

COMPLEX DISTILLATION COLUMNS DISC

R Smith, J Klemes, K A Amminudin, D R Webb, S Skogestad, I J Halvorsen,
E Marechal, G Heyen, O Nicolas, L. Puigjaner, A. España, A. Delgado,
M. Graells, A. Huercio, A. Mehlhorn, J.M. Nougués, M. Serra, F. Wilkendorf,
C Caracostis, M. S. Imellos, A Lopez-Garcia, F Lestak, D Egenes, J Fletcher,
A B Hinchliffe

**University of Manchester Institute of Technology, Department of Process
Integration, UK (UMIST)**

University of Trondheim, Norway (UT)

LASSC, University of Liege, Belgium (ULg)

Paragon S A, Athens, Greece (PARAGON)

**Universitat Politècnica de Catalunya, Chemical Engineering Department,
Spain (UPC)**

INFOSERVICIOS S. A., Madrid, Spain (INFOR)

M W KELLOGG Ltd, Kellogg Tower, Greenford, Middlesex, UK (MWKL)

University of Aston, Birmingham, UK (ASTON)

Contract JOE 3-CT 95-0035

PUBLISHABLE FINAL REPORT

1 April 1996 to 31 March 1998

Research funded in part by
THE EUROPEAN COMMISSION
in the frame of the
Non Nuclear Energy Programme
JOULE III

Abstract

Previous work has seen (1) the development of a short cut design technique for thermally coupled distillation systems and (2) initial studies on the control and operability aspects of the Dividing Wall Column (DWC). The objective was to improve the existing short cut design techniques to cater for more realistic industrial applications. UMIST developed a novel methodology for steady-state design optimisation, to be applied to a wider range of problems, and multicomponent rather than ternary separations, the use of stripping steam and the other systems. The development of software supporting this new methodology was substantial contribution.

UT studied control issues. Results show that the DWC can be controlled by conventional control structures. The optimal operation point is strongly dependent on feed composition and on the product specifications. When three product composition loops are closed, adjustment of liquid and vapour flow splits can be used to minimise energy consumption. From analysis of the shape of the solution surface can be seen that at least one of these inputs should be adjustable on-line in order to maintain close to minimum energy consumption when feed parameters may be varying.

PARAGON has developed: a) A Fluid mechanics code for the modelling of the flow, b) An optimisation code based on Genetic Algorithms for the optimisation of the operating degrees of freedom, and c) An Artificial Neural Nets (ANN) for the modelling of the DWC.

UPC and INFOR have developed an intelligent system framework supporting the DWC control system, including Fault Diagnosis. First, UPC performed several steady state and dynamic studies, leading to design and control strategies that optimise energy consumption and improve controllability indexes. A novel DWC dynamic model useful for forecasting and predictive control was designed. The model, based on ANN, can be continuously actualised by a genetic algorithm (evolutionary model) and has been integrated in the centralised control strategy of the whole DWC finally developed.

ULg has studied the implementation of DWC in two processes. They extended the modelling capabilities of available simulation software to DWC: the heat transfer across the dividing wall can now be simulated accurately. The modified simulation software was used to carry out a detailed case study of an existing gas separation plant.

MWKL, utilising their wide base in the chemical, gas and refining industries, completed a rigorous analysis, using actual plant/design data. It demonstrated that DWC's provide a significant reduction in energy demand. The highest energy savings of 33 % were predicted for a refinery fractionation problem producing gasoline-blending components.

ASTON completed work on the air-water simulator to determine the liquid distribution in a packed section in a DWC.

Keywords: Dividing Wall Distillation Column, Novel Methodology, Energy Saving

1 Partnership including names and addresses of co-ordinating institutions and one contact person per partner

Co-ordinator:

University of Manchester Institute of Technology, Centre for Process Integration (UMIST), PO Box 88, Manchester, UK; leading scientist in charge of the project Professor Robin Smith, contact person Dr Jiri Klemes.

Partners:

Department of Chemical Engineering, University of Trondheim - NTH, Sem Saelands vei 6, Trondheim, Soer-Troendelag, N-7034 Norway, contact person Professor Sigurd Skogestad

Laboratoire d'Analyse et de Synthèse des Systemes Chimiques, Universite de Liege, Sart-Tilman -B6A, Region Wallone, Liege, B-4000, Belgium, contact person Dr Georges Heyen

Paragon Ltd, Niovis 8, Galatsi, Attiki, Athens 11146, Greece, contact person Dr C Caracostis

Universitat Politècnica de Catalunya UPC, Department of Chemical Engineering. Av. Diagonal 647, 08028 Barcelona, Spain; contact person Professor Luis Puigjaner.

