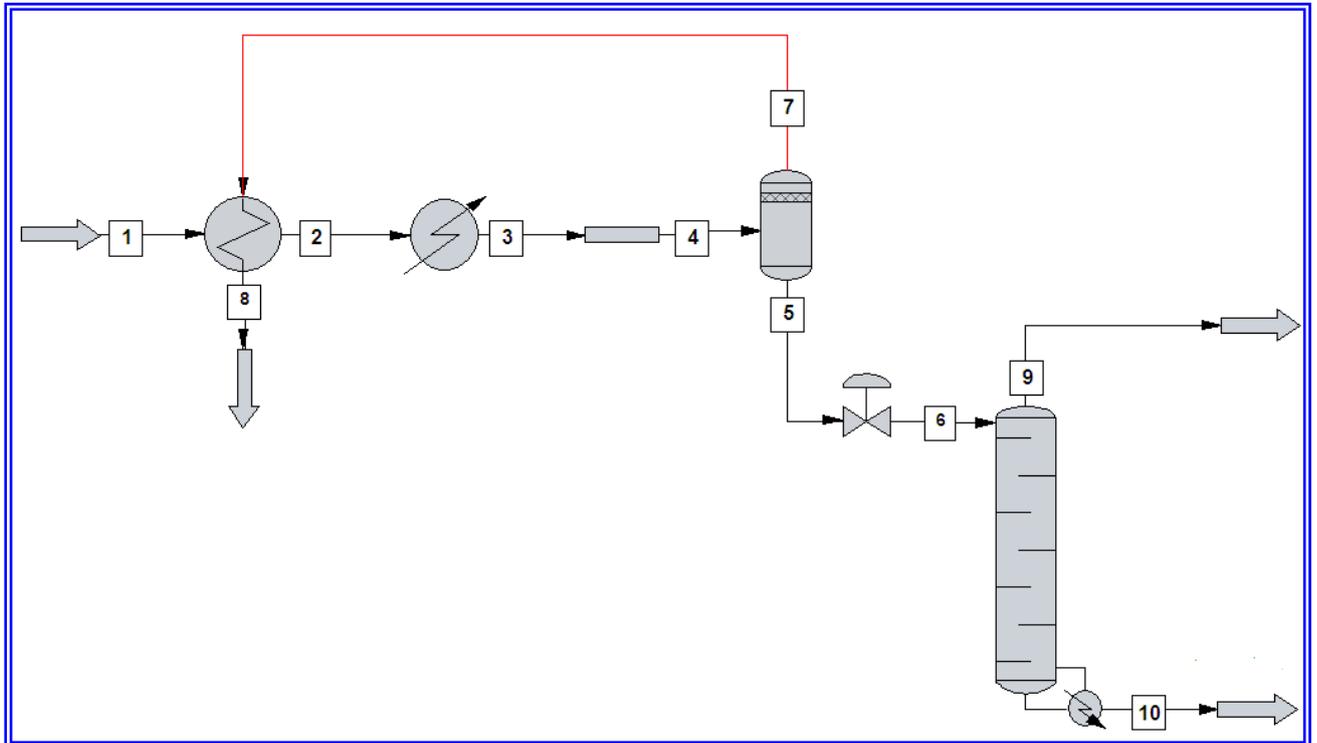


# ***CHEMICAL ENGINEERING***

## ***IN PRACTICE***

### ***Design, Simulation and Implementation***



***John E. Edwards***

***Process Simulation Engineer, P & I Design Ltd***

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[jee@pidesign.co.uk](mailto:jee@pidesign.co.uk)

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## *Preface*

This book is based on 50 years experience gained whilst working in the process engineering and simulation fields. It is not suitable for academic study, as it is intended for the practicing engineer. There is nothing original here, as the information has been developed from experience and based on many classic texts in Chemical Engineering literature, not least the following:

- Kern, Process Heat transfer, McGraw Hill
- Treybal, Mass Transfer Operations, McGraw Hill
- Norman, Absorption Distillation and Cooling Towers, Wiley
- Olson, Fundamentals of Engineering Fluid Mechanics, Intertext
- Fielder & Rousseau, Elementary Principles of Chemical Processes, Wiley
- Smallwood, Solvent Recovery Handbook, Edward Arnold
- Kohl & Nielsen, Gas Purification, Gulf
- Newbury, A Concise Organic Chemistry, Harrap
- Warn, Concise Chemical Thermodynamics, Van Norstrand Reinhold
- Shinsky, Process Control Systems, McGraw Hill
- Spink, Flow Meter Engineering, Foxboro
- Flow of Fluids 410, Crane
- Control Valve Handbook, Fisher Control Company

This book provides a synopsis of each section topic coupled with a concise data set, gleaned from many sources. Applications are presented from real situations whether it be design, simulation or operations.

Any originality may be in the presentation format and as such some would consider this to be a Handbook or Workbook. Many modern text books in Chemical Engineering do not adopt this approach which is not very helpful to the engineer challenged with providing a solution in a timely manner. The text books noted above seem to have a clarity of presentation missing from many modern text books.

This book has been collated from individual technical papers and guidance notes that have been written in support of our engineering activities and simulation work. As such each topic is in the form of a condensed refresher and provides useful practical information and data.

Each section is numbered uniquely for contents and references with the appendices and nomenclature being section specific. The references are not a comprehensive list and apologies for any unintended omissions.

Process simulation examples are based on CHEMCAD simulation software but the general principles should be adaptable to other simulation software.

Examples are included for each section topic and in many cases are based on actual designs or situations. Units used are not consistent, between Sections, as selection depended on the preferred units for a particular study. This should not be an issue as all simulators have powerful unit conversion facilities.

The simulation cases are available in electronic format. To run the simulations you will need a CHEMCAD software licence.

To obtain a software license and the cases please contact [support@pidesign.co.uk](mailto:support@pidesign.co.uk) who will organise a 30 day licence with Chemstations based in Houston.

## Section 1

### Introduction

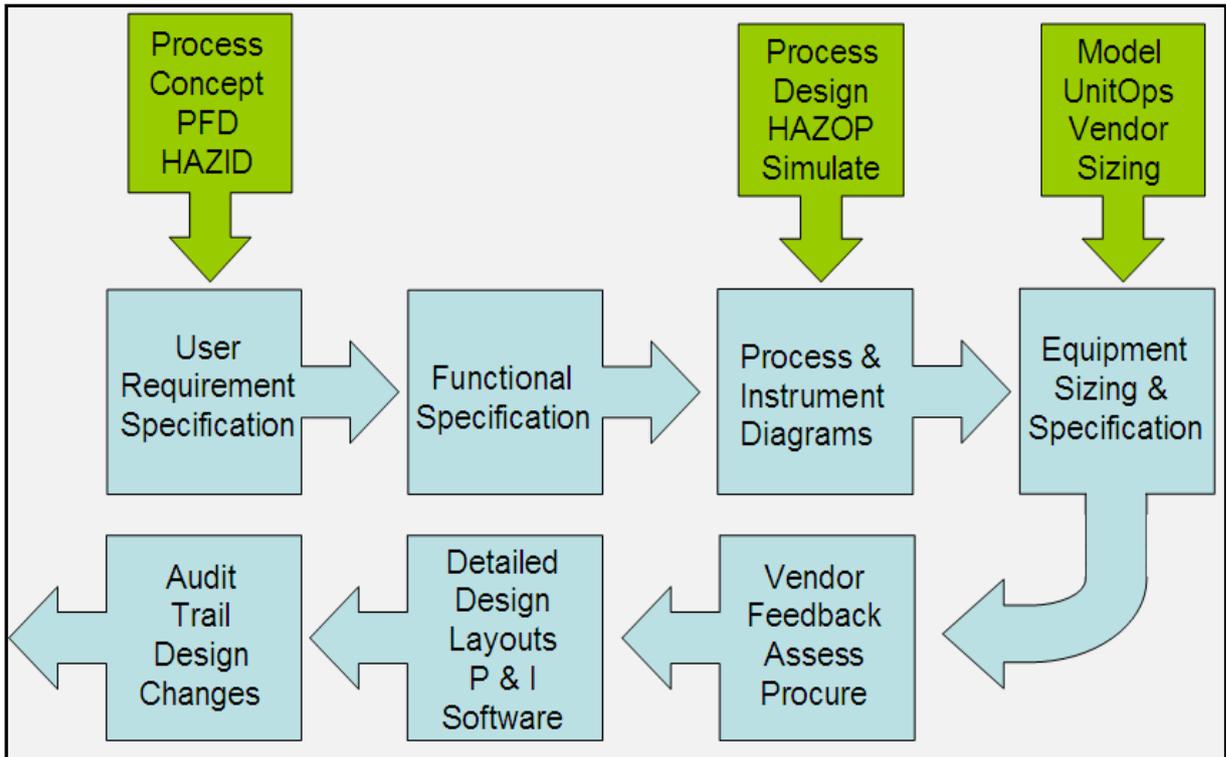
The process industry covers a broad spectrum of activities that involve the handling and treatment of gases, liquids and solids over a wide range of physical and processing conditions. The scope of this variety is shown in the following chart.

