decisions without any kind of analytical calculations. Then he/she uses these ideas as a basis to start detailed

calculations, and through constant revisions, reaches the problem solution. The system developed here imitates the designer's approach to the synthesis problem. The results of the expert part are used as the first approximation to the solution and form the basis of more detailed calculations.

The coupling of the expert and the procedural parts is implemented as different levels of detail are added, and not as a series of sequential development stages. In the beginning of the design, the expert part is assigned the decision making procedure about the structure of the plant without performing detailed calculations. In the next phase, after the structure of the plant has been defined, the procedural part is assigned the evaluation of the mass balances and evaluation of the characteristics of the plant.

The inference engine of the expert system performs the linking of the expert and the procedural part of the system. As the structure of the plant is defined based on heuristics and basic design principles stored in the knowledge base, the mathematical model that describes each object is used to evaluate the characteristics of the plant. Aside from methods of each object that represent the inference engine of the expert system and the procedural part of the design system the methods that gather the information derived from each object and handle the interaction of the system and the user are implemented in the object that plays the role of the designer.

3 The design problem

3.1 Reverse osmosis desalination

The basic layout of a reverse-osmosis desalination plant is presented in Figure 1. The feed stream of a desalination plant could be brackish water or seawater with total dissolved solids (TDS) in the range of 2,000 - 50,000 ppm. Pretreatment consists of a number of processes aiming to protect the membranes from salt or metal oxides precipitation, colloids fouling, suspended solids and biological growth on the membrane surface. Depending on the feed quality, pretreatment may include one or more of the following processes: acidification, conversion control, addition of precipitation inhibitors, ion exchange, pH control, filtration, coagulation - flocculation, chlorination. The high-pressure pump raises the feed pressure to 2.5 - 8.25 MPa, which is necessary for reverse osmosis. The pressure depends on the feed quality and the structure of the membrane system.

The structure of the membrane system may be one of the following:

- Single stage: The feed stream is distributed in a set of parallel-connected permeators.
- Multiple stages: The brine stream of the first stage is the feed stream of the next stage. The brine stream can pass through a third stage. This connection is repeated until the brine stream of the last stage is rejected. The product streams are mixed in the final product stream.

- Product staging: The first-stage product stream passes through a second high pressure pump and then into a second stage.

The membranes product stream contains a low concentration of TDS, which usually needs no further treatment for the reduction of its concentration. The post-treatment aims at refining the characteristics of this stream to meet the specific requirements of the plant product stream.

3.2 Identification of objects

Available data, calculations needed and the knowledge used define the objects of a model. In the case of the hybrid system for the basic design of a reverse osmosis desalination plant, the objects that constitute the abstract model are presented in figure 2. The basic object is the ROPlant object which is the reverse osmosis plant itself. The most important components of a reverse osmosis plant are the pre-treatment process and the membrane system that consist of a number of stages. The interrelation of these entities is represented in the abstract model by a whole-part connection where the ROPlant is the whole object and is connected to a Pretreatment object and a number of Stage objects. This connection between entities is implemented with additional attributes and services in the ROPlant object. These attributes are used to carry the characteristics of the part-objects to ROPlant, and the added services are assigned the connection and interaction between those objects.

The pre-treatment used in a reverse osmosis plant depends on the quality of the feed stream and is different for sea and brackish water. The objects *SWPretreatment* or *BWPretreatment* represent these processes respectively

and are connected to the *Pretreatment* object by a general-special connection which means that a number of the characteristics of the general object is inherited to the special objects.

The Stage object consists of a number of parallel connected permeators that are represented in the model with the object Membrane. Three subclasses of the object Stage are used in order to distinguish between the first (FirstStage object), the brine (BrineStage object) and the product (ProductStage) stages of the plant.

The streams of the plant are represented by the objects *ROStream*, *FeedStream*, *BrineStream* and *ProductStream*. Recycle streams are not treated differently by the expert-procedural system since this type of streams does not add any new behaviour. Their interaction with the rest of the plant is described within the relative objects (*Mixer* and *Splitter* objects describe the mixing and splitting of streams)

Attributes and services expand the model with details about the knowledge and the calculations for each object. The abstract representation of objects in Figure 2 becomes more detailed as shown in Table 1, where the attributes and services necessary to describe the characteristics and behaviour of the ROPlant object is presented. Attributes that describe a whole-part connection are, in fact, the representations of the part objects stored within the whole object (i.e. attribute InletStream of the ROPlant object represents a ROStream object). Services that implement the interaction of an object with its parts are either services that set the value of the relevant attribute, denoted by the name of the attribute followed by the character “:” (i.e. service “InletStream:”

defines the attribute *InletStream*) or services that return the value of the relative attribute, denoted with the name of the attribute (i.e. service “*InletStream*” returns the object represented by attribute *InletStream*). Table 2 shows the attributes and services of the object *ROPlant* after the software design level where the attributes and services that implement the object connections are presented. The same procedure is used for all objects, and the result of this stage of development is the class hierarchy shown in Table 3 (the abbreviations *SW* and *BW* stand for Sea Water and Brackish Water, respectively).