Inforservicios, S.A. Sociedad Anonima, Technical Department, Emilio Munoz 31, Comunidad de Madrid, 28037 Spain, contact person Technical Manager J Rodríguez-Violta.

M W Kellogg Ltd, Process Engineering, Kellogg Tower, Greenford, Middlesex, UK, contact person Dr Frigyes Lestak.

Department of Chemical Engineering, University of Aston, Aston Triangle West Midlands, Birmingham, B4 7ET, UK, contact person Dr John Fletcher

2. Objectives

Distillation consumes large quantities of energy in the petroleum, petrochemical and chemical industries. Process integration has proven to be very successful in reducing the energy costs for conventional distillation arrangements. However, the scope for integrating conventional distillation columns is often limited. These limitations can be overcome by using non-conventional column designs.

One of the most significant non-conventional arrangements involves “thermal coupling”. Thermal coupling (Fig 1) is used at present in the form of side-stripper arrangements in the petroleum industry. Such arrangements have not been used outside of the petroleum industry. More effective thermally coupled arrangements than side-strippers are possible.

The thermally coupled arrangement is often much more effective than a side-stripper and has been known for over 50 years. It has been established that, when the thermally coupled design in Fig. 2 can be applied, energy savings of 30% are typical when compared with a conventional arrangement. In addition, the thermally coupled design, known as the DWC, can in new designs save up to 30% of the capital cost in addition to 30% energy saving, compared with a conventional arrangement.

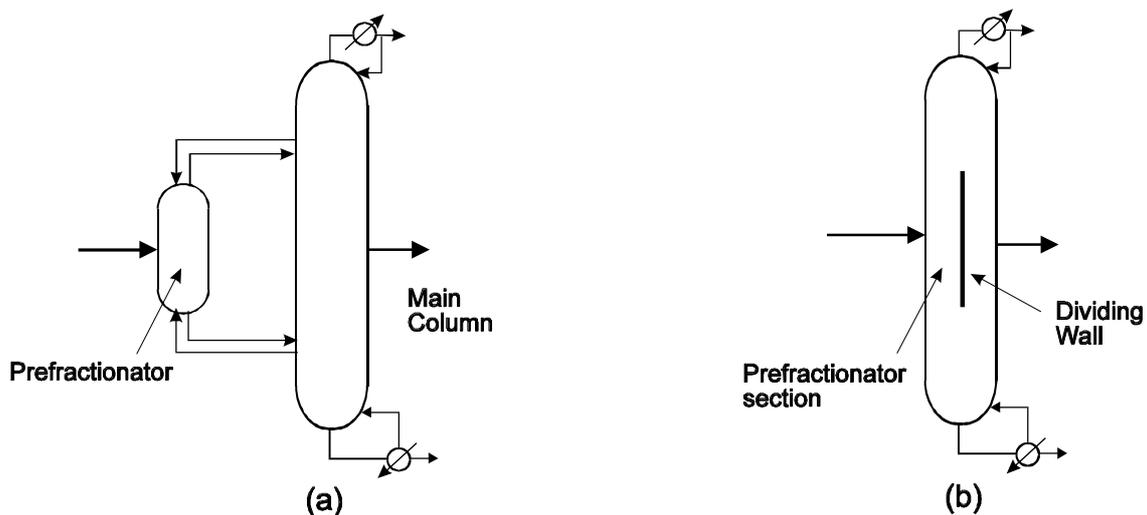


Fig 1: The fully thermally coupled column (a) and the DWC (b) are thermodynamically equivalent.

Although designers have been aware for many years of the improved energy efficiency possible with the designs shown in Fig 1b, such designs have until recently not been used. The sole exception is the recent use of the design by BASF. The reason for reluctance to use these designs is rooted in three reasons:

- (i) Lack of established design procedures
- (ii) Fear of control problems
- (iii) Reluctance to use untried technology.

New design methods for the arrangements in Fig 1b have to be established which optimise the design for minimum energy consumption and allow initialisation of the rigorous simulation. Control had to be studied theoretically at UMIST using dynamic simulation and in a new DWC pilot plant (0.3m diameter, 10.5m height). The control schemes studied indicate that the DWC can indeed be successfully controlled. An evolutionary modelling tool for the dynamic

simulation of the DWC based on artificial neural networks and genetic algorithms has been proposed by UPC to be part of a centralised (model predictive) control system.