Utility Systems	Steam Generators	Cooling Systems	Compressed Air Systems	Heat Transfer Fluid System
Raw Material Storage	Feedstock Tank Farm	Liquid Nitrogen	ICB & Drum Handling	Bottled Gases
Primary Production	Continuous Process Unit	Batch Process Unit	Solvent Extraction	Evaporation Equipment
Purification Process Unit	Solids Separation	Drying Equipment	Ion Exchange	
Waste Treatment	Solvent Recovery	Wet Scrubbers	Thermal Oxidizer	Liquid Treatment
Product Despatch	Product Tank Farm	Tanker Loading Bay	Drum Filling & Storage	Solids Handling

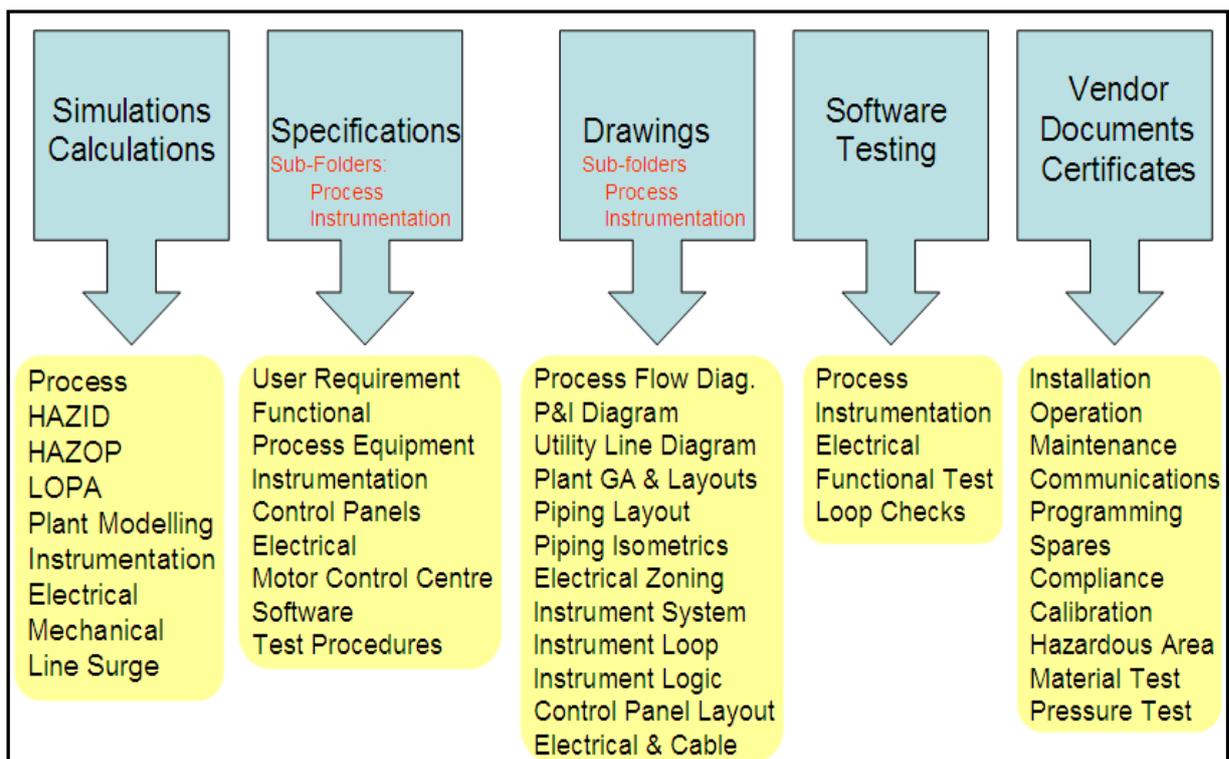
The development of a process and the steps taken to achieve an operational full scale unit are complex and involve many disciplines to achieve a successful result. Typical activities are shown in the following chart.

Process Chemistry	Thermodynamics Reaction Kinetics	Physical Properties	Optimize Process	
Process Concept	Process Simulations	Raw Material Assessment	Process Economics	Environment & Hazards
Flowsheet Developed	Mass - Energy Balances	Process Flow Diagrams	HAZID	
Scale-up	Process Steps	Test UnitOps	Budget	
Concept Design	Process Flow Updates	Process Inst Diagrams	HAZOP	Planning & Compliance
Detailed Design	Plant & Piping Layouts	Equipment Specification	LOPA	
Implement Phase	Project Management	Testing Calibration	Start up	Troubleshoot Optimization

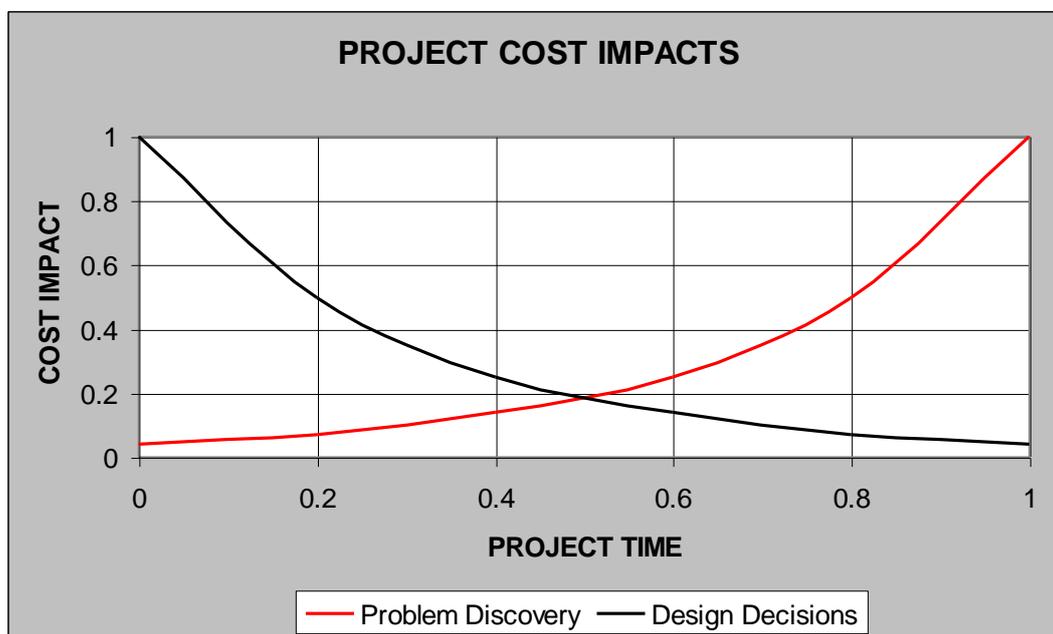
Project implementation involves many disciplines, including process, mechanical, electrical and control engineers, working as a team in a coordinated manner. The main work phases, together with the documentation required, are summarised in the following charts.



The process engineer, working in this environment The process engineer is required to provide safe, practical and timely solutions to design problems without having the opportunity to study the topic in great depth. This book is an attempt to provide a comprehensive review of the fundamentals, definitions and design principles to allow the solution of cases encountered in normal practice. For more complex cases or when in doubt reference should be made to an appropriate authority or specialist in the field.



The design process should attempt to identify potential problems and errors at the earliest stage possible in the life of a project. Many techniques have been developed to achieve this, namely HAZID, HAZOP, LOPA together with process simulation. The project cost impact curves show the benefits of stress testing the designs using these techniques to avoid the increased costs of correction, even if economically possible, late in the project life cycle.