The expert-procedural system for the basic design of a reverse osmosis desalination plant can propose the appropriate plant based on the inlet stream definition and the product stream requirements by the user. The decisions that must be taken, before the detailed evaluation of the plant, are the definition of the plant structure, the selection of the most suitable pretreatment, the selection of the membranes that will be used, and the evaluation of conversion for each stage.

The definition of the plant structure is assigned to the *ROPlant* object. The flowrate and quality of the feed and product streams of the plant are defined by the user and the *ROPlant* object selects the appropriate plant structure according to its knowledge base which contains the rules to select among plants with a single stage or multiple brine stages or product stages. Should the system has a recycle stream is decided by the user and is taken into account during the mass balance calculations. The selection of the appropriate pretreatment is assigned to the object *Pretreatment* which selects whether to activate the *BWPretreatment* or the *SWPretreatment* object according to the

quality of the input stream. The selection of the membranes to be used is assigned to the *Stage* object and which activated every time a new stage is created. The estimation of the initial values of the conversion for each stage is performed by the *ROPlant* object in order to initiate the detail calculation of the plant. These conversions are re-evaluated during the mass balance calculations. Some examples of the rules available in the knowledge base on which the decisions of the expert system are based are presented in Table 4.

4 Implementation algorithms

The system designs a new plant with the user's specifications given in a dialogue. The user must specify: (a) feed characteristics (flowrate, detailed analysis), (b) product characteristics (flowrate, quality, pressure), and (c) the definition of plant parameters (pretreatment processes, energy recovery and brine recycle if necessary, number of plant trains). The detailed analysis of the feed stream is defined by another dialogue box. The user must specify the temperature, pressure, pH and ion concentrations of this stream, and the system checks the correctness of the stream characteristics.

When the user specifications are complete, the system performs the design, and the results are shown in the window as a process flow sheet. The detailed results that concern the plant in general, are shown through a dialogue box (inlet, brine and product streams, total conversion, pressure and temperature). Another dialogue box is used for the results of the design for one of the plant stages (conversion, pressure drop, number of membranes, membrane model, analysis of inlet and outlet streams). The user may modify

the conversion and the membrane model. This allows the evaluation of alternative schemes in order to optimise the results.

5 Case study

The case study that will be used to test the expert system developed here is the re-evaluation of the reverse-osmosis sea-water desalination plant that operates on the island of Myconos, in the Aegean Sea in Greece. The reverse-osmosis plant on Myconos consists of two parallel units with capacity of 600 m³/d each. The expert system will be used to design one of the parallel units. From the vast array of membranes available for desalination plants, only membranes made by Dupont are included in the database, because these were originally used in the plant (see reference on PERMASEP, 1982, 1984a,b).

The analysis of the sea water and the design variables are presented in Table 5 . The plant that meets these requirements is presented in Figure 3, and the detailed results from the overall plant calculations are presented in Figure 4.

As shown in Figure 4, the expert-procedural system proposes that a single-stage plant is adequate for the separation needed. Figure 5 shows the detailed results for this single stage of the plant. The difference between the TDS concentration in the plant inlet stream and the first-stage inlet stream is due to the pre-treatment used. The product has a TDS below the user specifications indicating that one stage with the selected membranes is adequate for the production of potable water.

The expert-procedural system checked the permeators (i.e. membranes defined by DuPont by their "type", e.g. B-9 or B-10, and "model", e.g. 6840T, etc.) available in the database through an iterative procedure, which decides on the basis of rejection criteria whether a permeator "model" can be used or not. The system rejected all the membrane "models" that cannot be used and proposed to the user one of the remaining permeators (DuPont B-10 "model" 6840T). It should be noted that in the existing plant, the DuPont B-10 "model" 6840T permeators were used based on the designer's expertise. This shows the ability of the system to make proper decisions.

The final decision remains with the user, who may accept the system selection or start again the procedure with a different layout. The system proposals help the user to avoid iterations to the wrong directions and concentrate on the solution paths that are more likely to reach the correct results. The user does not have to waste time checking all the membranes in the database.

The expert system also suggested an alternative that can be used in the present case study for the permeators, i.e. the DuPont B-10 "model" 6842TR. Figure 6 shows the detailed calculation results for the single stage with the above membrane "model". The use of this alternative affected the number of the membranes and the quality of the product and brine streams.

The expert system was used to compare 6840T and 6842TR permeators in a wide range of overall conversion. The results are shown in Figure 7. The product quality is almost identical but there is a slight difference in the number of permeators needed. The "models" 6840T or 6842TR cannot be used for

overall conversion over 40% because the brine stream produced in each permeator is not within the manufacturer's specifications.

In an effort to test the expert system for different cases, the same procedure was used to compare four membrane "models" with the operating pressure set at 6.89 MPa. The lower pressure is necessitated because of limitations in the use of the two new membrane "models" (6840, 6842R). The results are presented in Figure 8. "Models" 6840T or 6842TR result in more permeators than "models" 6840 or 6842R. The difference is due to the fact that the former two are designed to operate at the higher pressure of 8.25 MPa. The product stream has more TDS when the pressure is reduced.

