

A MODULAR SYSTEM FOR DISTILLATION
COLUMN DESIGN BUILT ON EXCEL

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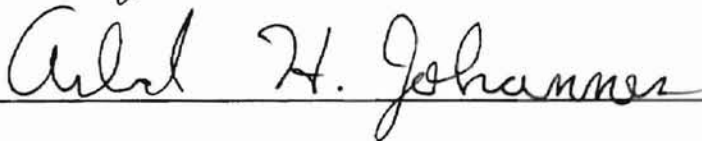
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CHAPTER I

Introduction

The rapid development of new technology in computer science exceeds its application to other fields. In fact, it is estimated (Yourdon, 1996) that one-year's progress made in computer science is equivalent to seven-year's progress made in other fields such as chemical engineering. The impact of new advancements in computer science is so great that it has created a brand new economy. It is clear that the new technology developed in computer science is not used fully in possible application areas. The potential of new technology in computer science has not been explored well in fields such as the chemical process industry (CPI) and chemical engineering.

This study aims to narrow the gap in advancement between computer science and the chemical process industry, to explore the potential uses of computer science technology in chemical process industry, and to demonstrate the economic benefits in CPI brought by new products developed in computer science. More specifically, this study explores and demonstrates the use of Microsoft Excel in distillation column designs to serve as an example of engineering applications with new interfaces for CPI.

This study uses Excel sheets as a uniform user interface for distillation column design, rating, and optimization (Lockett, 1987; Kister, 1992). The Excel application also is used as a tool to integrate different legacy Fortran applications together, then to serve

as a medium of communication between different Fortran applications and other applications through an array of Access databases. The proposed system can be considered not only as new interfaces for legacy Fortran applications, but also a technology based management system (TBMS) to manage the various technologies in large corporations.

The distillation process to separate mixtures (such as crude oil) into useful products (such as gasoline) is one of the most important processes in CPI. It accounts for 1/3 of all CPI investment and consumes 1/3 of energy used in CPI. Consequently, the design and performance of distillation columns is the most thoroughly studied topic in chemical engineering. Many design methods have been obtained and accumulated within the industry. However, these design methods that were developed in the past 50 years are still in the form of disconnected Fortran programs or codes. Some of these Fortran programs or codes are still running on mainframe machines. Since chemical engineers must use these Fortran applications on a daily basis, CPI should have graphical user interfaces (GUI) for its existing Fortran applications to improve productivity. For a wider access and easier maintenance of applications, CPI also should transform mainframe Fortran applications to PC based applications. Chemical engineers must use many Fortran applications to perform a design. It is very desirable to have an integrated system with uniform graphical use interfaces for all Fortran applications.

Although disconnected applications for a specific column internal design are available, an integrated modular system including all column internals has yet to be

developed. There are a few books and articles dealing with computational procedures for the overall design of columns. These studies primarily consider isolated design steps for a single column internal with the integration of the steps considered only partially. In the design procedures published by Chase (1967), Fair (1963), and Economopoulos (1978), one or two trays of a single tray internal is treated as representative of conditions throughout an entire column. An expert system for selecting column internals was developed by Chuang et al. (1992). Barnicki and Davis (1989) presented algorithms and design methods for sieve tray columns without considering other column internals. Optimal design of a column requires considering of all possible column internals. Therefore, an integrated modular system including all column internals is an essential tool for design engineers to arrive an optimal design for a specific application.

CHAPTER II

Systems Analysis

This chapter defines the problem domain, analyzes the system requirements and tasks, and designs corresponding objects and functions. It also reviews issues related to system integration and user interface design (Treu, 1994). Task analysis helps developers to understand what and how the users want to accomplish.

2.1 Distillation Column Design

Distillation columns contain either trays or packing, termed column internals (Kister, 1992). Trays include sieve trays, valve trays, fixed valve trays, and dual flow trays. Packings cover random packings and structured packings. For a specific distillation task, there is only one best choice for column internals. With the best choice, there is only one optimal design. For a new application, chemical engineers face great difficulties when they try to find the best design by using a trial and error method with different Fortran applications to model the internals for each column. For an installed application, engineers must know either the exact performance of the column when the column loadings are changed or they need to retrofit the column to achieve the maximum capacity. To accomplish these tasks, they again must use different Fortran applications with inputs tailored to each application. The main goal of this study is to provide a uniform graphic user interface for different column internals by using Excel spread sheets

and to integrate different Fortran applications with the Excel application, so chemical engineers easily can access all design methods for different internals at the same time in a PC based Windows environment. The system helps and guides chemical engineers to perform following tasks productively, accurately and efficiently.

2.1.1 Selecting Column Internals

Engineers use the system to design different columns with different internals simultaneously based on the provided flow rates and physical properties. Each design with particular internal is optimized by the system. The column size and column height resulted from each internal given by the system can be compared and analyzed. According to requirements for specific applications, a decision on the selection of column internals can be made for a minimum column size for a given through put or a maximum through put for a given column size, achieving the maximum column capacity. For the best mass transfer efficiency, the internal resulting in the minimum column height can be chosen.

2.1.2 Design Column

If an internal is chosen, then the user can load the specific interface for his internal. The system designs the column based on the provided flow rates and physical properties by using the selected design method and knowledge base. For tray columns, some of the tray dimensions, such as tray hole size and open area, are selected and given by expert systems.

2.1.3 Sizing Column and Downcomer

For tray columns, if tray essential dimensions such as hole size, hole area, and weir height, are given, the system determines and optimizes the column and downcomer size based on the specified design method. Tray downcomer size optimization is an key factor to obtain the maximum column capacity.

2.1.4 Rating

With hardware dimensions and flow parameters given, the system calculates and gives the completed column performance parameters at the given design point.

2.1.5 Plotting

With hardware dimension and flow parameters given, the system makes full performance diagram plots as a function of liquid rate and hydraulic and efficiency plots as a function of vapor rates (C_b). On the performance diagram, user can specify the maximum liquid rate to be plotted or let the system decide. One full performance diagram is for each panel. On the hydraulic plots, user can choose between constant liquid and constant liquid over vapor rate ratio (L/V ratio) for plots. Further, user can specify the liquid rate and the ratio of L/V for plots or choose default at the design point.

2.1.6 Tray Dimension Calculations

With a given column size, number of flow passes, and type of tray panels (either equal flow pass length or equal bubbling area), the system will determine all tray

dimensions based on the specified downcomer area or width or their combinations. It handles both sloped and straight downcomers up to four passes.

2.1.7 Unit Conversion

The system converts between British and metric units. Unit conversion includes the conversion of units used in the figures and table titles. The system recognizes which database to access based on the selected unit system.

2.1.8 Comparison of Different Design Methods

For each internal, four performance model libraries or four different design methods are constructed. The performance of different models or design methods can be compared easily. For sieve tray, as example, create two sieve tray interface pages, read the same run from the database but choose different models to performance calculation. The two sets of performance figures can then be copied on to a new sheet for comparison side by side or on one figure. If the run is not in the database, then input through one interface and write the inputs to a database and retrieve them from the other interface.

2.1.9 Comparison of Different Internals

The system compares the column performance of different internals side by side or on one figure. For trays as example, create one sieve tray interface and one valve tray interface, read inputs from the database and perform calculations. The results can then be copied on to a new sheet for comparison.

2.1.10 Comparison of Different Designs

Different designs of the same internal can be compared by the system side by side or on the same figure. For trays as example, create several sieve tray interfaces for different designs on the same workbook and perform calculations and plotting. The results can then be copied on to a new sheet for comparison.

2.1.11 Workgroups

Group leader sends the input into a central database and engineers worldwide who can access to that database can design the column simultaneously and write back the results to the central database for discussion. Or one engineer designs a column and writes to a central data base and other engineers who can access to that database retrieve the design for discussion and modification.

2.1.12 Internet Publishing

Since the user interface is separated completely from the main system, the user interface sheet containing the calculation results can be published on the Internet from Excel 2000. The user interface is a small file. This small interface file can also be sent as an attachment via E-mail. When this interface file is received via E-mail, it can be connected to the system automatically to perform additional calculations if necessary.

2.1.13 Information Managing

If engineers write to a central database regularly, the group leader can see who design what and when and how the design was done. When the system writes to a

database, it automatically attaches a time stamp. The group leader can use the system to distribute the workload, to check the designs from different engineers, and to manage the daily business activity.

2.1.14 Control Column Operation

The system can be connected to a control system to do a model predictive control. When the system is connected to on line input real time, the process outputs can be compared to the model predicted outputs at any desirable interval and to adjust the model parameter to fit the real process (educating). After the system is educated, the system can be used for model predictive control of columns.