Processes can be batch, semi-continuous or continuous and the selection depends on many factors.

Batch processes are used in the manufacture of a wide variety of fine and speciality chemicals and involve the following general criteria:

- Low to medium capital investment
- Low to medium cost to rectify design errors
- Low volume high value products
- Low to medium production costs
- Limited savings from yield improvements and reduced cycle times
- Multi-purpose capability often required

Batch processes are inherently transient in nature and to the equipment design needs to be analysed using the physical properties of the process and service fluids under a wide range of operating conditions.

Continuous processes are used in the oil and gas processing and petrochemicals industries and have the following characteristics:

- Heavy capital investment
- Expensive to rectify design errors
- High volume low to medium value products
- Well established process or high level of confidence in design for new process
- Large savings in raw materials and energy achievable with process optimization
- Product change capability required in some processing units

Process simulation tests the capability to achieve stable and reproducible operating conditions to achieve the product purity, yield, cycle times to satisfy the commercial requirements and the safety and environmental issues for the regulatory authorities.

The characteristic properties and design parameters of the process are analysed in this book using the CHEMCAD™ range of software by Chemstations of Houston.

## ***Section 2***

# ***Fundamentals***

### **Contents**

- 1.0 Introduction**
- 2.0 Units**
- 3.0 Mass and Energy Balances**
- 4.0 Simulation Principles**

### **Appendices**

- I Nomenclature**

### **References**

- 1 R.M.Felder and R.W. Rousseau, "Elementary Principles of Chemical Processes", Wiley, 2<sup>nd</sup> Edition, 1986.**
- 2 F.G.Shinskey, Process Control Systems, McGraw Hill, 1<sup>st</sup> Edition, 1967**

## 1.0 Introduction

This Section reviews engineering units and their application to prevent misuse in certain applications. Mass and energy balance principles and the fundamentals of steady state and dynamic simulation are reviewed.

## 2.0 Units

### Molality, Molarity, Mole Fraction and Mole Ratio<sup>(1)</sup>

Molality,  $m_i$  (mol/kg) denotes the total number of moles of solute species  $i$  per 1000g of solvent (not solution).

Molarity,  $M_i$  (mol/litre, kmol/m<sup>3</sup>) denotes the total number of moles of species  $i$  per litre of solution, sometimes referred to as Normality  $N$  which is essentially the same as mol/litre.

Mole fraction,  $x_i$  denotes the number of moles of species  $i$  divided by the total number of moles in a solution.

$$x_i = \frac{m_i MW_s}{1000}$$

Mole ratio  $X_i$  denotes the number of moles of species  $i$  divided by the number of moles of species  $j$ . For a binary solution we have:

$$X_i = \frac{x_i}{x_j} = \left( \frac{x_i}{1 - x_i} \right)$$

The weight fraction  $w_i$  of, for example, an alkanolamine aqueous solution is calculated from:

$$w_i = \frac{M_i MW_i}{\rho_{Soln} 1000}$$

Consider a reactant species A with a flowrate  $W_A$  (kg/h) and molecular weight  $M_A$  (kg/kmol) and inert species B with a flowrate  $W_B$  (kg/h) and molecular weight  $M_B$  (kg/kmol), we have:

Mole fraction component A 
$$y_A = \frac{W_A / M_A}{W_A / M_A + W_B / M_B}$$

Mole fraction component B 
$$y_B = 1 - y_A$$

Mean molecular weight 
$$M_{AB} = \frac{W_A + W_B}{W_A / M_A + W_B / M_B}$$

For a system pressure  $P=1.01325$  bar and temperature  $T^\circ K$  the inlet gas density is given by:

$$\rho_1 = \frac{M_{AB}}{22.4} \left( \frac{273}{273 + T} \right)$$

The gas inlet concentration of component A can be converted from mole fraction to mg/m<sup>3</sup> from:

Units in mg m<sup>3</sup> 
$$y_A \cdot 10^6 \left[ \frac{M_A}{22.4} \left( \frac{273}{273 + T} \right) \right]$$

Weight fraction is converted to mole fraction as follows:

$$x_i = \frac{w_i / MW_i}{w_i / MW_i + (1 - w_i) / 18}$$

## ppm(w), ppm(v), mg/m<sup>3</sup>, mole fraction and weight fraction

As always, units need to be approached with care. Frequently the basis used in published data assumes the reader knows the unit convention being used due to a particular industry practice. Concentrations are frequently quoted in ppm, which is a measurement of concentration on a weight or volume basis, frequently unspecified, depending on whether referring to contaminants in gases or liquids. We will use subscript v for vapour and w for weight.

### Pollutants in gases

Consider 
$$\text{ppm}_v = \frac{\text{mg}}{\text{m}^3} \times \frac{22.4}{\text{MW}} \times \frac{273 + t}{273} = \frac{\text{mg}}{\text{m}^3} \times \frac{24.055}{\text{MW}} \quad \text{at } 20^\circ\text{C}$$

$$\text{ppm}_v = \text{mf} \times 10^6$$

### Pollutants in liquids

Consider 
$$\text{ppm}_w = \frac{\text{mg}}{\text{L} \times \rho} = \frac{\text{mg}}{\text{L}} \quad \text{for water, where L is a litre and } \rho \text{ is liquid density}$$

$$\text{ppm}_w = \text{wf} \times 10^6$$

$$\text{wf} = \frac{\text{ppm}_w}{10^6} \qquad \text{mf} = \frac{\text{ppm}_w}{10^6} \times \frac{\text{MW}_{\text{Solvent}}}{\text{MW}_{\text{Contaminant}}}$$

For example, trichloroethylene (MW 131.4 g/mole) has a consent limit for drinking water, using preferred units, of 0.005 mg/L = 0.005 ppm(w). Therefore the consent limit as a weight fraction is  $0.005 \times 10^{-6}$  and as a mole fraction is  $0.000684 \times 10^{-6}$ .

For water contaminated with 100 ppm(w) trichloroethylene the inlet mole fraction is  $1.36 \times 10^{-5}$  and for a target purity of 1 ppm the outlet mole fraction is  $1.36 \times 10^{-7}$ . We will be looking at this air stripping example<sup>(13)</sup> later in Section 6.

The following table shows the relationships between volumes, moles, and mass.

Molar and Mass Relationships for Mixture with "i" Species								
Component	MW	% v/v	Volume in 1 m <sup>3</sup>	Mass in 1 m <sup>3</sup>	% w/w	Mass Flow	Molar Flow	% mol
	kg/kmol		m <sup>3</sup> /m <sup>3</sup>	kg/m <sup>3</sup>		kg/h	kmol/h	
A	M <sub>A</sub>	P <sub>A</sub>	$V_A = \frac{P_A}{100}$	$\frac{P_A M_A}{2241.5}$	$\frac{100 P_A M_A}{\sum P_i M_i}$	$\frac{W P_A M_A}{\sum P_i M_i}$	$\frac{W P_A}{\sum P_i M_i}$	P <sub>A</sub>
B	M <sub>B</sub>	P <sub>B</sub>	$V_B = \frac{P_B}{100}$	$\frac{P_B M_B}{2241.5}$	$\frac{100 P_B M_B}{\sum P_i M_i}$	$\frac{W P_B M_B}{\sum P_i M_i}$	$\frac{W P_B}{\sum P_i M_i}$	P <sub>B</sub>
C	M <sub>C</sub>	P <sub>C</sub>	$V_C = \frac{P_C}{100}$	$\frac{P_C M_C}{2241.5}$	$\frac{100 P_C M_C}{\sum P_i M_i}$	$\frac{W P_C M_C}{\sum P_i M_i}$	$\frac{W P_C}{\sum P_i M_i}$	P <sub>C</sub>
Total		100	1	$\frac{\sum P_i M_i}{2241.5}$	100	W	$\frac{100 W}{\sum P_i M_i}$	100

We have defined: 1 g-mole of any gas occupies 22.415 litre(dm<sup>3</sup>) at 0°C and 1 atmosphere.