A direct comparison between the scenarios presented in Figures 7 and 8 shows that membrane "models" at a higher pressure produce better product quality (lower TDS content) for a comparable number of membranes. An extra parameter that can influence the choice of design is evidently the total cost. The operating pressure is the main factor influencing the total cost of the plant. However, cost calculations and cost optimisation are beyond the scope of this work.

In order to evaluate alternative design scenarios the system has been used to design the plant in Myconos island with a brine recycle stream. The ratio of the brine stream that has been recycled to the feed stream has been set to 10, 20, and 30% while the stage conversion has been kept to 35%. The result of these alternatives are presented in Table 6. When the ratio of the brine stream that is recycled to the feed increases, the TDS of the product stream increases, but remains within the user specifications for the values selected.

When the 30% of the brine is recycled to the feed and the overall plant conversion is further increased the system proposes a two stage plant.

The results of these scenarios prove that the system is capable of performing the necessary calculations at a variety of user specifications and can come up with the plant structure that best fits the user specifications. The selection of the structure that will finally be adopted may then be based on cost assessments.

6 Conclusions

The main contribution of the present work is the introduction of a new unified approach for tackling: (i) requirements analysis, (ii) application design, and (iii) implementation of computer-aided process synthesis. The consistent approach to all the development stages of a computer-aided process synthesis tool has been achieved with the use of an abstract "model" that represents the physical entities of a reverse-osmosis desalination plant. The abstract "model" has been integrated into an easy-to-use tool for the basic design of the plant through an iterative procedure for addition of details and revisions.

The results from the case study of a desalination plant on the island of Myconos in Greece show that the expert system has come up with the proper solution and, can be used to reliably solve a reverse-osmosis desalination synthesis problem. The expert system results are in agreement with the current operating plant characteristics, but the expert system also provides more alternatives or scenarios to be investigated. Expansion of the present expert-procedural system to the direction of detailed calculations for mass transfer

coefficients and cost optimisation, and expansion of the knowledge base for detailed design of the pretreatment and post-treatment stages and for selection of an appropriate high pressure pump, are obvious future goals.

Computer-aided process synthesis and expert systems are highly active research areas. The expert-procedural system presented in this work is an example that process design can be simulated and implemented through a computer application when the proper development tools are used.

Acknowledgments

Financial assistance from the Natural Sciences and Engineering Research Council (NSERC) of Canada for one of the authors (E. Mitsoulis) is gratefully acknowledged.

References

Bikos, S. C. and J. R. Flower, "Preliminary Design and Energy Analysis of Evaporative Desalination Cascades", *Desalination*, 81, 483-503 (1991).

Clive, L. D. and L. E. Raymond, "Knowledge-Based Systems in Engineering", McGraw-Hill, Singapore (1991).

Coad, P. and E. Yourdon, "Object-Oriented Analysis", Prentice-Hall, New Jersey (1991a).

Coad, P. and E. Yourdon, "Object-Oriented Design", Prentice-Hall, New Jersey (1991b).

Douglas, J. M., "A Hierarchical Decision Procedure for Process Synthesis", *AIChE J.*, 31, 353-362 (1985).

Douglas, J. M., "Conceptual Design of Chemical Processes", McGraw-Hill, New York (1988).

El-Halwagi, M. M., "Synthesis of Reverse-Osmosis Networks for Waste Reduction", *AIChE J.*, 38, 1185-1198 (1992).

Evangelista, F., "Improved Graphical-Analytical Method for the Design of Reverse-Osmosis Plants", *Ind. Eng. Chem. Process Des. Dev.*, 25, 366-375 (1986).

Fujiwara, I., M. Sato, E. Kunugita, N. Kurita and M. Mitsuhashi, "EXPRESS: An Expert System for Synthesizing Chemical Reaction Cycles", *Comp. Chem. Eng.*, 18, 469-480 (1994).

Gani, R. and J. P. O'Connell, "A Knowledge-Based System for the Selection of Thermodynamics Models", *Comp. Chem. Eng.*, 13, 397-404 (1989).

Lien, K., G. Suzuki and A. W. Westerberg, "The Role of Expert Systems Technology in Design", *Chem. Eng. Sci.*, 42, 1049-1071 (1987).

Muratet, G. and P. Bourseau, "Artificial Intelligence for Process Engineering - State of the Art", *Eur. Symp. Comp.-Aid. Proc. Eng.*, October 1992, Toulouse, France, and also *Comp. Chem. Eng.*, 17, S381-S388 (1993).

Papafotiou, K., D. Assimacopoulos and D. Marinos-Kouris, "Synthesis of a Reverse-Osmosis Desalination Plant", *Trans. IChemE*, 70, Part A, 304-312 (1992).

Paranjape, P. K. and A. P. Kudchadker, "A Knowledge-Intensive Methodology for Thermodynamic Choices", *Comp. Chem. Eng.*, 17, 717-738 (1993).

"PERMASEP ENGINEERING MANUAL", E.I. Du Pont DeNemours, USA, December 1982.

"PERMASEP B-9 TECHNICAL INFORMATION MANUAL", E.I Du Pont DeNemours, USA, December 1984a.