2.1.15 Connect to Process Simulators

The system is able to receive data flow from process simulation programs and send the outputs back to the process simulation programs via the databases.

2.1.16 Connect to CAD systems

The system can be connected to CAD systems, so that the user can view the tray and column designs in CAD systems.

2.1.17 Connect to VR (Virtual Reality) systems

The system can be connected to VR systems, so that the user can walk through the designed column or tray three dimensionally.

2.1.18 Preserve Knowledge

The live knowledge base can acquire the knowledge about column design and internal selection over time and preserve the knowledge for future generations.

2.1.19 Training Engineers

The system can be used to train new engineers in this field by comparing the designs from the new engineers to that by the system.

2.1.20 Input Checking

The system checks all inputs and accepts only the correct inputs. If inputs are not in range, then the system rejects the inputs and gives an error message.

2.1.21 Database Access

The system accesses an array of databases including some third party proprietary databases for information storage and retrieval. Different levels of access control to the databases can be made to manage information sharing.

2.2 System Integration

Distillation columns can contain various internals. Each internal has its own design method and performance models. For the same internal, design methods and technologies from different sources are also different. For an optimal design of column, it is necessary to check the performance of all internals with all available design methods. If four sets of design method or four design applications for each internal are available,

design engineers may have to use 24 different applications for six kind of internals to arrive an optimal design for column. It is likely that different inputs are required for each application. Therefore, it is very desirable to integrate various applications into one system with common interfaces. Design engineers have options to choose on which design method is used and which column internal is selected. The system is able to handle and contain as many cases as necessary for different designs, different internals, and different design methods.

2.2.1 Integrated Modular System

An integrated modular system with open structures is essential, so that different design methods from various sources for different internals can be loaded into the system on demand. The system consists of several sub-systems for each internals. Each sub-system can be installed and used independently or jointly with any combination of the sub-systems. The sub-systems can be added to or deleted from the system without affecting the performance of other sub-systems.

2.2.2 Sub-Systems

Sub-systems are built for each internals. They are completely independent of each other. Each sub-system accesses, holds, and uses four or more different design methods for the internal from different sources. Each design method is self-contained and independent of other design methods. Design methods are also loaded on demand.

2.2.3 Databases

An array of databases are integrated into the system. Databases are used for design information storage and retrieval. They are also used to connect the system to foreign applications such as process simulation and CAD systems.

2.3 User Interface

User interface is an important part of the system that allows a user to enter, manipulate, store, and retrieve data, and to initiate commands (Laurel, 1991). It presents and displays system outputs and results visually to users. It enables communications among the user, the system, and the computer. It gives the first impression of the system and determines the usability of the system. A good user interface is an essential requirement to achieve the increase in productivity that is promised by the system and the use of computers.

From the command line data entry such as a DOS interface to the current generation of graphical user interface (GUI) such as Windows, user interface technology has evolved significantly over the years. A command line interface requires users' memories of commands. A menu driven interface eases the burden on user's memories and gives the available commands visually for users to select (Mayhew, 1992). Menus are often presented hierarchically where the main menu leads to sub-menus that lead to

sub-sub-menus. It is difficult for interface designers to decide which options are to be accessed from which menus and in what sequence (Thimbleby, 1990).

The current graphical user interface or the point and click GUI is now used in most applications (Collins, 1995). The most popular GUI consists of Windows, Icons, Menus and Points (WIMPS). WIMPS are used with Microsoft Windows, X Windows, and Apple computers and are accepted by a wide variety of users. The GUI is a logical choice for user interface of the system developed in this study.

It is a very complex task to design a good user interface. The interface should reflect user's capabilities and respond to any specific needs. The main goals of the interface design are to increase user's productivity and efficiency and to decrease training time, user error, development time, and customer support cost. A good interface can result in increased users and sale of the system. On the other hand, a poor design is an expense mistake. No matter how good or advanced the technology might be, they are wasted if they are not readily available to users. (Fabian, 1991; Hix and Hartson, 1993). The good design of user interfaces in this study is emphasized. The following characteristics of the user interface of the system are required and designed.

2.3.1 Customizable Interface

The user interface is customizable so that users can have their own choice for the color for fields and font sizes and types for texts. Users can add their own comments and

hints to the buttons and fields. The output results in figures or drawings or tables can be edited to any desirable formats.

2.3.2 Rich Visual Presentation

Inputs and outputs of the system are displayed in a variety of formats such as drawings or figures, tables, and color text. If necessary, video and sound clips can also be attached to the interface to add the communication between users and the system.

2.3.3 Simple Interaction

The user interacts with the system by using a simple pointing device such as a mouse in most cases. A complex action can be completed with pointing and clicking. Simple interaction results few human errors in using the system.

2.3.4 Easy Transfer of Data

Input and output data are often transferred or exchanged within the system or between different applications. It is convenient to use the clipboard or drag and drop function to move data or objects between different applications.

2.3.5 Multitasking

It is important that the interfaces can be duplicated to create multitasking, so that different cases can be loaded or contained into the system at the same time. The system can switch between multiple tasks or interfaces to achieve maximum efficiency (Wood, 1998).

2.3.6 Uniform Interfaces

Different user interfaces are made for different internals because of different inputs. However, different interfaces are designed to be similar. Some of the data blocks are the same for all interfaces if there is no difference in input and output data. If the user is familiar with one interface, then he should have no problem to use other interfaces. Thus, the learning time of users can be greatly reduced.

2.3.7 Compatibility

User compatibility, task compatibility, and product or system compatibility are designed and provided. Users are often with different levels of sophistication from experts in the field to naïve or casual users. A common mistake of developers is to assume that all users are all alike (Zetie, 1995). This assumption often leads to a wrong conclusion by developers that if the interface is fine to developers themselves or to a few users, it will be good enough to all users. Actually, users differ significantly from developers in sophistication, motivation, experience, and needs. Thus, a good interface design should accommodate the different needs and different aspects of all users. The task compatibility requires that the structure and flow of the system should match the tasks that users must do to complete the job. The task-oriented style is preferred to application-oriented style. The organization of functions and actions allows smooth transition between tasks. The system compatibility means that the system should be compatible with other common used GUI that users may be already familiar with. Compatibility across system reduces learning time and errors significantly.

2.3.8 Consistency

Since 1980s, GUI industry and research organizations have developed guideline documents and general design standards to help maintain design consistency. Consistency among interfaces enables users to reason by analogy and to predict how to use the system even if they have never encountered before (Jewell, 1994). Inconsistency surely increases learning time and learning requirement. Excess learning requirement and learning time post a major barrier for users to accept and use the system (Lionel, Morasca and Basili, 1999). High degree of consistency is maintained among different interfaces, so that users need to learn only a small portion of the system to master the whole system.

2.3.9 Simplicity

A simple interface helps user gain confidence in using the system. A complex interface is confusing and overwhelming to users and often makes user give up the system at the beginning (Cockbum, 1998). Simplicity can be achieved by using default options, layered approach, and simple common tasks. Default options hide some advanced functions from novices and make the system easy to start with. A layered approach introduces the functions gradually from simple and common ones to complicated and more advanced ones. A layered approach makes novices more comfortable by introducing functions and system components one step at a time (Thimbleby, 1990). Most users may perform only simple common tasks at most cases. Making common tasks simple and easy to access increases the overall system efficiency and improves the acceptance of the system.

2.3.10 Flexibility

Different users have different knowledge, different experience, and different preference and consequently have different needs. System and interface flexibility reflects system's capability to satisfy different needs (Marcus, 1992). A customizable interface allows users tailoring and accommodates different preferences.

2.3.11 Control

Users prefer to control the system than to be controlled by the system. Users often get angry or frustrated if the system constantly forces them to do certain things in order to proceed. It is important for users to feel that they are in control over the system at all times.

CHAPTER III

System Design and Implementation

This chapter presents the design and implementation of the system described in Chapter II. Based on the requirements of the system and design principles given in Chapter II, various functions are constructed. User interfaces are designed and created. The system consists several sub-systems that are independent of each other. Each sub-system contains several independent modules that are physically in different files. Components of the system can be deleted, modified, and added as desired without affecting the whole system or re-compiling the whole system. Each component of the system is independent and loaded on demand. The system can be used and installed as a whole or as a part.

The overall system is an integrated modular system with open structures. It includes: (1) Technology (tech) modules for different design methods for different internals; (2) Application interface modules for each internal; (3) Databases for information storage and retrieval; (4) Utility modules such as for unit conversion and tray dimension analysis; (5) Uniform user interfaces for each internal.