If the full potential for thermal and mechanical coupling was applied effectively throughout the European petroleum, petrochemical, and chemical industries it would create substantial enormous energy savings, capital reduction and/or yield improvements. Before the full potential of thermal coupling can be established across the European chemical industry further work is required:

- (i) to refine the design procedures to allow a wider range of designs to be analysed
- (ii) to investigate theoretically and practically the hydraulic design of thermally coupled columns
- (iii) to examine a range of generic processes (eg petroleum refining, ethylene production, etc.) to find suitable applications of the technology.

The fluid mechanics of the fluid flow inside complex columns modelled with a Finite Element model. Design methods for the material and energy balance, hydraulic design and control will be developed and tested using simulation and pilot plant tests.

3. Technical description

WP 1 Development of novel technology to allow complex columns to be used on a wider range of problems.

WP 1.1 Development of design methodology (UMIST)

UMIST is a co-ordinator of the project and assumes a leading role in the development of the new methodology (WP1). The objective has been to develop a methodology for steady-state design optimisation, to be applied to a wider range of problems, and multicomponent rather than ternary separations, the use of stripping steam and the other systems.

The novel design procedure is essentially the extension from Triantafyllou and Smith (1992) short cut method. It incorporates new design features such as the calculation of product distribution and an improved optimisation procedure. The revised method can extend its applications to more than one middle key component; account for non-sharp separation for lighter than light key (LLK) and heavier than heavy key (HHK) components; and employ mathematical programming for design optimisation purposes. The design obtained from the revised method is used to initialise the rigorous simulation using a commercial process simulator.

The procedure is tested on the case study of applying the DWC to replace both the debutaniser and depropaniser in the separation trains of the refinery complex. The short cut design result provides an initialisation for the subsequent rigorous simulation. Nevertheless, the simulation needs to be fine-tuned in order to meet the desired product specifications. No convergence problems are noted during the runs. The results confirm that the use of DWC could generate significant energy savings (up to 35%) when compared with the conventional column arrangement.

WP 1.2 Software development (UMIST, ULg, UPC, INFOR, ASTON)

UMIST developed the prototype software. Novel extended methodology was implemented into software that should be robust enough to deal with a wide variety of feed or product

specifications such as low middle key feed component and impurity specifications. In addition, this software should be extended to retrofit scenarios as revealed in the column revamping study.

The novel short cut design procedure, which was presented earlier in this report, is developed into software employing mathematical programming package, GAMS TM. This software enables the user to develop the model and to solve for optimum configuration of the DWC. Due to its thermodynamically equivalent, the column is modelled as a fully thermally coupled column with a provision that there is no heat transfer across the wall.

For comparison and evaluation purposes, UPC has analysed the most appropriate design parameters for minimum energy consumption. Parameters α (molar fraction of the light component in the bottom product) and β (fraction of all the middle component in the feed that exits the prefractionator with the head product) have been identified as appropriate for this purpose. The search of appropriate α and β parameters has been done in a systematic way. Therefore, a design strategy based on shortcut and rigorous simulations has been developed for a separation problem defined by:

- the composition of the mixture,
- the conditions of the feed and
- the required purity of the three product streams.

In order to illustrate the strategy, the energy consumption required by different designs of the divided wall columns has been calculated. The systems benzene-toluene-orthoxylene and ethanol-propanol-butanol have been studied. Shortcut as well as a rigorous steady state simulation of the DWC have been implemented in the program ProVision / ProII (a flowsheeting simulation package developed by SimSci).

As the final criterion for the application of divided wall columns in industry is the economics of this configuration in comparison with other separation techniques, optimisation of the design should always take into account the total costs of the solutions proposed. Therefore, UPC has proposed a cost function that allows to compare the influence in the final cost of all the design variables. Analysing the DWC it can be concluded that the main emphasis in design should be the reduction of the energy required. Other objectives like similar number of trays on both sides of the wall for smaller shells are only interesting if there is no significant penalty in energy. Nevertheless, the size of the column and therefore the energy savings are limited by other restrictions than cost as pressure drop, fluid dynamics or construction aspects.

UPC has also developed a novel neural network simulator (UPC proprietary software) for use in real time simulation and control of the DWC. Simulation results have been tested against modelling of the DWC developed using SPEEDUP commercial package (see WP 5.1).

ASTON developed software for analysis of the results of the hydrodynamic experiments and comparison with the performance of the UMIST column.