"PERMASEP B-10 TECHNICAL INFORMATION MANUAL", E.I Du Pont DeNemours, USA, December 1984b.

Renard, F. X., L. Sterling and C. Brosilow, "Knowledge Verification in Expert Systems Combining Declarative and Procedural Representations", *Comp. Chem. Eng.*, 17, 1067-1090 (1993).

Savic, D., "Object-Oriented Programming with Smalltalk/V", Ellis Harwood, Chichester, West Sussex (1993).

Serra P., M. Sanchez, J. Lafuente, U. Cortes, M. Poch, "ISCWAP: a knowledge-based system for supervising activated sludge processes", Comp. Chem. Eng., 21, 2, 211-221 (1997).

Shafer, D., "Smalltalk Programming for Windows", Prima Publishing, Rocklin, California (1993).

Stephanopoulos, G., "Artificial Intelligence in Process Engineering - Current State and Future Trends", Comp. Chem. Eng., 14, 1259-1270 (1990).

Venkatasubramanian, V., "Knowledge-Based Systems in Process Engineering", CAChE Monograph, Columbia University, New York (1987).

Voros, N., Z. B. Maroulis, D. Marinos-Kouris, "Optimization of reverse osmosis networks for seawater desalination", Computers chem. Engng, 20, Suppl, S345-S350 (1996).

"Smalltalk/V Windows Manual Encyclopedia Of Classes", Digitalk, 1992a.

"Smalltalk/V Windows Manual Tutorial And Programming Handbook", Digitalk, 1992b.

Table 1. **ROPlant** object with its attributes and services.

ROPlant Object	
Atributes Names	Services Names
Stages	OverallConversion
NumberOfTrains	Recycle
OverallConversion	NumberOfTrains
Recycle	MaterialBalance
BasicRequirements	

Table 2. **ROPlant** after the design level.

ROPlant Object	
Attributes	Services
Stages	Stages
NumberOfTrains	AddStage:
OverallConversion	CalculateNumberOfTrains
Conversion	OverallConversion:
ConversionSpecified	OverallConversion
Recycle	Conversion:
BasicRequirements	Conversion
InletStream	ConversionSpecified
BrineStream	Recycle:
ProductStream	Recycle
ReverseOsmosisInletStream	BasicRequirements
Pretreatment	MaterialBalance
	MaterialBalancePerIon
	InletStream:
	InletStream
	BrineStream:
	BrineStream
	ProductStream:
	ProductStream
	ReverseOsmosisInletStream:
	ReverseOsmosisInletStream
	Pretreatment:
	Pretreatment
	NoPretreatment

Table 3. Application hierarchy

Root Object	Classes	SubClasses
ROClass	Membrane	SWMembrane
		BWMembrane
	Pretreatment	BrackishWaterPretreatment
		SeaWaterPretreatment
	Mixer	
	Pump	
	ROPlant	
	ROStream	FeedStream
		BrineStream
		ProductStream
	Splitter	
	Stage	FirstStage
		BrineStage
		ProductStage

Table 4. Examples rules on which the expert system decisions are based

Definition of the plant structure
<p>If Overall Conversion 10 - 60 And Feed Stream TDS 2000 -15000 ppm Then use one stage</p> <p>If Overall Conversion 60 - 70 And Feed Stream TDS 2000 -15000 ppm Then use two stages</p> <p>If Overall Conversion 70 - 80 And Feed Stream TDS 2000 -15000 ppm Then use three stages</p> <p>If Overall Conversion 10 - 40 And Feed Stream TDS >15000 ppm Then use one stage</p> <p>If Overall Conversion 40 - 50 And Feed Stream TDS >15000 ppm Then use two stages</p> <p>If Overall Conversion 50 - 70 And Feed Stream TDS >15000 ppm Then use three stages</p>
Definition of the pre-treatment
<p>If Feed Stream TDS < 15000 ppm Then use BrackishWaterPretreatment</p> <p>If Feed Stream TDS > 15000 ppm Then use SeaWaterPretreatment</p>
Selection of the stage membrane
<p>If Stage Inlet Stream TDS < 10000 ppm Then use Brackish Membrane</p> <p>If Stage Inlet Stream TDS > 10000 ppm Then use Sea Water Membrane</p>
Estimation of conversions for each stage
<p>If ROPlant has one stage Then Stage Conversion = Overall Conversion</p> <p>If ROPlant has two stages And uses Sea Water Membranes Then First Stage Conversion = 35% And Brine Stage Conversion estimated estimated</p> <p>If ROPlant has two stages And uses Brackish Water Membranes Then First Stage Conversion = 50% And Brine Stage Conversion estimated estimated</p> <p>If ROPlant has three stages And uses Sea Water Membranes Then First Stage Conversion = 35% And 1st Brine Stage Conversion =25% And 2nd Brine Stage Conversion estimated</p> <p>If ROPlant has three stages And uses Brackish Water Membranes Then First Stage Conversion = 50% And 1st Brine Stage Conversion =40% And 2nd Brine Stage Conversion estimated</p>

Table 5. Design variables and feed stream analysis.