3.1 System Architecture

The system presented in this study is a component-based system as introduced earlier. It consists of different components or modules that are independent of each other. Each component is made into an independent file. All components are dynamically linked and loaded on demand.

3.1.1 Overall System Architecture

Figure 1 shows the overall system architecture. GUIs contain an array of individual sheets that can be duplicated. Five unique interface sheets are built for the five

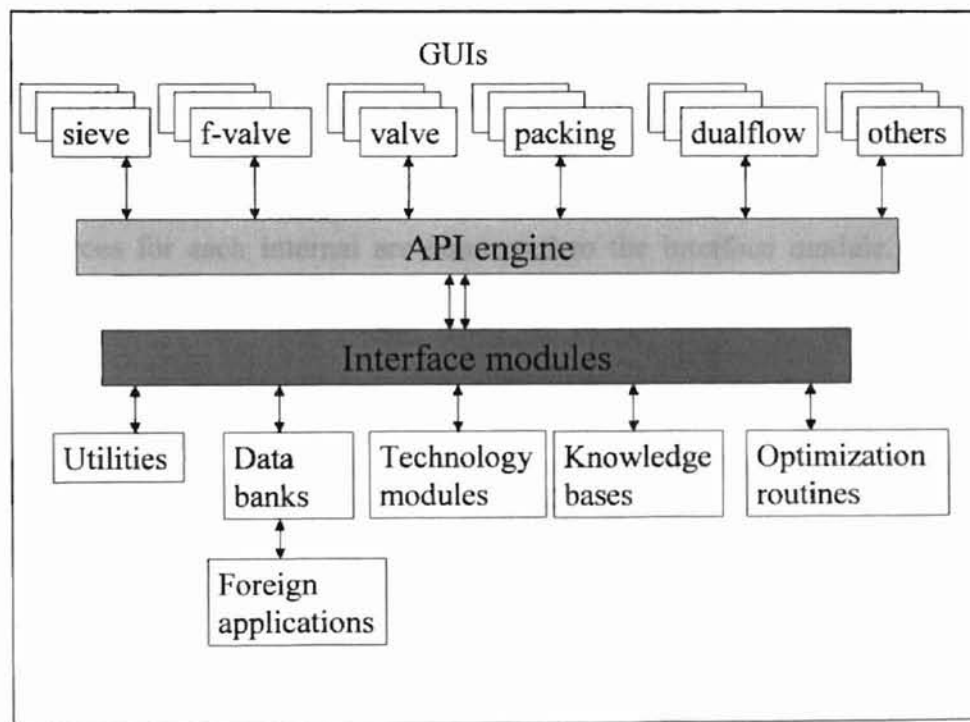


Figure 1. Overall System Architecture

different column internals. One additional sheet is reserved for other uses. Any combination of GUI sheets can be loaded into the system, so that users are able to design

columns with different internals simultaneously and compare the performance of columns with different designs. Interface modules connect among the GUIs and technology modules and other part of the system. Design modules contain distillation column design technologies to be accessed by users through GUIs.

3.1.2 Interface Modules

Interface modules are dynamically linked to the system. One independent module is built for each column internal. Each module contains necessary sub-routines to perform specific tasks. These tasks include design, rating, plotting, database access, unit and interface conversion, etc., as specified by system analysis in Chapter II. These interface modules work as bridges to connect user interfaces and technology modules. They can connect to as many user interfaces and tech modules as necessary. In this study as an example, four tech modules representing four sets of different design technology from various sources for each internal are connected to the interface module. The interface module accesses to three knowledge bases for design cases by using expert system. Figure 2 presents the architecture of the interface module for sieve tray column engineering. Similar interface modules for valve tray, dualflow tray, and packings are also designed and made.

Sub-module Learn in Figure 2 acquires necessary knowledge in the current design and preserves knowledge by updating or expanding knowledge base 2. Knowledge base 2 is named as live knowledge base in the user interface. Knowledge base 1 is provided by

third part. Knowledge base 3 is made from in-house technology. Options are provided for users to choose a particular knowledge base for using in design.

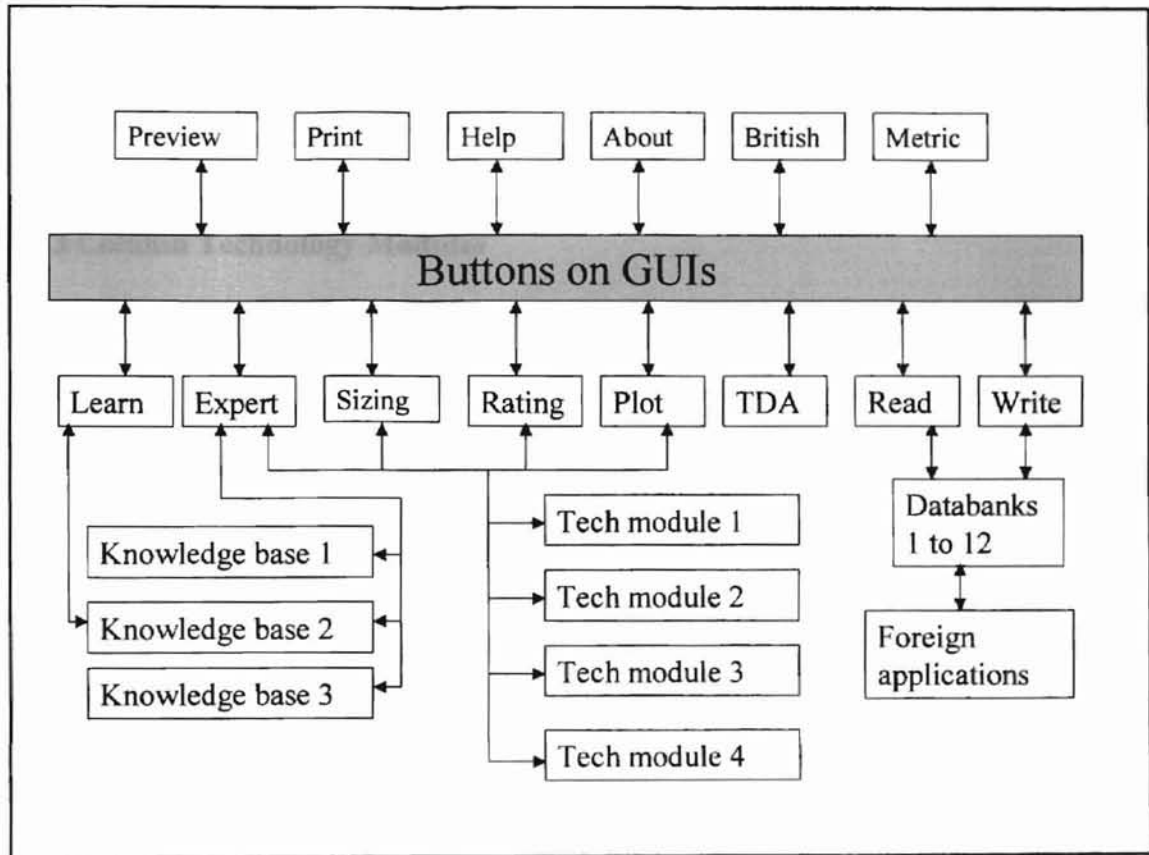


Figure 2. Interface Module Architecture for Sieve Tray Column

Four sieve tray technology modules from 1 to 4 are provided for using in expert design, sizing, rating, and plotting. They are independent of each other and made into independent files. Technology module 1 is a default option and contains technologies available in public domain. Technology module 2 contains propriety technologies developed by third parties who are specialized in this area. Technology module 3 is reserved for future technology abstracted and developed by the system based on the

selected data points in the database. Technology module 4 is made from in-house technologies. These four technology modules are provided as options for users to choose from the user interface to accomplish design and engineering tasks. Similarly, interface modules for other internals can also access four technology modules and three knowledge bases.

3.1.3 Column Technology Modules

Column design technologies are built into technology modules. These modules are linked dynamically to the system on demand. Four independent tech modules are design and built for each of the five column internals. Thus, a total of 20 tech modules are made. Each tech module contains a complete set of technology for a specific column internal. Since tech module is independent, it can be deleted, added, and modified at any time without affecting the other part of the system.