WP 1.3 Pilot Plant Tests (UMIST)

The pilot plant tests generated sufficient pilot plant data and were carried out during the reported period. The pilot plant data collected during the project were presented in Deliverables No 9 and have been widely used by project partners.

WP 1.4 Extension of developed methods (ASTON, PARAGON)

The Artificial Neural Network (ANN) developed and trained in the WP 4.3 was applied for the prediction of two fully thermally DWDs. The State-of-the-art in the ANNs was examined and reported in Deliverables No1. From this State-of-the-art examination results the recommendation that most appropriate ANN type for prediction purposes is the widely used Back-Propagation Neural Network (BPNN). UPC were not initially planned to be involved in the WP 1.4. UPC offered their collaboration to contribute by their expertise on ANNs. In this sense, UPC has collaborated in the selection and development of the most appropriate ANN for the modelling of DWC, as reflected in Deliverable No 1.

WP 1.5 Experimental testing of the hydraulic simulation model (ASTON)

ASTON undertook experimental studies to observe and quantify liquid distribution in a packed column close in specification to the pilot scale divided wall column at UMIST using an air water system to simulate the conditions. Experiments have been made to study flows in a D section column and quantify the distribution of the liquid in the packing.

WP 1.6 Evaluation of the industrial applications (MWKL)

A number of industrial applications were investigated where the application of DWC technology could save energy and/or capital. The applications covered the refinery, chemicals and gas processing industries.

Energy savings up to 33 % were reported by MWKL. Other case studies reached 27 % and 19 % energy savings. Significant capital saving were also achieved.

DWC's are not only beneficial for energy savings, but also for capacity increase and improvements in product quality.

WP 2 Identification of control problems and analysis of controllability**WP 2.1 Identify control problems (UT)**

The focus has been on identifying control problems, and in particular on any problems related to operate the column close to minimum energy consumption. This is an important issue for the DWC since saving energy is one of the motivating factors for using this kind of column design.

From a control point of view it is interesting that we have more degrees of freedom in the control inputs, than specifications of products. Then the extra degrees of freedom may be used for other purposes, like minimisation of energy consumption.

It has been shown that when three product compositions are specified, the use of the extra degrees of freedom are quite important. If the liquid and vapour split ratios are not carefully set, according to product specifications and feed conditions, the result may be very large energy consumption, or failure to fulfil specifications.

Based on RGA analysis and simulation results, the regulatory problem of keeping product purities at the specified values is similar to conventional columns. That is, we have strong interactions, and analysis to choose good pairings is important for the control performance.

WP 2.2 Dynamic Behaviour (UT, ULg, UPC)

A dynamic model of the DWC has been developed by UT and has been used for dynamic simulations and steady-state computation in order to get an understanding of the column behaviour.

UPC has implemented a dynamic shortcut model of the divided wall column in the commercial software package SPEEDUP. For several separation problems, the dynamic behaviour of the divided wall column when leaving the nominal operation point have been studied. The benzene-toluene-xylene (BTX) and methanol-isopropanol-butanol systems have been analysed. In order to compare with real results, the pilot plant of UMIST was one of the simulated columns.

ULg has developed a dynamic model of a thermally coupled distillation system using its own dynamic simulation program DYNA. DYNA is based on general DAE formulation (differential algebraic equation) and uses rigorous thermodynamics to compute the liquid-vapour equilibrium.

Co-operation between ULg, UT and UPC has allowed the development of the same process using models of different complexity and different systems. The BTX model developed within DYNA uses the identical command parameters [Rl, Rv, L, S, V] as the UT model (steady state results are nearly identical). ULg has also computed the gain matrix and transfer functions with the DYNA model and the associated package. The comparison shows a reasonable good match, and differences can be explained by details in the different complexity level.

Further enhancement could include better hydraulics modelling such as variable tray hold-up and pressure drop. In particular for studying the effect on the vapour split. A series of simulations have been carried out on the different systems.

The dynamic behaviour of the DWC is quite complex. But there are obvious similarities to binary columns, at least for the top and bottom product compositions. The available models seem to be able to predict the dynamic behaviour quite well.

The BTX separation process studied in WP 3.1 was used as a base case. Below, the steady-state composition profiles from ULg's DYNA and UT's simple staged modes were compared. The result is quite good. The dynamic responses were also quite similar.