Therefore we can say that the same g-mole of any gas will occupy the same volume giving:

$$\text{Mole \%} = \text{Volume \%}$$

For a Total Flow of  $W$  (kg/h) and a mixture density of  $\rho_{G0} = \frac{\bar{M}}{2241.5}$  (kg/m<sup>3</sup>) we have:

$$\text{Volumetric Flow } Q = \frac{W}{G_0} = \frac{2241.5 W}{\sum P_i M_i} \text{ (Nm}^3\text{/h)}$$

$$\text{where average mw } \bar{M} = \frac{\sum P_i M_i}{100} \text{ (kg/kmol)}$$

To correcting for temperature and pressure gas density calculations are calculated from:

$$\rho_G = \frac{M_w}{22.415} \times \frac{P_f}{Z_f} \times \frac{273}{T_f} \text{ kg / m}^3$$

where 22.415 is in units of litre(dm<sup>3</sup>)/g-mole or m<sup>3</sup>/kg-mole of any gas at NTP(0°C,1atm),  $M_w$  is molecular weight g/mol or kg/kmol.

### Example

For example a 30.2% w/w MEA solution in water has an MEA (MW=61.09 g/mol) mole fraction of 0.558, a mole ratio of 1.26 and molarity (density= 1.01 g/litre) of 5.0 N. 15.2% w/w is 2.5N.

Now consider the vapour liquid equilibrium of a gas containing CO<sub>2</sub> in air being scrubbed with a 30% MEA aqueous solution using with K model-AMINE.

A TPxy plot provides equilibrium data for the CO<sub>2</sub>/MEA/Water system in mole or weight fractions which include or exclude the third component, water. If CO<sub>2</sub>/MEA liquid mole ratio  $X$  is required then use data excluding the third component and for mole fraction  $x_{CO_2}$  include the third component.

In the gas phase the air needs to be considered.

A TPxy plot, at constant temperature, provides a report which provides the sum of component partial pressures,  $p$ , for values of  $x$ , allowing the CO<sub>2</sub> mole fraction  $y_{CO_2}$  to be calculated from the total pressure.

$$y_{CO_2} = \frac{P - P_{MEA} - P_{H_2O}}{P_T} = \frac{P_{CO_2}}{P_T}$$

Consider a system at 1.01325 bar (101.325 kPa) with components CO<sub>2</sub>/MEA/H<sub>2</sub>O with H<sub>2</sub>O as 3<sup>rd</sup> component having a constant mole fraction of 0.866.

A single set of data from the TPxy plot, at constant temperature of 50°C, gives:

$$p_{MEA} + p_{H_2O} = 0.1242 \text{ bar when } x=y=0, \text{ ie no CO}_2 \text{ in system.}$$

CO <sub>2</sub> /MEA/H <sub>2</sub> O	$x_{CO_2} = 0.0335$	$y_{CO_2} = 0.01633$	$p_{CO_2} + p_{MEA} + p_{H_2O} = 0.126 \text{ bar}$
CO <sub>2</sub> /MEA	$x_{CO_2} = 0.25$	$y_{CO_2} = 0.94587$	$p_{CO_2} + p_{MEA} + p_{H_2O} = 0.126 \text{ bar}$

The equilibrium curve liquid composition axis can have units of mole fraction 0.0335 or mole ratio CO<sub>2</sub>/MEA  $0.25/(1-0.25) = 0.333$ . The vapour composition axis can have units of partial pressure  $p_{CO_2} = (0.126 - 0.1242) \times 101.325 = 0.18 \text{ kPa}$  or mole fraction  $0.18 / 101.325 = 0.00178$ .

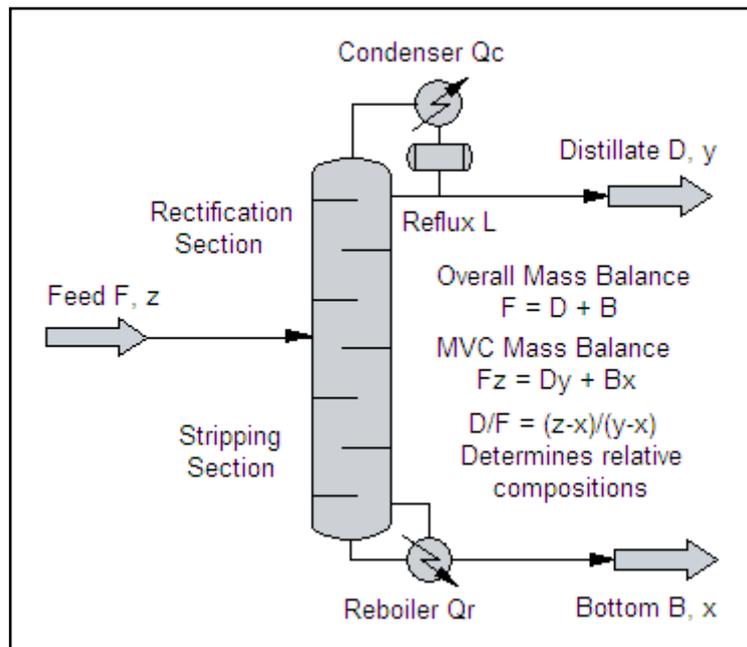
Note TPxy data gives CO<sub>2</sub> mole fractions in vapour as mol CO<sub>2</sub>/(mol CO<sub>2</sub> + mol MEA + mol H<sub>2</sub>O) or mol CO<sub>2</sub> / (mol CO<sub>2</sub> + mol MEA) which can be misused in absorption of species from inerts.

### 3.0 Mass and Energy Balances<sup>(1,2)</sup>

The law of conservation of mass, which states that mass can neither be created or destroyed, enforces the requirement that a process design is not complete until all inputs and outputs of the overall process and individual units satisfy a mass balance for each component.

For a batch process no mass crosses the system boundaries between the time the feed is charged and the product is removed and for a continuous process inputs and outputs flow continuously. A semi-batch process combines both characteristics.

Consider the mass balance across a Distillation Unit. At steady state the overall material balance must be satisfied for each component. Only one product stream can be set independently making the other product stream a dependent variable. In general, the distillate flow is manipulated, directly or through varying reflux ratio, requiring the bottom outlet flow to be adjusted to maintain the material balance which is achieved by holding the reboiler liquid level constant.



The material balance based on the more volatile component (MVC) yields:

$$\frac{D}{F} = \frac{z - x}{y - x}$$

This shows that the flow ratio **D/F** determines the relative composition of each product such that if feed composition **z** changes then **D/F** must be manipulated to maintain constant **x** and **y**.

Note how the mass balance equations imposes restraints on the inter-dependency of feed and product stream flow rates and compositions. This feature is used to develop control strategies such as feedforward control.

The law of conservation of energy, which states that energy can neither be created or destroyed, is the First Law of Thermodynamics, discussed later in Section 3. The rate at which energy (kinetic+potential +internal) accumulates in a system is the net energy transferred (heat and work) to the system from the input streams minus the output streams. A batch process is a closed system, in that energy does not cross the system boundaries and a continuous process is an open system.

For the distillation column a simplified overall energy balance yields:

$$Q_r + F_H = C_c + D_H + B_H + \text{losses}$$

The process design objective is always to minimize the use of energy consistent with achieving the desired product quantity and quality. Consider a batch distillation where the objective is to minimise the batch cycle time which implies maximising the heat input and minimising the reflux ratio to achieve the required separation. The process variables are interdependent as determined by the mass and energy balances and the mode of operation.