3.1.4 Data Banks

An array of data banks is provided for information storage and retrieval with the system. Each databanks contain a set of completed tables to store all inputs and outputs from all user interfaces with all column internals. A main table is created and shared by all internals. This main table is to store physical properties and flow rates that are common to all internals. Separate tables are designed for different internals. Figure 3 shows the Tables of the data banks used by the system. A unique design ID is used to related tables. The system is able to write all data including inputs and outputs shown on user interfaces into the data banks. These data can be late retrieved to any interfaces by the system. Through the data banks, the system is able to communicate with foreign

applications such as process simulators and CAD systems. Additional data banks for storing common dimensions of valves and packings are also created for user's convenience, so that users enter only the packing or valve name instead of all dimensions. With the provided name, the system retrieves all necessary dimensions. For a new packing or a new valve design, users enter the dimensions only once in the first time. The system writes all dimensions entered into the data banks for new packings and new valve designs.

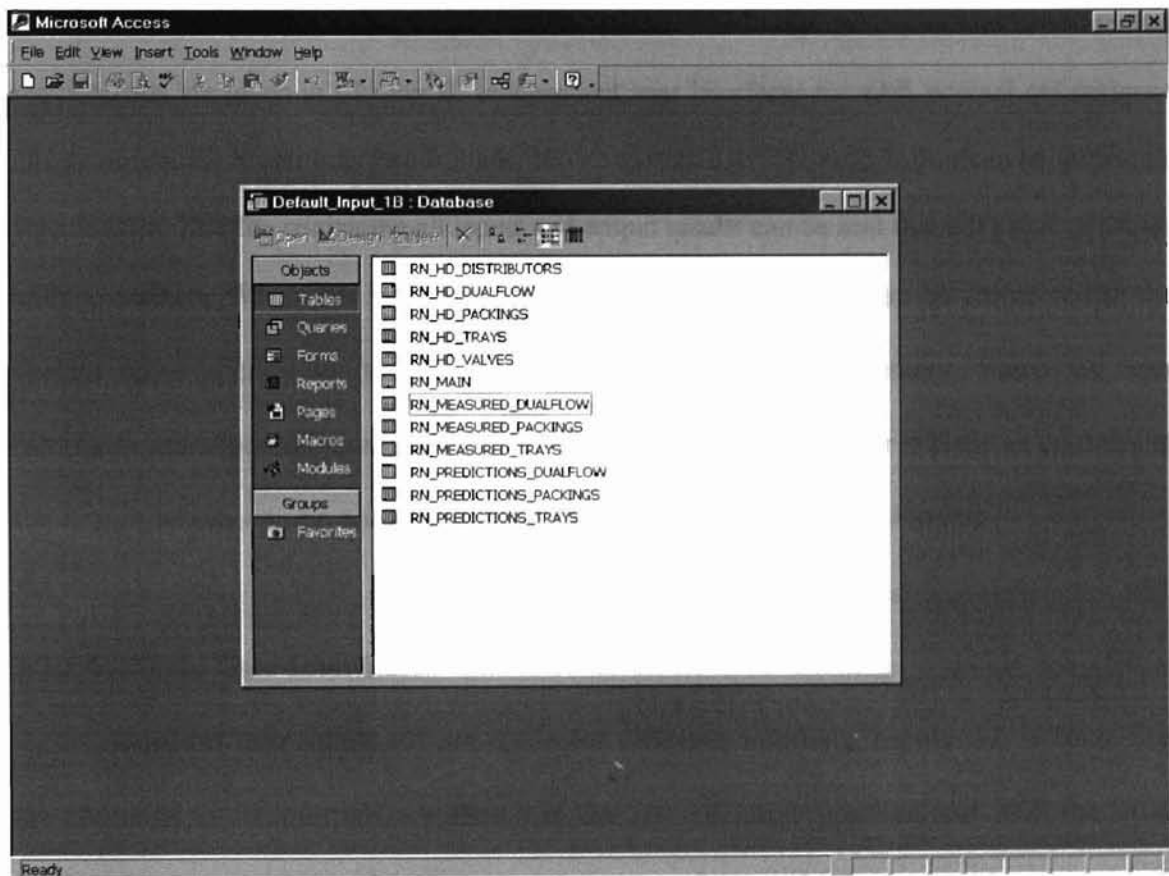


Figure 3. Tables of Data Banks Used by the System

3.1.5 Other Modules

A separate module, TDA module, is made for tray dimension analysis. This module also contains some utility routines such as for optimization. TDA module can be accessed from all interface modules. Future improved routines for optimization will also be built into this module.

3.2 User Interface Design

User interfaces are integral part of the system. The design principles and user interface requirements are given in Chapter II. Independent user interfaces for each internal are designed and provided. Each user interface is made into a separate interface module that can be saved in a separate file. This file containing all inputs and output results can be sent through email or shared with co-workers. When this interface file is received via e-mail, it can be connected to the system automatically to perform additional calculations if necessary. Since the user interfaces are separated completely from the main system, the user interfaces containing the design results can be converted and published on the Internet or intranet.

3.2.1 Uniform User Interfaces

Uniform user interfaces are made for different internals. Inputs and outputs that are common to all internals are shown in the same relative position and with the same format. The position of tool buttons and the name of the tool buttons are also the same if they perform the same action.

3.2.2 Tool Buttons

Consistent tool buttons are designed and used for all interfaces. These tool buttons are connected to the various sub-modules within the interface modules for different internals. The tool buttons for sieve tray sub-system is shown below in Figure 4. The tool buttons for other internals are almost identical to those shown in Figure 4.

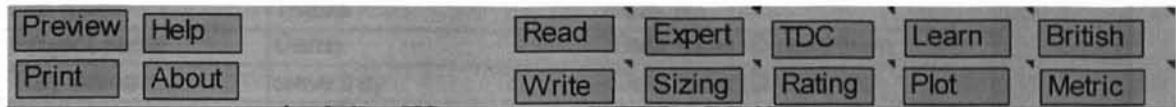


Figure 4. Tool Buttons of the Sieve Tray Sub-System

Comments also are attached to the tool buttons if necessary. These comments are shown when the mouse moves over the tool buttons to guide user's action. Additional identical tool buttons are also embedded at proper locations through out the user interface for easy access.

3.2.3 Grouped Inputs and Outputs

The inputs and outputs on the interface are grouped properly with its own name or title. Each group can be hidden or visible by clicking the + or – sign on the left. Additional rows can be added between two groups of inputs or outputs for further customization. The interface is designed to accommodate 1 to 4 pass trays for tray internals. When used for a 1-pass tray, for example, figures and tables that are not related are hidden automatically by the system. Figure 5 shows a sample of grouped data presentation. Addition comments for each data shown are given if necessary with a red mark at the corner of data labels. These comments are shown automatically when the mouse move on the data label. Comments give users additional guidance and help to

understand the data shown. Data groups that are the same to different internals are presented with the exactly same way in different user interfaces for consistency and uniform appearance.

Preview	Help	Read	Expert	TDC	Learn	British
Print	About	Write	Sizing	Rating	Plot	Metric
General Information			11/15/00 16:44			
File name	Thesis	Run_ID	Test 1			
Project name	Demo	Data base ID read from	1			
Tray name	sieve tray	Data base ID write to	1			
System name	C6/C7	Language	English			
System pressure	24 psia	In & output units, Br.=0, SI=1	0			
Notes	example	User name	XXX			
Calculation Options						
Numerical routine library	1	Performance model library	1			
Design percent of jet flood, %	85	AIE system library	1			
Design percent of DC flood, %	85	Entrainment fraction, level 1	0.1			
Weir constriction factor	1	Entrainment fraction, level 2	0.2			
		Weep fraction	0.2			
Physical Properties						
Liquid density, lb/ft ³	49.509	Vapor density, lb/ft ³	0.077			
Liquid viscosity, cp	0.264	Vapor viscosity, cp	0.0084			
Surface tension, dyn/cm	18	Column pressure, psia	24			
For Efficiency Calculation						
Liquid diffusivity, cm ² /s	5.09E-05	Vapor diffusivity, cm ² /s	0.0212			
Liquid molecular weight		Vapor molecular weight				
Liquid Schmidt number		Vapor Schmidt				
Slope of VLE, m	0.76614					
Column Loads						
Liquid mass rate, klb/h	30.24	Vapor mass rate, klb/h	5			
Liquid volumetric rate, gpm		Vapor volumetric rate, ft ³ /s				
Lambda, mG/L	0.5	G/L, Molar ratio	0.7			
<input type="button" value="Expert"/> <input type="button" value="Sizing"/>						
Column Specifications						
Column diameter, inch	48	Number of liquid flow pass	1			
DC area top/DC area bottom	1	Type of tray panels				
Tray spacing, inch	15	Vapor tunnel, Yes=1, No=0				

Figure 5. A sample of Grouped Input

3.2.4 Output Results in Figures and Drawings

In addition to the grouped output results, figures and drawings are used extensively to show the trends of various results and functions. Two kinds of figures are designed and made. One is the column performance diagram that shows the column performance as a function of liquid rates. The other kind is the hydraulic and mass transfer performance diagrams. Options for constant liquid rate or constant liquid over vapor ratio are available. Further, the liquid rate or liquid over vapor ratio for plotting can be set as desired. The appearances of these figures are consistent across various interfaces for various internals. The examples of figures for sieve tray design are shown in Figures 6 and 7.