The main properties of the composition and temperature profile are calculated by the MATLAB model with the assumption of constant relative volatility in sections. This is not surprising, since this can be expected for many hydrocarbon mixtures.

```
Title: fig/cprof_c.eps
Creator:  MATLAB, The Mathworks, Inc.
CreationDate:  10/06/97  11:43:02
```

WP 2.3 Propose control schemes for divided wall column (UT, UPC)

UT has used the dynamic model from WP2.2 as a basis for studies on control schemes. In order to achieve operation close to the theoretical minimum energy consumption, and at the same time keeping product specifications within specifications, it is important to use active control. At the same time it is also important to know the kind of design decisions which makes control easy or difficult. The proposed control schemes are kept as simple as possible and we use conventional structures. This makes implementation in existing industrial control systems straight forward.

UPC has calculated steady state gains of different process transfer functions for the DWC studied in WP 2.2. A measure of the resiliency of these processes has been given by the Morari Resiliency Index (MRI). Unworkable pairings of variables have been detected through the Niederlinski index (NI). An analysis of the interaction among control loops has been developed through Relative Gain Array matrix (RGA).

WP 3 Integrated study of dividing wall distillation columns

WP 3.1: Feasibility of implementation of thermally coupled distillation in a process (ULg, UPC)

UPC has analysed three different separation problems that are common in the industrial practice: ethanol-propanol-butanol, benzene-toluene-ortho-xylene and benzene-toluene-paraxylene. Conventional designs for multicomponent separations namely, the trains of columns have been compared with the best solution given by a divided wall column. Solutions have been obtained using the design methodology for minimum energy developed (WP 1.2). Steady state simulations of the divided wall column as well as simulations of direct and indirect trains have been implemented in the program ProII / ProVision. The results have been obtained in close collaboration with ULg and are presented with more detail in the deliverable of WP 3.1. Important energy savings (20 % - 39 %) could be achieved for the DWC in all these cases.

ULg objective was to develop a model for steady-state simulation of a state of the art industrial process and identify parts of the process that can be replaced by Thermally Coupled Distillation (TCD) systems. Next a new model has been developed for the same process that includes the TCD columns. Finally, one had to perform the heat integration of both processes to compare with energy savings that can be gained using existing energy integration techniques.

The BTX separation process was chosen because it is a multicomponent separation and because in the first part of the process, the feed stream is split into three fractions. Thus it appears to be a suitable candidate for implementation of TCD technology. The feed stream includes the following chemical compounds: benzene, toluene, ethylbenzene, o-xylene, p-xylene, m-xylene.

Process simulation

1. The conventional arrangement design has been made considering the feed and products specifications. For classical columns arrangements ULg uses its own short cut models.
2. Rigorous and multicomponent simulation has been done. Rigorous simulation results are analysed to find which parts of the process can be replaced by TCD columns. This analysis is based on qualitative rules (feed composition, composition profile, and pressure level). Two conventional arrangements were candidates to be converted to TCD system but only one has been selected.
3. UPC has designed the TCD column using a short cut method based on the one presented by UMIST.
4. The multicomponent simulation model has been then developed in the steady state simulation software for the whole process.
5. Results of rigorous simulations of multicomponent systems have been compared with simplified simulations of ternary columns carried out by UPC.

Simulation results: the conventional arrangement needs 14.5 kW while TCD column only needs 12 kW for the same separation. The TCD reduces the energy requirements almost 20%. Energy saving is clearly identified by the load of the two columns replaced by TCD. Other requirement demands are the same.

Heat integration.

The objective was to realise the heat integration of both conventional and TCD systems. Currently, conventional process heat integration has been done. The TCD system heat integration is almost completed too; some fine-tuning is still necessary to obtain definitive conclusions. This fine-tuning will not affect the trends already identified.

Heat integration description.

Pressure in the second column which has been replaced by TCD system is decreased so that the overhead vapour of first column (separation of benzene from toluene and xylene) can be used to provide its heat content for boiling up the second column (separation of toluene from xylene).

This modification does not reduce the Minimum Energy Requirement (MER) but allows mechanical vapour recompression to be applied to another distillation column. Pressure in TCD column is slightly increased to allow mechanical vapour recompression to be applied to another distillation column. Heat integration results: the Minimum Energy Requirement of the

process including the TCD system (12,927 kW) is about 8% lower than for the conventional process (13,985 kW) when energy integration has been performed in both cases.

WP 4.1 Fluid Mechanics modelling (PARAGON)

Initially the publicly available FE fluid mechanics codes were examined. None of them offered the flexibility required by modifying and becoming a two-dimensional divided distillation column model. As a next step PARAGON examined the appropriate commercial Finite Element packages available in the market (Algor, Phoenics, COSMOS/M, etc). Due to the complexity of the problem and the fact that the use of this model is needed later to the project, it was decided to devote a little more time for the selection of the appropriate software package. At this moment PARAGON examines the possibility of developing the Fluid Mechanics code in a language.