Ca ⁺⁺	493
Cl ⁻	23597.4
Mg ⁺⁺	1572
SO ₄ ⁻	3272
Na ⁺	13391.7
HCO ₃ ⁻	174
K ⁺	0.0
SiO ₂	18
Fe ⁺⁺	0.0
CO ₂	1.4
Total conversion:	35%
Capacity:	600 m ³ / d
Product stream TDS:	500 ppm

Table 6. Results for the Myconos plant with the use of a brine recycle stream

	Scenario 1	Scenario 2	Scenario 3	Scenario 4	Scenario 5
Recycle Ratio (% of brine)	0	10	20	30	30
Overall Plant Conversion (%)	35	37.5	40.3	43.5	49
Number of Stages	1	1	1	1	2
Stage Conversion (%)	35	35	35	35	Stage 1: 30 Stage 2: 17.3
Product Flowrate (m ³ /d)	600	600	600	600	600
Product TDS (ppm)	386.4	420.4	466.6	482.8	524.4

List of Figures

Figure 1. Reverse-osmosis desalination plant.

Figure 2. Objects and model structure.

Figure 3. Single-stage plant for the case study of a desalination plant on the island of Myconos, Greece.

Figure 4. Overall plant design results for the case study.

Figure 5. Particular stage calculations for the case study with the DuPont B-10 "model" 6840T membranes proposed by the expert system and actually used in the plant.

Figure 6. Particular stage calculations for the case study with the DuPont B-10 "model" 6842TR membranes (alternative suggested by the expert system).

Figure 7. Comparison of DuPont B-10 "models" 6840T and 6842TR membranes for different conversions (operating pressure 8.25 MPa).

Figure 8. Comparison of DuPont B-10 "models" 6840, 6842R, 6840T and 6842TR membranes for different conversions (operating pressure 6.89 MPa).

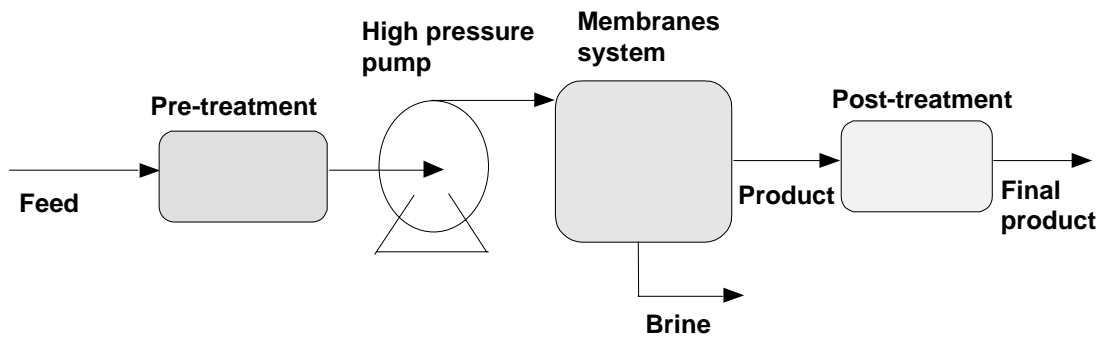


Figure 1. Reverse-osmosis desalination plant.