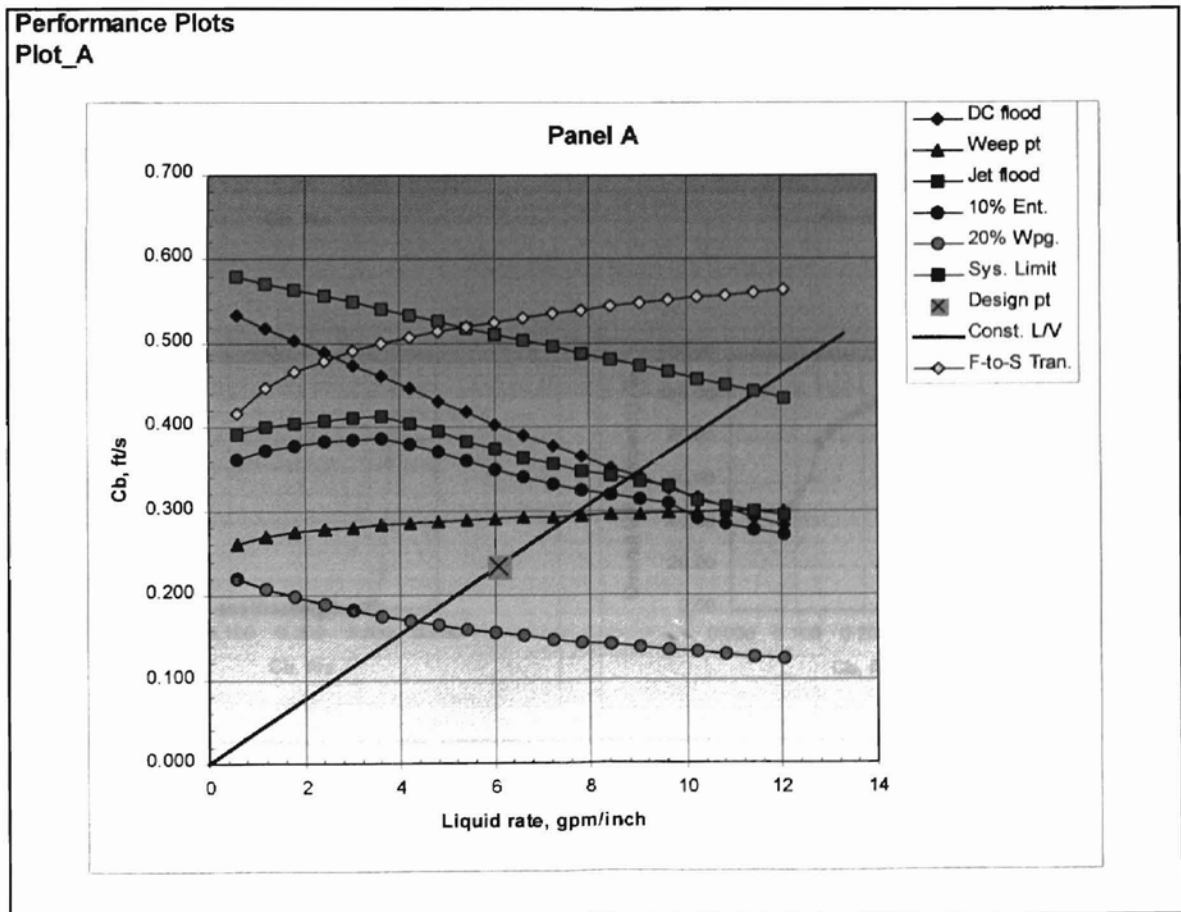


Figure 7. Column Performance Diagram

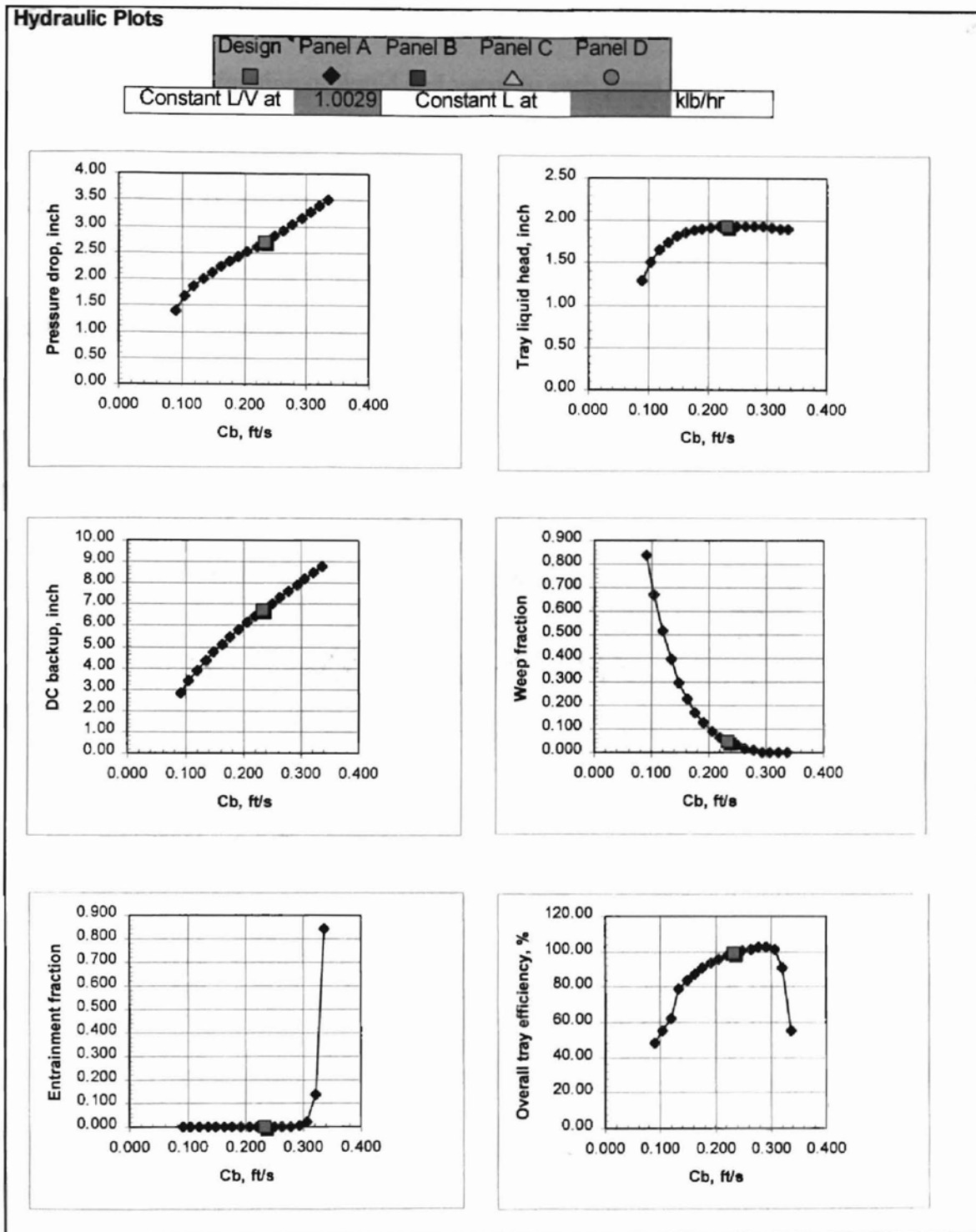


Figure 8. Hydraulic and Mass Transfer Efficiency Plots

For trays more than one flow pass, performance diagrams for each pass are made and additional lines are added for different passes to the hydraulic and mass transfer

efficiency plots. Similar plots are also made for tray point efficiency and tray Murphree efficiency and the fraction of liquid and vapor to each panel for multi-pass trays.

3.2.5 Tabulated Output Results

The data points used in the figures are also presented in a tabulated form, so that additional figures may be made as necessary. A sample of tabulated results for panel 1 is shown in Figure 8, which is used to construct the column performance diagram.