WP 4.2 Optimisation of the degrees of freedom (PARAGON)

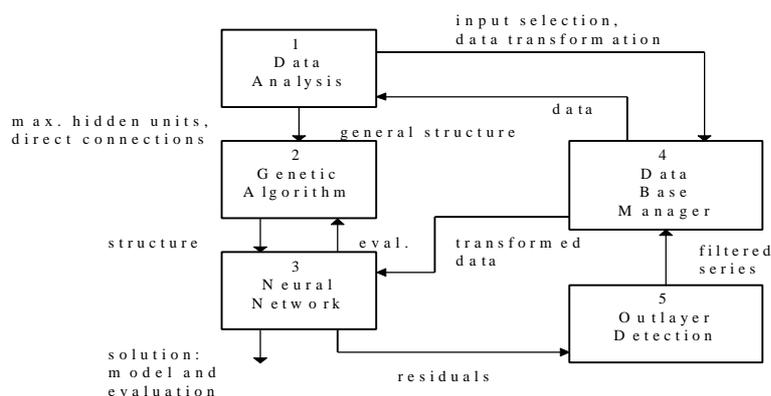
A GA algorithm had to be developed in FORTRAN computer language. At this point the basic GA operators, as well as the main code have been developed. The developed operators are the Reproduction (also known as selection), the Crossover (also known as recombination) and the Mutation.

WP 4.3 Neural Network (PARAGON)

WP 5.1 Evolutionary models (UPC, INFOR)

From the dynamic studies carried out in WP2, it has been confirmed that the dynamic response of a DWC to changes is usually very slow. So predictive models that are continuously fine-tuned with real-time information can be very relevant to improve forecasting and control. In this sense, UPC and INFOR have been developing a novel approach that includes the use of Artificial Neural Networks (ANN) as the core of evolutionary model building.

A general view of the entire system proposed to model dynamically the divided wall column is shown in the figure:



Global Proposed Modelling System

- The first module corresponds to the Data Analysis component. In this part data are analysed to have a previous idea of the general structure. This module should determine the length of the string used in the GA and its composition using a flexible structure. Using

heuristic rules it is possible to reduce the time of processing and to guide the search in a wide spectrum containing the optimal model to be found.

- The second module is a Genetic Algorithm. This module provides to the NN module the structure to be evaluated and using an iterative process the best structure built is returned as the system solution.
- Module 3 estimates the parameters and returns to the GA module the fitness function taking into account the parsimony principle. The stopping criterion used allows us good generalisation of the NN structure found.
- In module 4 all the information is processed depending on the Data Analysis result. The NN module uses the training set transformed to the best form.
- An additional module (outlayer detection) detects values with a higher modelling error than the average and analyses their influence on the model quality. Based on this information some values may be excluded from the learning set.

As the Genetic Algorithm actualises the structure and the parameters of the ANN, the artificial neural network simulates the real conditions in the column including influences which cannot be described by rigorous (first principles) models. Therefore it is especially appropriated for Model Predictive Control.

WP 5.2 Expert system and neural network (UPC, INFOR)

Simulation tools for control purposes have to model the real operating conditions of the dividing wall column as exactly and quickly as possible and to obtain forecasting results on-line. The combination of Artificial Neural Networks (ANN) and Genetic Algorithms (GA), which has been developed by UPC and INFOR in WP5.1 satisfies these requirements. This models are integrated into a general control system of the Divided Wall Column.

The general schema of the proposed controller consists of a Predictive Model Control System that is able to modify the appropriate set point in the inner control loops and a Diagnosis Expert System that identifies the current general operation status of the DWC. The Diagnosis expert system can also:

- Generate event and alarm messages to the user interface
- Determine the NN model to be applied in each situation according with the current behaviour of the system and, eventually, ask for new model building.
- In case of undesired situations (i.e., equipment breakdown, information incoherence, etc.), take care of driving the system to a predictable and safe situation, by passing the control structures provided.

The predictive control presented is a centralised control integrated into an intelligent system framework that support the whole control strategy of the DWC. INFOR has developed this Intelligent System framework and a Fault Diagnosis for the DWC. The Expert system interacts with the Data Acquisition system and feeds its variables. Then the Expert System evaluates the state of its rules and produces the diagnosis results. This diagnosis result is then displayed through the user interface.