The heat input for a variable top composition achieved by setting a fixed reflux ratio is given by:-

$$Q = \lambda (S_0 - S_1)(R + 1)$$

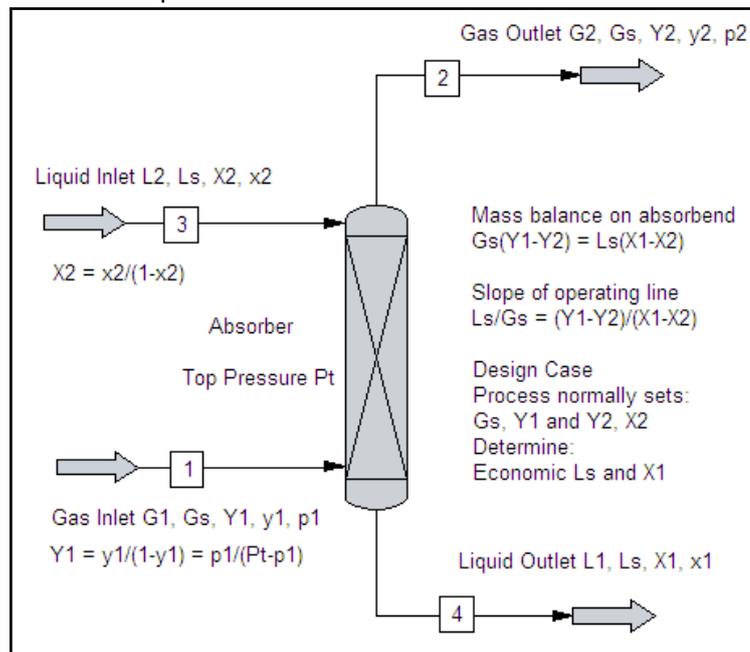
The heat input for a fixed top composition is achieved by varying the reflux ratio to maintain a fixed top temperature at constant pressure is given by:-

$$Q = \lambda(S_0 - S_1) \int_{R_0}^{R_1} (R) dR$$

Where  $\lambda$  mean latent heat  
 $S_0$  starting material  
 $S_1$  final material  
 $R$  reflux ratio

Both relationships indicate that the reflux ratio must be kept to a minimum, subject to satisfying the requirements for the desired separation specification, to optimise the heat input.

Now consider an absorber mass balance where the gas inlet stream condition and the liquid inlet composition are determined by the process with the liquid flow rate being the only variable to adjust the dependent outlet streams compositions.



The gas stream,  $G$  (mol/area-time), at any point in the tower consists of the diffusing species, mole fraction  $y$ , partial pressure  $p$  or mole ratio  $Y$  and the non-diffusing relatively insoluble gas  $G_s$  and are related as follows.

$$Y = \frac{y}{1-y} = \frac{p}{P_t - p} \quad G_s = G(1-y) = \frac{G}{1+Y}$$

The liquid stream  $L$  (mol/area-time), at any point in the tower consists of the dissolved species, mole fraction  $x$  or mole ratio  $X$  and essentially non-volatile solvent  $L_s$  and are related as follows:

$$X = \frac{x}{1-x} \quad L_s = L(1-x) = \frac{L}{1+X}$$

Since the inert gas  $G_s$  and solvent liquid  $L_s$  remain essentially unchanged in the tower the overall material balance is based on them and yields:

$$G_s(Y_1 - Y_2) = L_s(X_1 - X_2)$$

This is the equation of the operating line with slope  $L_s/G_s$  which passes through ordinates  $(X_1, Y_1)$  at the bottom (gas inlet/liquid outlet) and  $(X_2, Y_2)$  at the top (gas outlet, liquid inlet). We can conclude the following:

1. The composition of both product streams is dependent on  $L/G$
2. For a constant separation, setting the composition of either product results in control of the composition of the other product due to the relationship between  $x$  and  $y$  being fixed.

## 4.0 Simulation Principles

Simulators provide process engineers with a powerful tool to assist in the design, optimization and operation of processes. The simulator characteristics are determined by the process. Batch and semi-batch processes require dynamic simulation whereas continuous processes are studied with both dynamic and steady state simulators.

Dynamic simulators are based on real time or accelerated dynamic simulation principles and can provide a true representation of the plant behaviour, including retention times and thermal lags. Continuous steady state with varying throughput, start up, shutdown, feed change, composition change all can be studied. Dynamic simulators can also be used for operational plant troubleshooting, control loop tuning and real time optimization. Dynamic simulations require more information and more difficult to set up.

Steady state simulators model plant behaviour using continuous, time interval based, steady state approximations and require the least effort to set up and calibrate the flowsheet. Dynamic simulation can also considered to be a series of steady state simulations.

A process simulation involves taking the input stream flow rates, compositions and thermodynamic conditions, performing a series of iterative calculations as the streams are processed through Unit Operations and recycles, finally leading to the output stream flow rates, compositions and thermodynamic conditions.

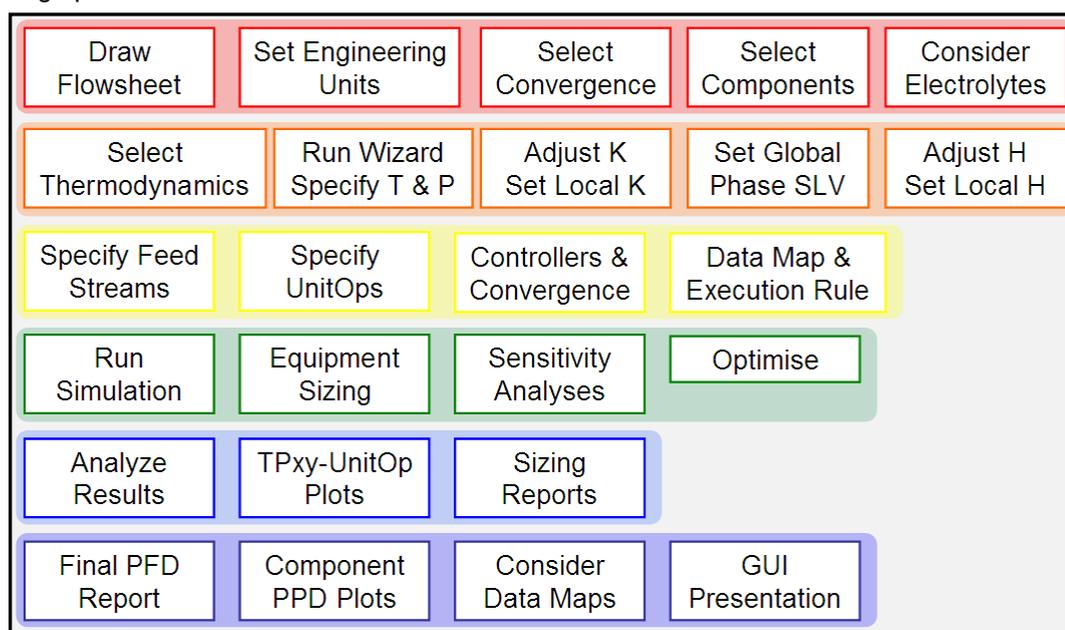


The iterative process can be based on

- Direct substitution, the value is recalculated after each iteration
- Wegstein acceleration, the value is recalculated after three iteration-speed up frequency 3
- Dominant Eigen value, the value is recalculated after three iteration-speed up frequency 4

The number of iterations is limited, default value 40, until the convergence parameters are satisfied, nominally set at an absolute value of 0.001.

A simulation carries out repetitive calculations, based on the thermodynamic models selected, to satisfy the mass and energy balances around individual Unit Operations with recycle streams and to satisfy the overall process balances. In typical integrated continuous processes this is not a trivial exercise due to the inter-dependency of all parameters. The chart below shows the steps involved in setting up a simulation.



Prior to the introduction of process simulators this exercise involved a team of engineers working many man hours and maybe not achieving a definitive result.

## Appendix I Nomenclature

G	total gas molar flow	mol/s-m <sup>2</sup>
G <sub>s</sub>	insoluble gas molar flow	mol/s-m <sup>2</sup>
L	total liquid molar flow	mol/s-m <sup>2</sup>
L <sub>s</sub>	non-volatile solvent molar flow	mol/s-m <sup>2</sup>
F	feed flow	kg/h
D	distillate flow	kg/h
B	bottoms flow	kg/h
S	batch quantity	kg
x	concentration in liquid (MVC in feed)	mole fraction
y	concentration in gas (MVC in distillate)	mole fraction
z	MVC concentration in bottoms	mole fraction

### Subscripts

0	initial condition
1	tower bottom, gas inlet, liquid outlet or final condition
2	tower top, gas outlet, liquid inlet