Table Results for Performance Diagrams							
PANEL_1				Constant L/V Line			
Design Point							
Liquid rate	6.08228 gpm/inch			0	6.08228	13.29657	
Cb	0.23324 ft/s			0	0.23324	0.5099	
Liquid rate	Cb_SL	Cb_DC	Cb_jet	Cb_10E	Cb_wp	Cb_20w	Cb_st
PANEL_1							
0.601792	0.5788	0.5336	0.3925	0.3619	0.2611	0.2203	0.4173
1.203584	0.5712	0.5182	0.3999	0.3714	0.2692	0.2078	0.4472
1.805376	0.5637	0.5028	0.4047	0.3774	0.2742	0.1978	0.4657
2.4071679	0.5561	0.4885	0.4083	0.3819	0.2779	0.1895	0.4793
3.0089599	0.5485	0.4735	0.4112	0.3854	0.2809	0.1826	0.4901
3.6107519	0.5410	0.4600	0.4121	0.3869	0.2833	0.1761	0.4992
4.2125439	0.5334	0.4458	0.4049	0.3801	0.2854	0.1703	0.5069
4.8143359	0.5258	0.4310	0.3944	0.3699	0.2872	0.1650	0.5137
5.4161279	0.5183	0.4175	0.3834	0.3593	0.2888	0.1602	0.5198
6.0179199	0.5107	0.4031	0.3731	0.3493	0.2903	0.1558	0.5253
6.6197119	0.5031	0.3899	0.3638	0.3402	0.2917	0.1517	0.5304
7.2215038	0.4956	0.3772	0.3554	0.3321	0.2929	0.1478	0.5350
7.8232958	0.4880	0.3646	0.3480	0.3249	0.2940	0.1442	0.5393
8.4250878	0.4804	0.3509	0.3414	0.3185	0.2951	0.1415	0.5433
9.0268798	0.4729	0.3395	0.3355	0.3128	0.2961	0.1382	0.5471
9.6286718	0.4653	0.3265	0.3303	0.3078	0.2970	0.1351	0.5506
10.230464	0.4577	0.3153	0.3122	0.2898	0.2979	0.1321	0.5539
10.832256	0.4502	0.3023	0.3055	0.2832	0.2987	0.1293	0.5571
11.434048	0.4426	0.2914	0.2994	0.2773	0.2995	0.1265	0.5601
12.03584	0.4350	0.2813	0.2939	0.2720	0.3003	0.1239	0.5630

Figure 8. Tabulated Results for Column Performance Diagram

Tabulated output results for hydraulic plots are show in Figure 9 for panel 1. Similar tabulated results are also given for other panels for multi-pass trays.

Table Results for Hydraulic Diagrams										
PANEL_A										
<i>Cb</i>	<i>DP</i>	<i>hcl</i>	<i>hdcl</i>	<i>wf</i>	<i>ef</i>	<i>Eo</i>	<i>Emv</i>	<i>Eog</i>	<i>Vapor</i>	<i>Liquid</i>
<i>ft/s</i>	<i>inch</i>	<i>inch</i>	<i>inch</i>			<i>%</i>	<i>%</i>	<i>%</i>	<i>Frac.</i>	<i>Frac.</i>
0.2332	2.703	1.925	6.703	0.048	0.000	98.82	98.84	73.77	1.0000	1.0000
PANEL_A										
0.3359	3.51	1.90	8.79	0.000	0.843	54.9449	55.46	76.14	1.0000	1.0000
0.3215	3.39	1.91	8.47	0.000	0.135	90.7339	90.91	75.88	1.0000	1.0000
0.3071	3.26	1.92	8.19	0.000	0.022	101.1078	101.08	75.60	1.0000	1.0000
0.2926	3.15	1.92	7.91	0.001	0.003	102.7300	102.67	75.30	1.0000	1.0000
0.2782	3.03	1.93	7.62	0.008	0.001	102.2968	102.25	74.97	1.0000	1.0000
0.2637	2.92	1.93	7.33	0.018	0.000	101.3749	101.35	74.61	1.0000	1.0000
0.2493	2.82	1.93	7.04	0.030	0.000	100.2769	100.27	74.22	1.0000	1.0000
0.2349	2.72	1.93	6.75	0.046	0.000	98.9650	98.99	73.80	1.0000	1.0000
0.2204	2.62	1.92	6.45	0.066	0.000	97.3925	97.44	73.33	1.0000	1.0000
0.2060	2.52	1.92	6.14	0.092	0.000	95.5021	95.59	72.82	1.0000	1.0000
0.1916	2.43	1.90	5.81	0.125	0.000	93.2234	93.35	72.24	1.0000	1.0000
0.1771	2.33	1.88	5.46	0.170	0.000	90.4614	90.64	71.58	1.0000	1.0000
0.1627	2.23	1.85	5.10	0.224	0.000	87.3092	87.54	70.83	1.0000	1.0000
0.1482	2.12	1.81	4.72	0.297	0.000	83.4622	83.75	69.95	1.0000	1.0000
0.1338	2.00	1.75	4.31	0.392	0.000	78.9179	79.26	68.88	1.0000	1.0000
0.1194	1.85	1.65	3.86	0.514	0.000	61.9326	62.42	67.53	1.0000	1.0000
0.1049	1.66	1.50	3.37	0.666	0.000	55.1817	55.69	65.74	1.0000	1.0000
0.0905	1.40	1.28	2.78	0.838	0.000	48.4290	48.95	63.17	1.0000	1.0000

Figure 9. Tabulated Results for Hydraulic Plots

Consistent tabulated results are also made for user interfaces of other internals. These figures and tabulated results can be copied and pasted to make additional new plots for column performance comparison among different designs of the same kind of internal or among different internals. The data points of new figures are still connected to the system and are updated automatically after a recalculation by the system. This feature is essential

for users to arrive an optimum design from all designs and all internals for a specific application.

3.2.6 Input Data Validation

Incorrect inputs lead to erroneous output results. Since reused old codes may not have adequate error detecting mechanisms, it is important to make sure at the user interface level that every input is correct and in the proper range. Only the correct inputs are accepted by the user interfaces. A message is displayed immediately if users try to input erroneous inputs. Input data validations are provided to every input at user interface level.

3.3 System Implementation

With the modular design given in the previous section, it is easy to implement the various components. Since components are completely independent of each other, they can be built with different program languages by different developers at different times. They can also be modified, deleted, or added at any time after the system is built. Modular component system design in this study has significant advantages in code reuse, code sharing, code development, and code maintenance.

3.3.1 Technology Modules

Distillation column technologies are developed over many years. Various specialized sources provide distillation technologies in different formats, such as in

Fortran codes or in C codes or others. These codes developed over the years from various sources will be reused with a minimum modification. Interface codes are added at the beginning of old Fortran applications. All input and output statements are removed from old Fortran application. Inputs and outputs are now passed through the interface of components that are in the form of dynamic link libraries (DLL). Sample codes to make a DLL from old Fortran codes are given as:

```
SUBROUTINE SIV_MAIN1(Z,Y)
!ms$attributes dllexport :: SIV_MAIN1
Other Fortran Codes Here
```

The first line is Fortran code where Z and Y are arrays for inputs and outputs. The second line specifies that the Fortran routine is to be a DLL. The name of the Fortran routine in DLL is SIV_MAIN1 that can be called from other applications. Three more DLLs for sieve tray internal are made from technologies from different sources. Similarly, for other internals, four DLLs are made for each internal. If the original codes are in C or C++, they can also be made into DLLs.

3.3.2 Interface Modules

Interface modules connect the inputs and outputs on user interfaces to various system components such as technology DLLs. They perform manipulations on the user interface and inputs and outputs. One independent interface module is made for each internal. Within the interface module, sub-modules as designed in previous section are created to perform specific actions. The interface module is also linked dynamically into the system on demand. Technology modules are called from interface modules. At the

beginning of the interface module codes, the file name containing DLLs and the subroutine name are specified fully as:

```
Declare Sub SIV_MAIN1 Lib "C:\Column\Model Library\Sieve_D.dll" Alias  
"_SIV_MAIN1@8" (Z As Single, Y As Single)
```

Normal procedures can be used to call Siv_MAIN1 routine in the interface module as:

```
Select Case ID_MODEL  
  
Case 1: Call SIV_MAIN1(Z(1), Y(1))  
  
Case 2: Call SIV_MAIN2(Z(1), Y(1))  
  
Case 3: Call SIV_MAIN3(Z(1), Y(1))  
  
Case 4: Call SIV_MAIN4(Z(1), Y(1))  
  
End Select
```

Based on the technology module selected by users at the user interface, the interface module calls the technology module DLL as specified by ID_MODEL. Thus, users can access to all technology modules from the user interface and compare the design results from various technology modules.