In the global framework, the DWC structure is modelled in a class system that will interact with the system rules to produce a diagnosis result. Taking the advantages of the OOP, INFOR developed once the method in the Super Class DWC, and all sub classes and objects inherit this method.

4. Results and conclusions

Previous work in the dividing wall column research has seen

1. The development of a short cut design technique for thermally coupled distillation systems and
2. initial studies on the control and operability aspects of the DWC. The first objective of the current research was to improve the existing short cut design techniques to care for more realistic industrial applications.

UMIST developed a novel extended methodology for steady-state design optimisation, to be applied to a wider range of problems, and multicomponent rather than ternary separations, the use of stripping steam and the other systems. The development of software supporting this new methodology was another substantial contribution and was completed in close collaboration with the project partners during the second half of the project.

UT have studied control issues. Results show that the column can be controlled by conventional control structures. The column has extra degrees of freedom that can be used for optimisation. The optimal operation point is strongly dependent on feed composition and on the product specifications. When three product composition loops are closed, adjustment of liquid and vapour flow splits can be used to minimise energy consumption. From analysis of the shape of the solution surface we can see that at least one of these inputs should be adjustable on-line in order to maintain close to minimum energy consumption when feed parameters may be varying. UT has also shown that this “optimising” adjustment can be done by a conventional controller through feedback from measurement variables which characterise the optimal operation point. The DWC column has several similarities to traditional binary columns with respect to interactions and other important properties for control, so usual design methods for selecting the best pairings etc. can be used. And as for conventional columns, there is no single configuration that is best for all kind of separation tasks, but the methods of control analysis are general. The best configuration for a particular column will depend on feed compositions, purity specifications, number of actual trays in sections, relative volatility, and requirements for flexibility both in the range of feed composition and product specifications.

PARAGON developed: a) A Fluid Mechanics code for the modelling of the flow in DWC, b) An optimisation code based on Genetic Algorithms for the optimisation of the operating degrees of freedom of the DWC, and c) An Artificial Neural Network for the modelling of the DWC.

UPC studied a steady state model of the DWC. Rigorous steady state simulations of the DWC as well as rigorous steady state simulations of conventional designs were developed using commercial packages for several mixtures to compare the number of plates and the energy consumption required in all cases. In order to optimise the energy consumption of the DWC, a design strategy has been proposed. The analysis of appropriate control structures for the DWC requires flexible and detailed simulation models.

UPC supported by INFOR also developed dynamic models of the DWC. These models were implemented using SPEEDUP. Through the simulations, the dynamic behaviour of the DWC was studied and some control characteristics derived. The identification of a modelled column was done and control indexes were calculated. A novel artificial neural network (ANN) for the dynamic simulation of the DWC was designed and trained. The results show that ANN are appropriate to simulate DWC. It has been seen that the ANN learning structure for dynamic

simulation combined with Genetic Algorithms (GA) can be used to readjust and optimise the ANN structure, giving place to real evolutionary modelling. SPEEDUP data from dynamic simulations were used to train the ANN and to model the DWC behaviour for forecasting purposes. The integration of the predictive model based on ANN into a centralised control strategy of the whole DWC and a general control system have been proposed. Supported by INFOR, a global framework including predictive control and diagnosis has been described.

ULg has studied in details the implementation of DWC in two processes: Thermally coupled distillation system requires less energy than conventional stand-alone systems, the real benefits of the introduction of TCD systems considering a whole process were investigated. ULg has also extended the modelling capabilities of available simulation software to dividing wall columns: the heat transfer across the dividing wall can now be simulated accurately. The modified simulation software has been used to carry out a detailed case study of an existing gas separation plant.

All the data needed to model the four column distillation sequence were obtained from industrial sources. The process modifications resulting from the installation of dividing wall columns have been investigated by detailed simulation, and a complete equipment costing and economic analysis have been carried out. Finally, ULg contributed in the analysis of control structures by collaborating with UT and UPC and delivering rigorous dynamic simulation results that were used to validate the simplified models required to design and tune the control schemes.

MWKL, utilising their wide base in the chemical, gas and refining industries, have completed a rigorous analysis, using actual plant/design data. It demonstrated that DWC's can provide a significant reduction in energy demand. The highest energy savings of 33 % were predicted for a refinery fractionation problem producing gasoline-blending components.

ASTON has completed work on the air-water simulator rig to determine the liquid distribution in a packed section in a DWC.