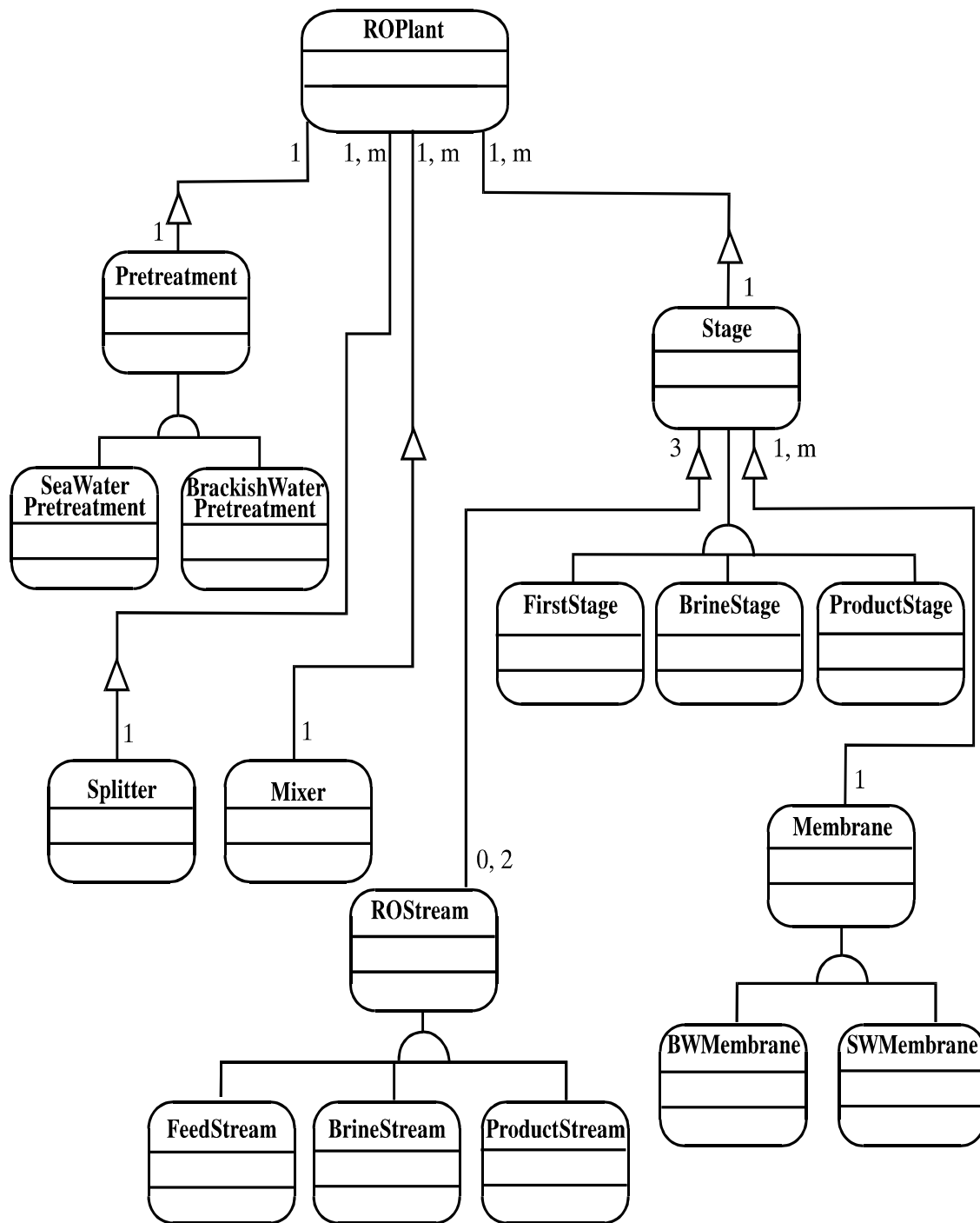


Figure 2. Objects and model structure.

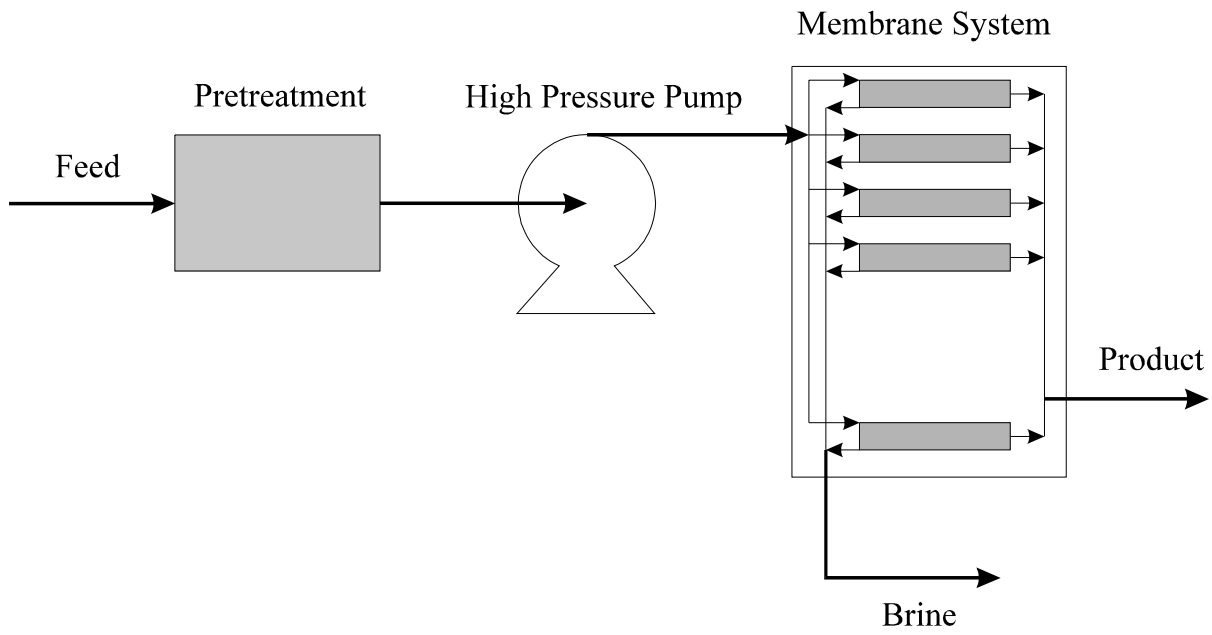


Figure 3. Single-stage plant for the case study of a desalination plant on the island of Myconos, Greece.