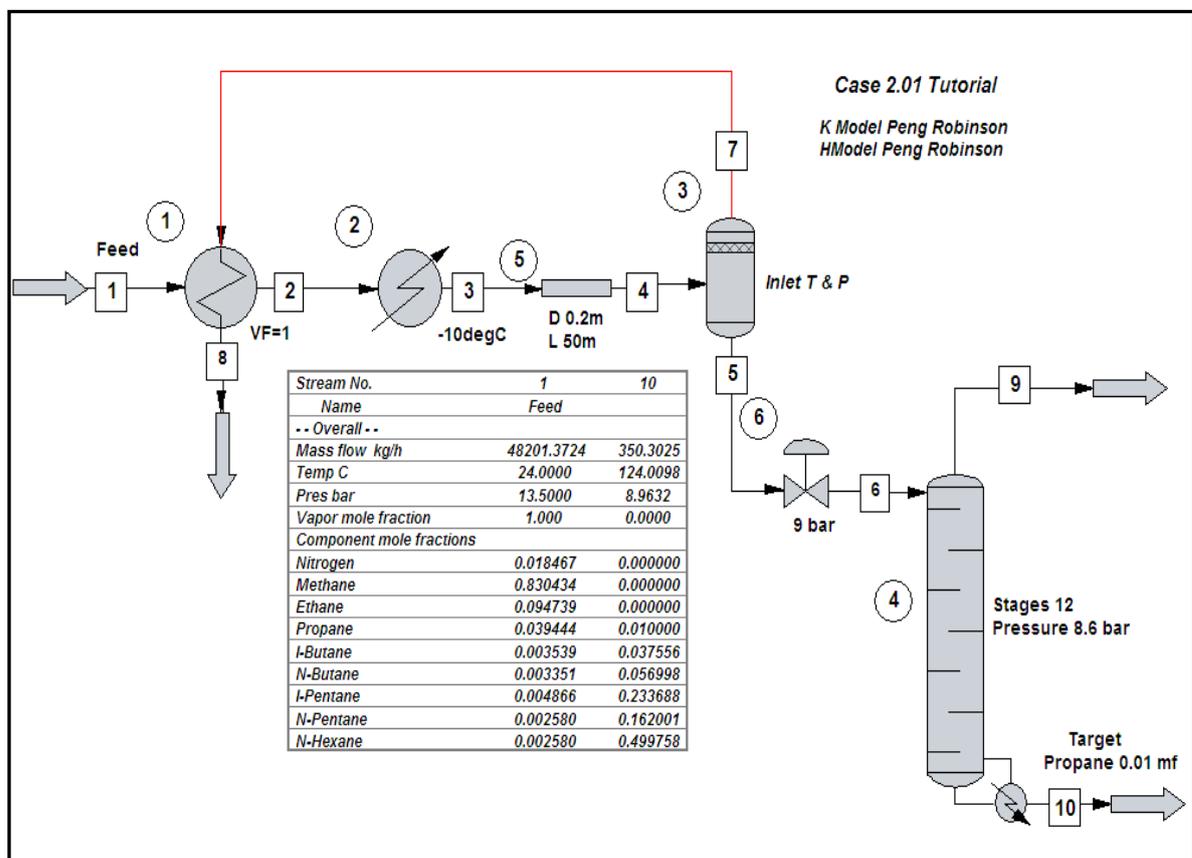
## Section 2

### Fundamentals Simulation Cases

In this section are presented cases to facilitate an understanding of the CHEMCAD steady state simulation. For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

Case/File Name	Description
2.01	Tutorial A1

This tutorial introduces UnitOps Heat Exchangers, Pipe Simulator, Flash Unit, Control Valve and SCDS Column and the handling of a recycle stream. The objective is to achieve a column bottoms propane concentration target of 0.01 mole fraction.



## ***Section 3***

# ***Process Control and Instrumentation***

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- 5 Controller Tuning
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- I Flow Meter Considerations

### **References**

1. F.G.Shinskey, Process Control Systems, McGraw Hill, 1967
2. J.E.Edwards, Level Sensor Selection, Chemical Processing, December, 2010

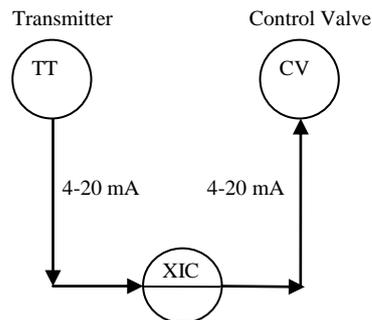
## 1.0 Introduction

An understanding of the fundamentals of process control is essential before beginning work on dynamic simulation. Process Control Systems by Shinskey is a landmark text in which Process Control is explained from first principles with due consideration given to real processes in regards to mass and energy balances.

The cases presented in this Section's Workbook provide an introduction to dynamic simulation and simple control loop applications.

## 2.0 Control System Basics

A basic control loop consists of an instrument measuring a process variable and converting it into a 4 to 20 ma dc signal for transmitting to a controller. The controller produces a 4 to 20 mA dc output signal based on the error between measurement and set point and the control parameters. The output signal is connected to a regulating device, such as a control valve or variable speed drive. A typical single loop showing this configuration follows:



The key points to consider when setting up a control loop with a controller and control valve combination are:

1. The measurement from a process is normally transmitted using a 4 to 20 mA dc signal representing the process variable calibrated range. For example a flow loop could be calibrated 4 mA = 0 kg/h (Enter 1E-06 not 0 in simulation) and 20 mA = 50000 kg/h. An elevated zero can be used - 4 mA = 10000 kg/h or a suppressed zero 4 mA = -50°C.
2. The measurement signal on modern systems, is normally linearised with signal conditioners, for example flow measurement with an orifice plate gives a signal proportional to the square of flow. The measurement units for level is Length and for mass flow is Mole/Mass.
3. Set Point value is the desired process value in the same units as specified for the measurement.
4. Controller Action determines the controller output (OP) in response to the error between Set Point (SP)  $\pm$  Measurement (MV).

For Reverse Action: If  $MV > SP$  the  $OP \downarrow$  and if  $MV < SP$  the  $OP \uparrow$

For Direct Action: If  $MV > SP$  the  $OP \uparrow$  and if  $MV < SP$  the  $OP \downarrow$

It is essential that this concept is understood because an incorrect selection will result in Positive Feed back with MV continually increasing or decreasing.

5. Control Valve failure action selection is determined by the process e.g. heating valve usually fails closed and cooling valve usually fails open. A fail closed valve requires an increasing controller output 4 to 20 mA signal to open (Signal to Open) and a fail open valve requires an increasing controller output to close (Signal to Close).
6. An incorrect match of controller action and valve action will result in Positive Feedback.
7. Tuning parameters for noisy control loops e.g. liquid flow, liquid pressure and level use a wide Proportional Band (PB in %) as controller gain is  $100/PB$  relying on short Integral Times ( $T_i$  in m) to eliminate  $SP \pm MV$  error. Never use Derivative on noisy signals as  $T_d$  operates on rate of change of error  $de/dt$ .

### 3.0 Controller Basics

The controller algorithm in CHEMCAD is representative of a model which does not exhibit interaction between control modes:-

$$\text{Controller output } P_{out} = \frac{100}{P} \left( e + \frac{1}{T_i} \int edt + T_d \frac{de}{dt} \right) + P_o$$

Where, P = proportional band, %  
T<sub>i</sub> = integral action time, min  
T<sub>d</sub> = derivative action time, min  
P<sub>o</sub> = steady state controller output  
e = ± (X<sub>set</sub> - X), the error between process measurement and set point

Inspection of the controller equation yields the following key points:

1. If no error the controller output equals steady state output P<sub>o</sub>
2. The controller gain is 100/P. Increasing P decreases the controller gain with % change of output for same % error change reducing and vice versa.
3. The integral term being 1/T<sub>i</sub>, increasing T<sub>i</sub> reduces its effect. Increasing error results in an increase in rate of change of controller output. For fast processes, such as flow, use low T<sub>i</sub> and for slow processes, such as temperature, use higher T<sub>i</sub> but do not set such that the process is too slow to absorb the energy change, which will result in cycling.
4. Decreasing derivative term T<sub>d</sub> reduces its affect. Increasing error rate change increases % controller output change. Do not use on noisy processes, such as flow, level and liquid pressure, as equipment damage will result!

The measurement calibrated range, in Engineering Units, is converted to a 4 to 20 mA signal as a linear or quadratic function. In modern control systems most inputs are now linearised.

Controller output direction in response to an error ( ± ) is determined by the controller action.