5. Exploitation plans and anticipated benefits

The following are some examples based on the proposed case. Exploitation plans are based on the project results benefits, its economic and social impact. As the leading partners have an excellent record in technology transfer, they will use their well-proven structures.

It has been envisaged that a THERMIE-JOULE project would be the most helpful step for the exploitation.

A detailed Technology Implementation Plan lists six main exploitable results:

- I. Novel Design Methodology for Optimisation of DWC (UMIST).
- II. Optimisation Algorithm for the DWC based on Genetic Algorithms (PARAGON).
- III. Software for rigorous steady state simulation of thermally coupled distillation columns (ULg).
- IV. Novel methodology for evolutionary modelling, optimum operation, diagnosis and control of DWC supported by prototype software (UPC).

V. Novel understanding of controllability and on-line optimisation of the DWC (UT).

VI. Industrial Applications of DWC (MWKL).

UMIST will use its industrial and academic contacts to transfer novel technology and design tools into European practice. UMIST will target other areas of European industry not directly covered by the project partners, which would benefit from the novel methodology and design tools, e.g. chemical and petrochemical plant, oil refineries.

UT will present results from DISC to Norwegian process industry and encourage the industry to find suitable applications for this kind of technology. UT has been working with dividing wall columns before start-up of DISC, and also running research in closely related areas. Results from UT will also be spread within our strong network of process system technology (PROST «Strong point centre of PROcess Systems Engineering»). This network has participants from several departments of UT and SINTEF, which is a Norwegian research foundation, and close contacts to Norwegian process industry.

PARAGON will further develop its results from the DISC project and will use them in applications in the Greek market and abroad. Furthermore, it will use the knowledge derived from this project in order to widen its collaborations in areas related to distillation processes.

UPC has a long tradition for co-operation with the industry. The Chemical Engineering Department has built-up through the years a strong interaction with the surrounding industrial environment in terms of consultancy, specific developments and projects. Industrial contracts amounted 1 MECU in 1996. Specifically, industrial contacts with interested parties (polymer and plastic materials manufacturers) in DISC developments (Evolutionary Modelling, the use of ANN for modelling and dynamic control purposes) have been established along the project lifetime and are to be continued for future possible specific applications.

ULg intends to exploit results from the DISC project in three ways:

- Updating course materials used for both university teaching and for industrial seminars, to disseminate information about novel technologies.
- Improvement and extension of simulation software codes especially in the framework of its collaboration with a spin-off company created by ULg.
- Publications and communications

MWKL will be pursuing applications within the process industries with the objective of engineering the first DWC outside of BASF. All relevant research results will be analysed and potentially utilised in the design.

Exploitation of the expected results will be also made through the Universities Technology Transfer Centre and Research Consortia which will provide vehicles for disseminating R & D results to the industrial environment by:

- **Organising seminars.**

Adequate technology transfer will be made, specifically in this case, by making use of the proven structures.

- **Contacting potential end-users.**

Feasibility studies are undertaken under contract. They will normally range from 3-6 months in duration with the aim of demonstrating the applicability of the software to specific problems and establishing the likely benefits. It is envisaged that such case studies will usually be a prelude to the granting of software licenses for direct use by the company.

- **Software licensing to end-users**

This will involve the granting of non-exclusive licenses to individual operating companies. The licenses will cover limited use within each company as specified by the relevant contract.

- **Software Applications**

This will involve study and development of specific applications to interested companies. This will be realised directly by the project partners or through software engineering houses specialising in the marketing and support of process engineering software. In all cases the project partners co-ordinate and control those activities.

- **Public Training Courses**

Short courses will be given in public venues to train practising engineers and academics to become familiar with the techniques developed.

It is worth emphasising that the CTT at UPC already has substantial experience with respect to all four modes of commercial exploitation of engineering research work. Technology transfer in the UPC amounted to 50 MECU in 1997. The CTT plays also the role of UPC internal administrator and organises the follow-up of activities for the duration of the contracts. Financial and technical reports are checked and commercial exploitation of results is also handled by the CTT office. Specifically, the software produced by UPC in this project will be eventually commercialised through CTT services. Contacting potential industrial partners and publicising the results obtained will also be carried out through CTT offices.

The partners intend to disseminate the project results through the common channels as technical paper in scientific journals, trade journals, demonstrations and presentations of software at conferences, workshops and seminars. The information about software will be also disseminated in the frame of European Symposiums on Computer Aided Process Engineering (ESCAPE series) and a specialised conference "Process Integration, Modelling and Optimisation for Energy Saving and Pollution reduction" - PRES'98 and PRES'99.