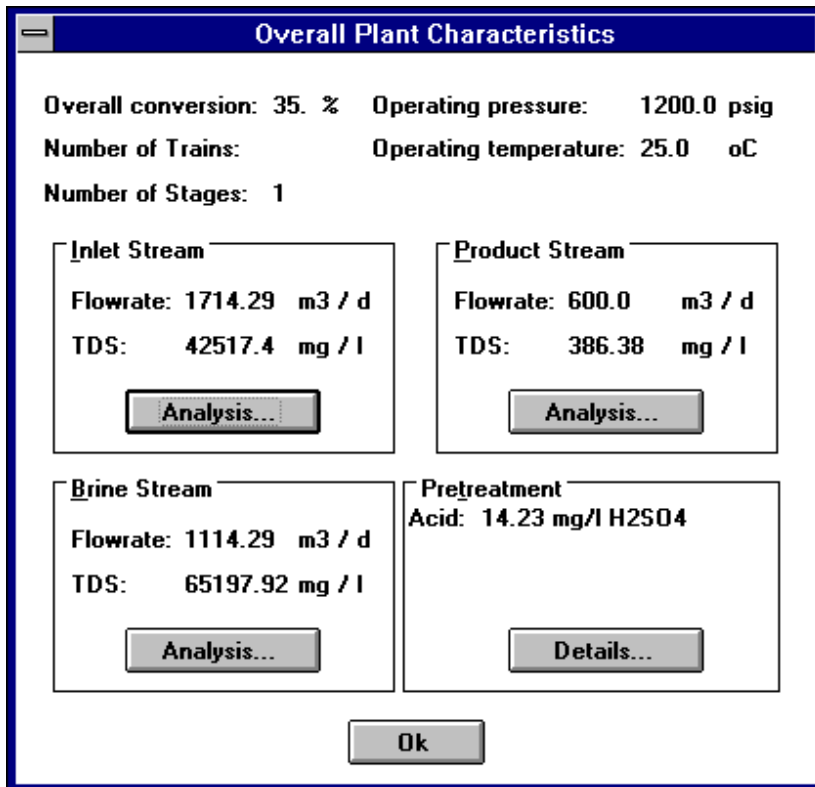


Figure 4. Overall plant design results for the case study.

Stage Characteristics	
Conversion:	35.0
Flow Balancing Pressure Drop:	20.0 psig
Number of Membranes:	35.0
Membrane	
Type:	B-10 Arami
Model:	6840T
Select...	
Inlet Stream	
TDS:	42513.88 mg / l
Flowrate:	1714.29 m ³ / d
Pressure:	1200.0 psig
Analysis...	
Brine Stream	
TDS:	65197.92 mg / l
Flowrate:	1114.29 m ³ / d
Pressure:	1159.89 psig
Analysis...	
Product Stream	
TDS:	386.38 mg / l
Flowrate:	600.0 m ³ / d
Pressure:	10.0 psig
Analysis...	
Ok Cancel Help	

Figure 5. Particular stage calculations for the case study with the DuPont B-10 "model" 6840T membranes proposed by the expert system and actually used in the plant.

Stage Characteristics	
Conversion:	35.0
Flow Balancing Pressure Drop:	20.0 psig
Number of Membranes:	37.0
Membrane	
Type:	B-10 Arami
Model:	6842TR
Select...	
Inlet Stream	
TDS:	42513.88 mg / l
Flowrate:	1714.29 m3 / d
Pressure:	1200.0 psig
Analysis...	
Brine Stream	
TDS:	65198.12 mg / l
Flowrate:	1114.29 m3 / d
Pressure:	1161.05 psig
Analysis...	
Product Stream	
TDS:	386.01 mg / l
Flowrate:	600.0 m3 / d
Pressure:	10.0 psig
Analysis...	
Ok Cancel Help	

Figure 6. Particular stage calculations for the case study with the DuPont B-10 "model" 6842TR membranes (alternative suggested by the expert system).