Direct action where increasing input gives increasing output or decreasing input gives decreasing output

$$e = X - X_{set} \quad (\text{Level with fail closed valve on tank output})$$

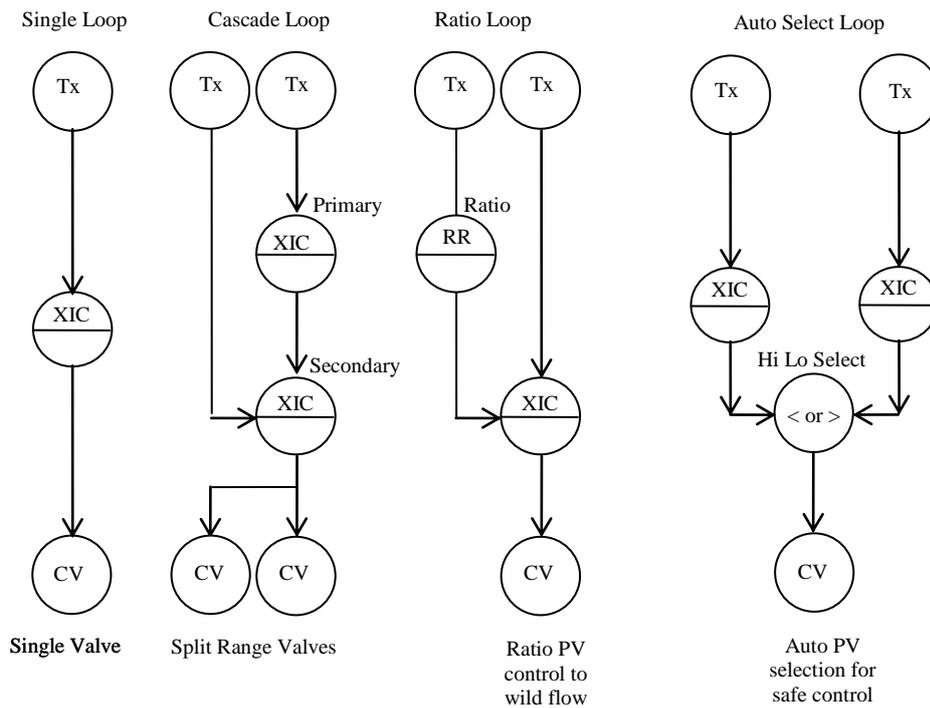
Reverse action where increasing input gives decreasing output or decreasing input gives increasing output

$$e = X_{set} - X \quad (\text{Heating valve will fail closed with fail closed valve cooling valve will fail open with fail open valve})$$

In CHEMCAD the controller output can be directed to one valve or two valves, in split range operation, or another controller set point for cascade operation.

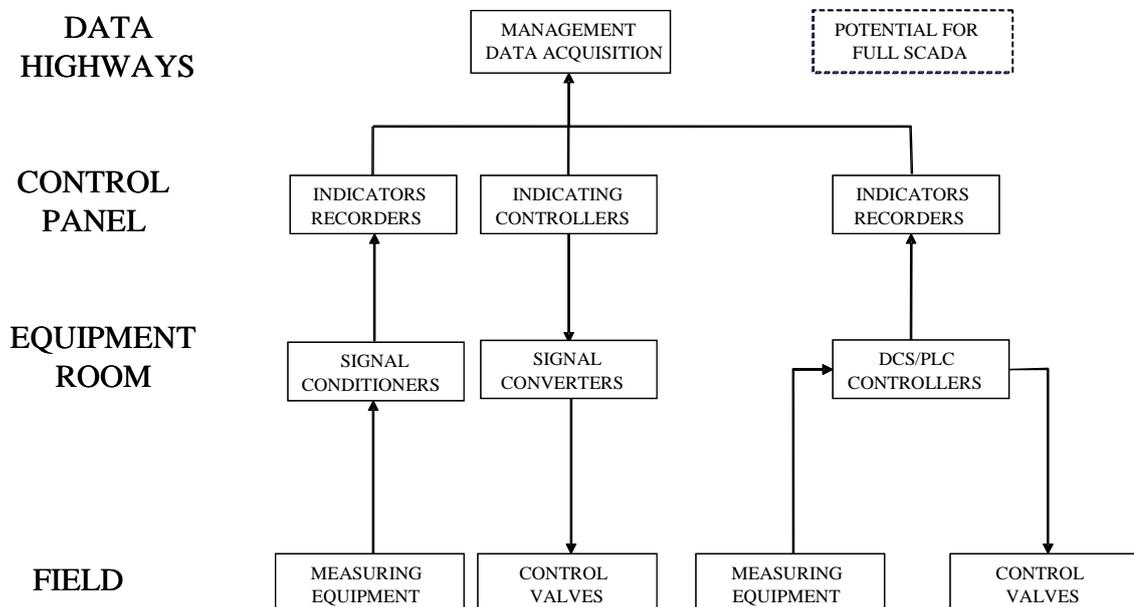
The measurement can be derived from a Stream or UnitOp variable. For UnitOp variable measurements always use the Calculated Value. Set the steady state controller output (P<sub>o</sub>) at the simulation start value which is derived from running the model in steady state with correctly sized control valves, using valve sizing feature.

The basic control loop consists of a field mounted transmitter, with the process variable (PV) range scaled to represent a 4-20 mA signal, a control room mounted controller and process parameter regulating device such as a control valve or variable speed drive. Common loop configurations are shown below:



All the above configurations can be achieved in CHEMCAD using the Excel mapping tool.

The diagram below shows the location and component configuration of a typical modern system:



#### 4.0 Control Valve Characteristics

The selection of a control valve, with the appropriate operating characteristics and sizing, is essential for satisfactory control loop performance. A valve has two characteristics namely the inherent characteristic (relationship between flow and stroke at constant  $\Delta P$ ) and the operational characteristic where the inherent characteristic is modified by the process pressure conditions.

An Equal Percentage valve operating characteristic tends towards a linear characteristic as  $\Delta P_{\max}/\Delta P_{\min}$  increases. A Linear valve operating characteristic tends towards a quick opening characteristic as  $\Delta P_{\max}/\Delta P_{\min}$  increases.

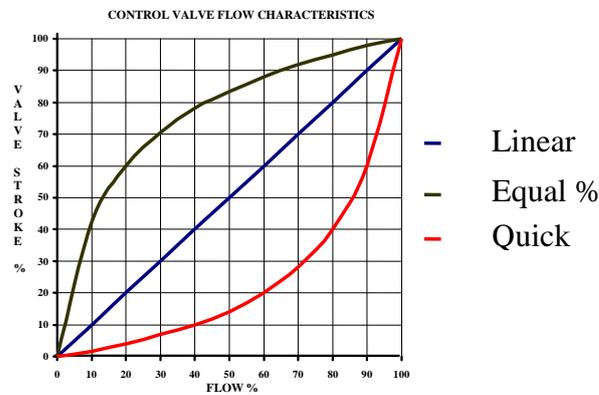
The following table gives a summary of selection criteria for good industry practice:-

Process Variable	$\Delta P_{\max} / \Delta P_{\min}$	Characteristic
Temperature	< 2	Equal %
Pressure	Constant	Linear
	< 2	Equal %
Level	< 2½	Linear
	> 2½	Equal %
Flow (linearised)	< 2½ (Note 1)	Linear
	> 2½ (Note 2)	Equal %

Note 1 Value  $\Delta P$  at flow maximum > 40% system  $\Delta P$

Note 2 Value  $\Delta P$  at flow maximum < 40% system  $\Delta P$

$\Delta P_{\max}$  will be close to the maximum shutoff  $\Delta P$  and  $\Delta P_{\min}$  at full flow should not be underestimated which favours an equal % characteristic. CHEMCAD allows dynamic analysis of the process to confirm appropriate characteristic selection. The graph of Valve Stem position vs Flow demonstrates the range of valve characteristics available:



The operational characteristic of a valve can also be modified by control system output signal characterisation using various techniques.