3.3.3 Data Banks

Data banks are made with Microsoft access as designed in the previous section. The database access object (DAO) provided by Microsoft is used to read from and write to data banks. The system can also customized to access third party data banks. Options are provided to users in the user interface on which data bank is to be accessed. All data

banks can be accessed from all user interfaces, so that inputs and outputs can be shared with different user interfaces for different internals.

3.3.4 User Interfaces

An independent user interface is made for each internal. The user interface is considered as a separate component or module. Based on user interface requirements and designs given in the previous section, user interfaces can be built in a sheet format by using Microsoft MFC. However, such user interfaces to satisfy all requirements are readily available. One example is the Microsoft Excel sheet that has all the desirable properties of a good user interface. Therefore, Microsoft Excel sheet is chosen and customized as the user interface. One unique sheet is made for each internal. Buttons, figures, comments, inputs and outputs, and data validation mechanism are all constructed on the Excel sheet. The user interface sheet can be further customized. It can be copied or duplicated within the Excel workbook or across different workbooks. Since one workbook can hold many different sheets, many different designs of the same internal or different internals can be contained in one workbook for unlimited comparisons between different designs. By copying and pasting of the figures, performance lines on figures from different user interface sheets for different cases can be displayed together in the same figure. Additional figures can be made within the user interface sheets or in new sheets with the tabulated results provided by the system. Figure 10 shows the hydraulic and mass transfer performances of three kinds of tray internals. The data points of lines shown in the figure are still connected to the outputs of the original user interface sheets.

Thus, these lines are updated automatically upon re-calculations by the system. Similar comparison plots can also be made for column capacity and other performance.

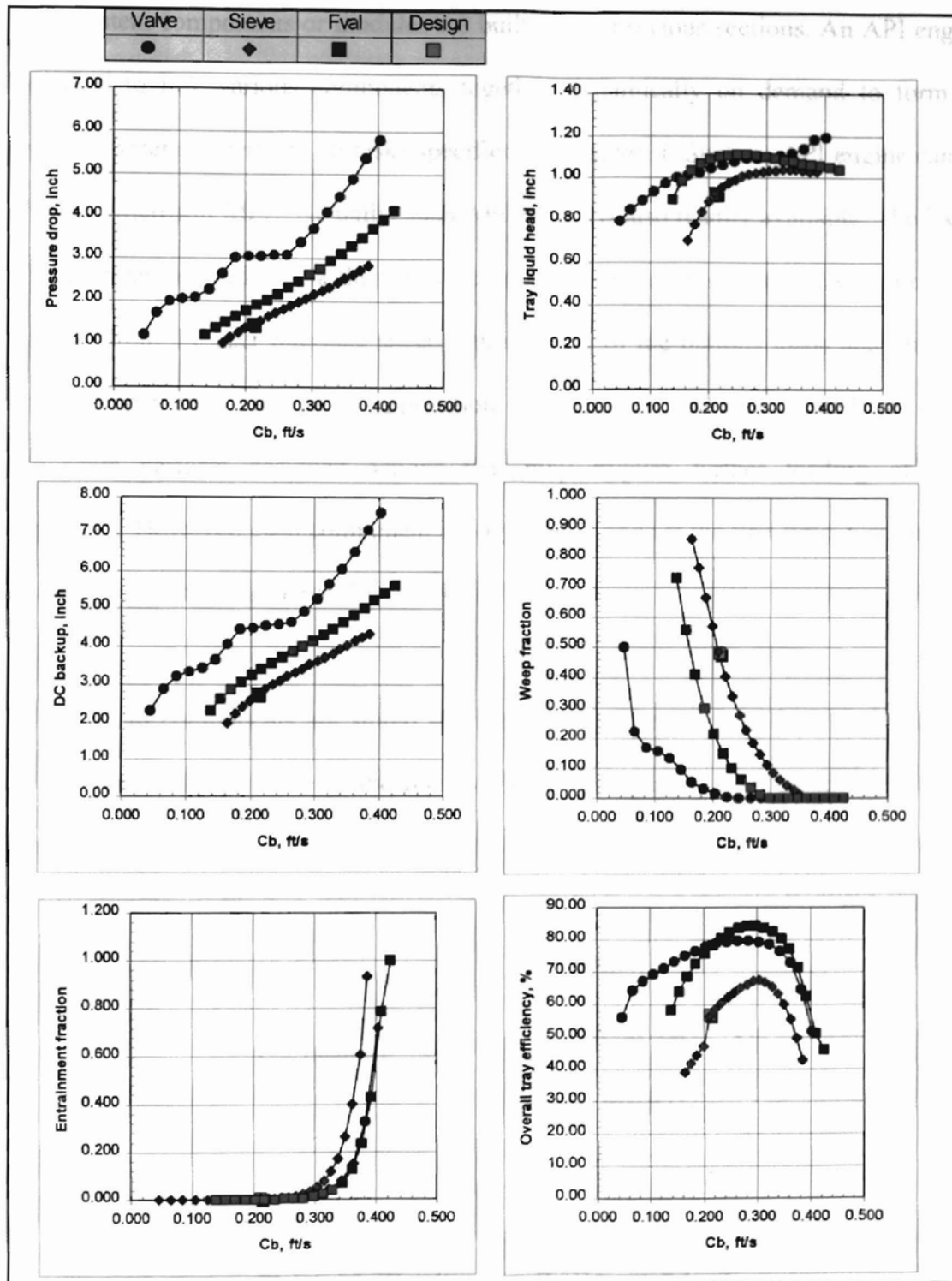


Figure 10. Performance Comparison Plot for Three Tray Internals

3.4 API Engine and System Integration

System components or modules are built in the previous sections. An API engine is required to link various components together dynamically on demand to form an integrated system to perform all tasks specified in Chapter II. Such an API engine can be built from Microsoft MFC. Actually, such API engine is also readily available. The Excel API engine can be used to link the various components together dynamically. Commands initialized from the user interface sheet with clicking of the buttons loads and links the proper components into Excel application dynamically and the loaded or linked components perform designed actions that may require further loading of other components. However, each component is only loaded once at the first time. Components not used or referenced are never loaded.

System components are stored in different sub-directories under a main one for easy reference. The structure of the files is shown in Figure 11. All components of the system are given in Figure 12.