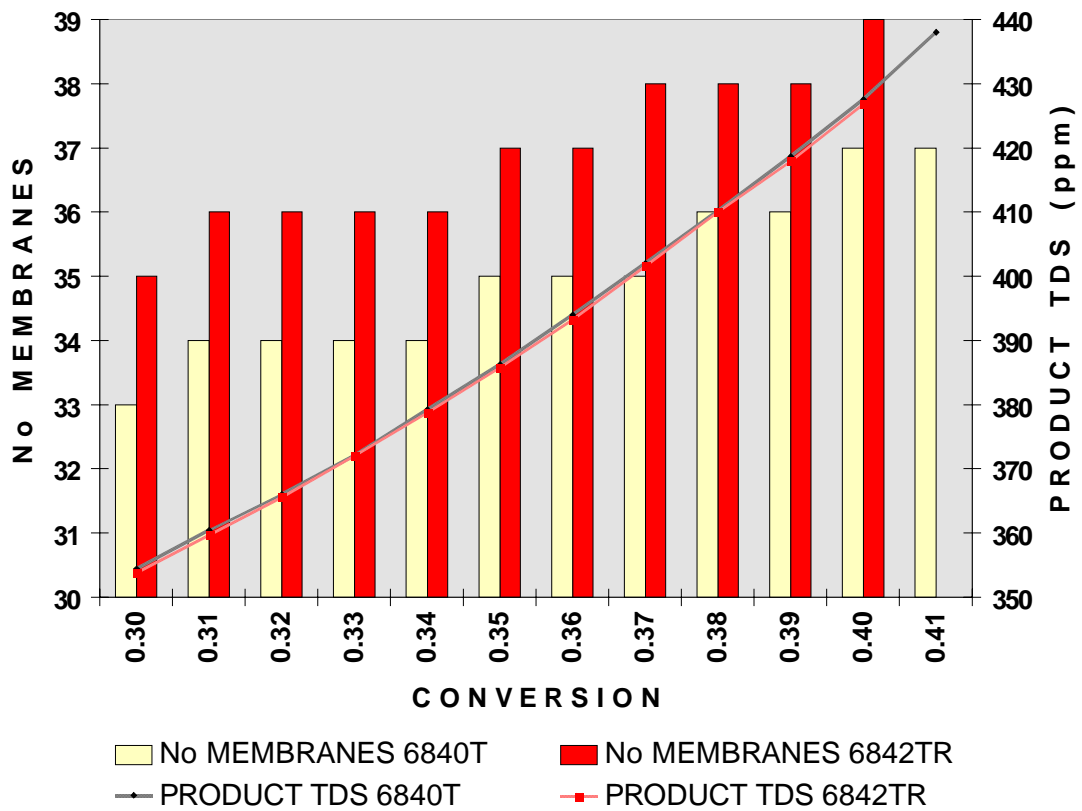


Figure 7. Comparison of DuPont B-10 "models" 6840T and 6842TR membranes for different conversions (operating pressure 8.25 MPa).

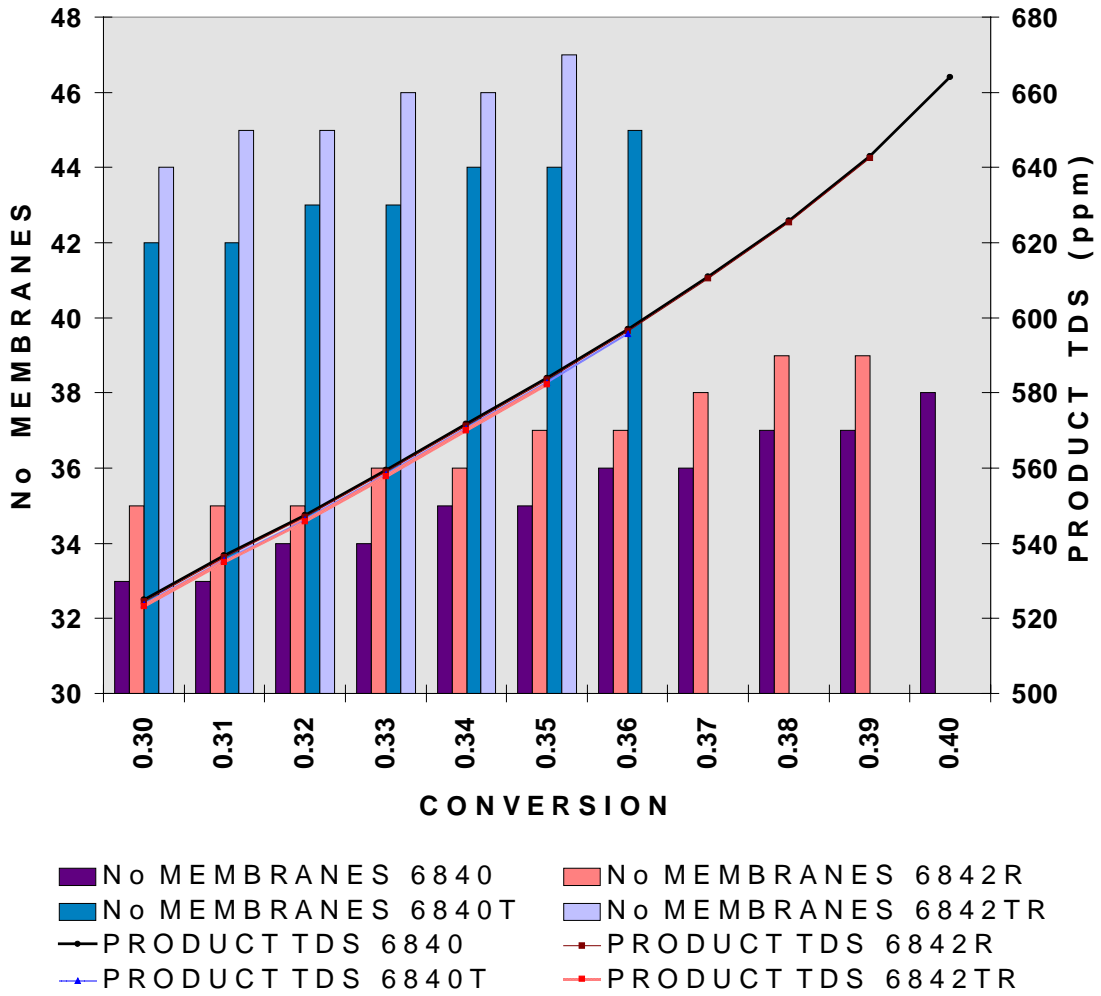


Figure 8. Comparison of DuPont B-10 "models" 6840, 6842R, 6840T and 6842TR membranes for different conversions (operating pressure 6.89 MPa).