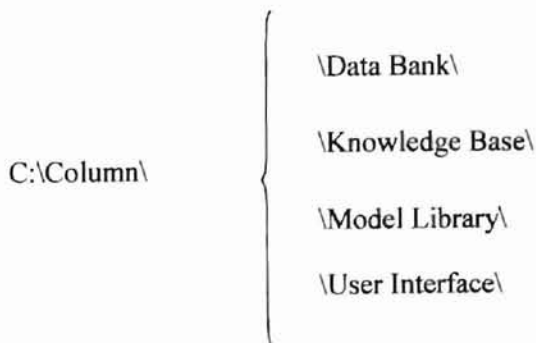


Figure 11. The directory Structure of the System

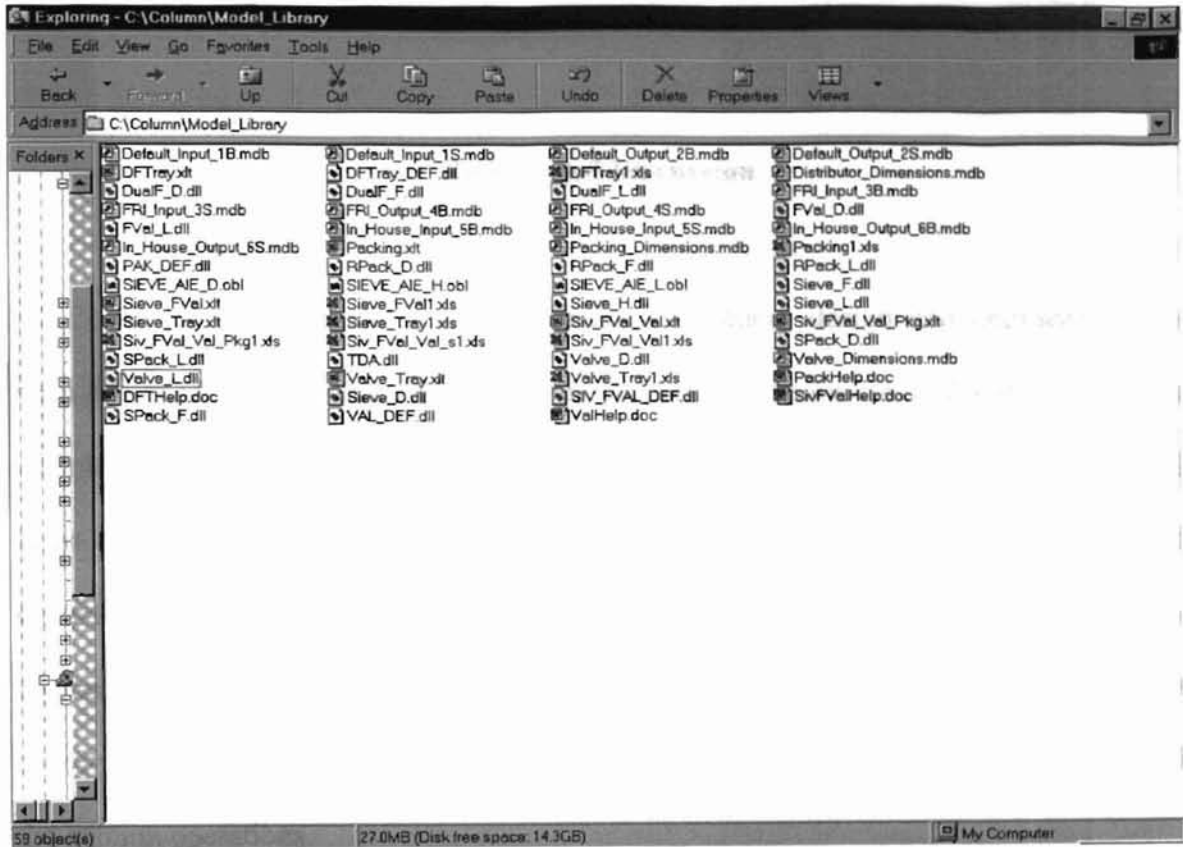


Figure 12. All Components Built and Used by the System

Excel files shown in Figure 12 contain various combinations of user interface sheets. The Access files are an array of data banks in both British and metric units. DLL files are technology modules and interface modules. Word files are help files that will be shown when Help button is clicked. The system can be partially or fully installed and can work as a whole or as a part.

CHAPTER IV

Results and Discussion

An integrated modular system distillation column design and engineering has been designed and constructed in previous chapter. It contains several sub systems for each kind of internals commonly used in columns including sieve tray, valve tray, dual flow tray, random and structure packings. The system uses up-to-date advanced technologies in computing science to help employ distillation knowledge in daily business of CPI. It can be used to manage the information flow and daily business activity, to help make decisions, to design and retrofit columns, to optimize and control the column operations.

4.1 Sample Runs

A few sample runs with tray internals are made to demonstrate the capability of the system. The results and conclusions obtained from tray internals can be extended to other internals included by the system.

4.1.1 Rating and Plotting

Column designs with different internals can be rated and their performances can be plotted by the system. For a sieve tray design of design ID T7777 as an example, the inputs of flow rates, physical properties, and tray and column dimensions are retrieved from the database into the sieve tray user interface. With various options

selected, clicking the rating button on the interface rates the column performance at the design point. Similarly, clicking the plotting button draws the performance diagram and hydraulic diagram.

4.1.2 Sizing

The system makes column sizing as easy as a button clicking. To size a column, a user first sets the design percent of jet and downcomer capacity. Then he clicks the sizing button on the interface. The optimal tray design is made by the system and the design results are shown on the user interface. Clicking the plotting button gives the performance plot for this design.

4.1.3 Design

A complete tray design can be made by the system with given flow rates and physical properties. The expert design module of the system is able to select the tray dimensions that are difficult to be optimized numerically such as sieve hole size and open area. With the inputs from the previous case in 4.1.2, clicking the expert button gives a full design of a sieve tray column.

4.1.4 Working with Data banks

Giving a unique Run_ID number and selecting a database, clicking the write button sends all information to the database. After the run is recorded in a database, it can be retrieved and loaded into any interface.

4.1.5 Comparison of Design Methods

The user interface sheet holding the previous example can be duplicated to create another user interface sheet. With different model options chosen for the two interfaces, the column performance predictions from the two set of models or design methods can be compared graphically and side by side.

4.1.6 Comparison of two Designs of the Same Internal

From the previous example with the same model option selected for the both interface sheets, the performances of two designs of the same tray internal can be compared and analyzed. A user can compare and study as many cases as necessary to reach a satisfied design.

4.1.7 Comparison of Two Different Internals

Similarly, the performances of different internals can be compared graphically by the system. A desired combination of different user interfaces for different internals are loaded into the same Excel workbook. The system can produce optimal designs for each internal. The column performances from different internals given by the system are then compared. According to results given by the system, a user can make a design decision based on the requirements of a minimum column diameter or a minimum column height or a minimum column volume. With the system, the optimal design of distillation columns can be easily realized based on selected design methods and available column design technology.

4.2 Discussion

Example runs show that the system is very easy to use. Users can access to different technologies in column design and engineering at the same time without switching among different applications. The system makes the optimum column design and the column internal selection as easy as just a few click of mouse. Unlimited design cases of the same internal or different internals can be compared graphically in any way users prefer. Test runs indicate that the system improves productivity by at least 10 to 100 times.

The results shown in the user interface sheets can be easily saved as a Web page in html format that can be published on the Internet or Intranet for sharing the information and results. The system can also be used to manage information and technology. Since the system has open structure, new technologies and column internals developed in the future can be made into additional components and added to the system. Due to the extensive uses of data banks, the system is easily connected to other foreign applications. The tray dimensions can be read by a CAD system. The physical properties generated by other applications are saved to the data banks and can be retrieved by the system.

The dynamically linked modular system developed in this study makes the memory uses more efficient that leads overall better performance. Since each component is independent of each other and is physically contained in an independent file, the

component can be added, deleted, and revised without affecting the other part of the system. This feature saves time and cost in the development and future maintenance.

The system can be viewed as a technology based management system (TBMS) that is similar to a data base management system. Each piece of technology can be considered as an object or ADT. Uses retrieve or use each technology through the uniform use interfaces. The uniform user interfaces are object-oriented. The system is able to contain as many technologies as desired for users to retrieve or use in their design and engineering for chemical process industry.

Since an Excel application can work both on a PC and in a network environment, the system is able to work in the network environment as well. As a result, the system delivers every piece of enterprise technologies to every engineer in everywhere at any time. Further, the system is also able to deliver technology through the Internet for a world-wide distribution and access because the new version of Excel application can run across the Internet.

CHAPTER V

Conclusions and Future Work

An integrated modular system is designed and developed as a part of this study. The system consists of many independent components and uniform user interface modules. Various components are loaded dynamically then linked on demand to an Excel application when users access the component and use the system. This study developed an effective way to reuse legacy codes in different languages to build new applications with uniform graphical user interfaces. The system developed in this study can deliver the technology that may be kept on mainframe machines in different format to users in a world-wide basis with a minimum development work.

The uniform graphical user interfaces are developed and used by the system. This study finds that using Excel sheets as user interfaces is an excellent means to give a new look to old applications. It has been shown that Excel sheets have many desirable features of user interfaces. With the uniform user interfaces and independent components, the system developed in this study can be viewed as a technology based management system.

Future work should focus on the development of more components for the system. Components such as those for data mining and modeling can be developed and

added to the system. An additional learning capability of the system can be incorporated to preserve knowledge for future generations.

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APPENDICES

APPENDIX A

ACRONYMS

API	Application Programming Interface
CAD	Computer Aided Design
CPI	Chemical Process Industry
DLL	Dynamic Link Library
DAO	Database Access Object
HTML	HyperText Markup Language
Tech	Technology
TBMS	Technology Based Management System
VR	Virtual Reality
WIMPS	Windows, Icons, Menus and Points

APPENDIX B

GLOSSARY

Distillation Column

A device contains column internals. It is used to separate chemical components from mixtures based on the difference in boiling points of different components.

Downcomer

Downcomer is used with trays. The liquid in the tray column flows down through the downcomer.

Dualflow Tray

It is similar to sieve trays but without a downcomer.

Packing

Packings are generally divided into random packing and structured packing. Random packings are discrete pieces of packing of a specific geometrical shape which are randomly packed into the column shell. Structured packings are crimped layers of wire mesh or corrugated sheets.

Sieve Tray

A piece of sheet metal having sieve holes for vapor to flow upward.

Valve Tray

It is similar to a sieve tray, but the holes are covered by valves.

Weir

Weir is used with trays to keep a layer of liquid/vapor phase on the tray deck.

VITA *γ*

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