For **Reverse** control action specify Controller Parameter **Error =  $X_{set} - X$**

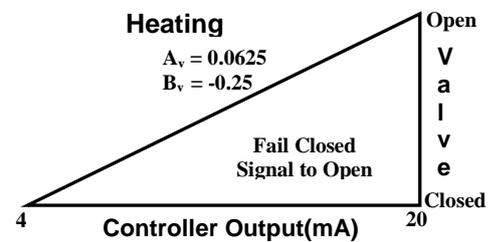
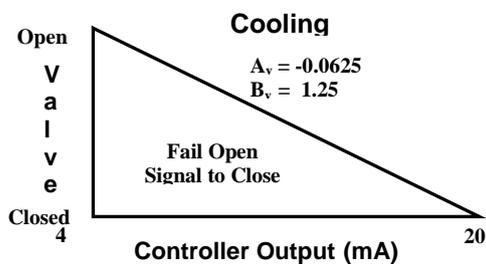
Increasing Measurement with Decreasing Controller Output gives Cooling for Fail Open Valve.  
Decreasing Measurement with Increasing Controller Output gives Heating for Fail Closed Valve.

For **Direct** control action specify Controller Parameter **Error =  $X - X_{set}$**

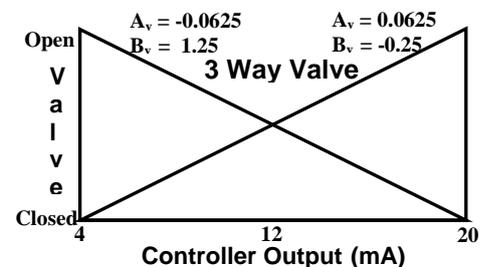
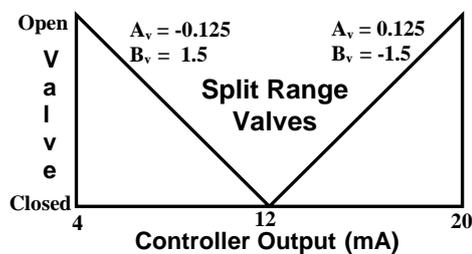
Increasing Measurement with Increasing Controller Output opens Fail Closed Valve e.g. Level control on tank outlet or Pressure control on tank outlet.

Decreasing Measurement with Decreasing Controller Output opens Fail Open Valve e.g. Level control on tank inlet or Pressure control on tank inlet.

SINGLE CONTROL VALVE OPERATIONS							
ACTION	CONTROL OUTPUT		POSITION	STATE	LOGIC EQUATION	COEFFICIENTS	
	mA	%				$A_v$	$B_v$
FAIL CLOSED	4	0	Closed	0	$0 = 4A_v + B_v$	0.0625	-0.25
	20	100	Open	1	$1 = 20A_v + B_v$		
FAIL OPEN	4	0	Open	1	$1 = 4A_v + B_v$	-0.0625	1.25
	20	100	Closed	0	$0 = 20A_v + B_v$		



DUAL CONTROL VALVE OPERATIONS IN SPLIT RANGE							
ACTION	CONTROL OUTPUT		POSITION	STATE	LOGIC EQUATION	COEFFICIENTS	
	mA	%				$A_v$	$B_v$
FAIL CLOSED	12	50	Closed	0	$0 = 12A_v + B_v$	0.125	-1.5
	20	100	Open	1	$1 = 20A_v + B_v$		
FAIL OPEN	4	0	Open	1	$1 = 4A_v + B_v$	-0.125	1.5
	12	50	Closed	0	$0 = 12A_v + B_v$		



## 5.0 Controller Tuning

When tuning control loops it is important to understand the impact the tuning parameters have on the process. The minimum effective values are:-

Proportional Band	P %	highest value (minimum gain)
Integral Action Time	$T_i$ min	longest time
Derivative Action Time	$T_d$ min	shortest time (or off)

The following ground rules should always be considered :-

### Proportional Band

Wide P (50 – 500%) on fast and noisy processes such as Flow, Liquid Pressure and Composition.  
Narrow P (1- 50%) on slow processes such as Gas Pressure, Temperature and Vapour Pressure.

### Integral Action Time ( $T_i$ )

Integral Action Time changes the controller output at a rate proportional to the magnitude of the error (e) and should never be set so short such that the resulting load change imposed exceeds the load response characteristics of the process. (Consider approaching a corner too fast in a car).

Short  $T_i$  (0.05 – 2 min) on fast and noisy processes such as Flow and Liquid Pressure.

Long  $T_i$  (2 – 120 min) on slow processes such as Temperature, Vapour Pressure and Composition.

$T_i$  is unnecessary on Gas Pressure and is seldom used on Liquid Level as steady flow is usually the required condition e.g. surge tanks between process units.

### Derivative Action Time ( $T_d$ )

Derivative Action Time changes the controller output at a rate proportional to the rate of change of error  $\left(\frac{de}{dt}\right)$  and as such should **never** be used on noisy processes such as Flow, Liquid Pressure and Liquid Level.

$T_d$  is used on Temperature, Vapour Pressure and Composition and should be set conservatively (short  $T_d$ ) to protect against control instability resulting from unanticipated load changes.  $T_d$  set in the range  $\frac{T_i}{4} < T_d < \frac{T_i}{2}$  is considered reasonable.

### Integral Action Time Saturation (Windup)

When a sustained error is maintained between set point and measured variable on a controller with  $T_i$  the output is driven off scale (valve full open or closed). Control action does not commence until the measured variable crosses the set point resulting in overshoot. This condition is typical of heating/cooling a batch reactor to a desired temperature and composition endpoint control. Controllers incorporating Proportional and Derivative modes only overcome this problem.

### Controller Loop Tuning Method

Ziegler and Nichols developed the Ultimate Sensitivity Method which provides a useful basis for control loop tuning as follows:-

1. Set the control modes to their minimum effective values.  
Maximum P, maximum  $T_i$ , minimum  $T_d$  (or off).
2. Reduce P whilst making small set point changes (both directions) until the measured variable begins to oscillate at constant amplitude. The proportional band  $P_u$  and the period  $T_u$  are noted.
3. Initial controller settings proposed are:-

Controller Type	P %	$T_i$ min	$T_d$ min
P only	2 $P_u$		
P + I	2.2 $P_u$	$T_u / 1.2$	
P + I + D	1.6 $P_u$	$T_u / 2.0$	$T_u / 8.0 = T_i / 4$

This procedure can be used as a 'starting point' for tuning control systems on batch processes,  $T_u$  being established at a stable condition. Typical periods ( $T_u$ ) for batch reactors vary in the range 15 to 60 minutes.

## 6.0 Dynamic Simulation Considerations

The following provides a summary of key points to achieve rapid results from the dynamic models.

Control valve rangeability based on the ratio of maximum to minimum controllable flows depends on the entire control loop. For simulation use 50 for equal % characteristic and 10 for linear characteristic.

The position of the control valve in the model is critical and the rules can be summarized:-

It requires inlet ( $P_i$ ) and outlet ( $P_o$ ) pressures to be specified where  $P_i$  is taken from the inlet stream.  $P_o$  can be specified directly or overtaken indirectly by an assigned UnitOp in the model.

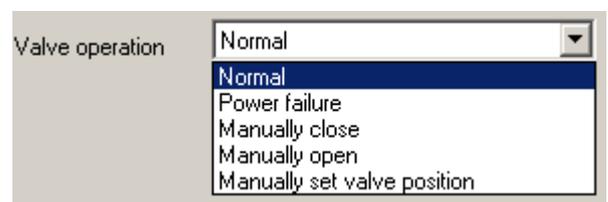
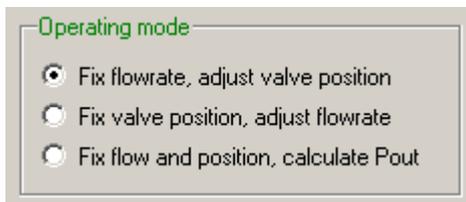
A mass balance must be maintained around the control valve. To achieve this, locate immediately after a Feed Arrow (direct flow adjust) or after Stream Reference (SREF) or Divider (DIVI) (indirect flow regulation). Dynamic Vessel, Dynamic Reactor and Dynamic Column can also be assigned for indirect flow regulation. The optimal mass flowrate transfer is used to set up Indirect Flowrate Regulation.

If a value for valve flow coefficient  $C_v$  is not known use the Equipment Sizing  $C_v$  option which will provide a value at stated stream conditions. An incorrectly sized valve will result in dynamic model convergence problems and an unstable condition in the model.

If the controller input goes out of the calibrated range the control output continues to change resulting in unreal conditions. To “debug” complex models there are several techniques available:

Under “Run – Convergence” use Run One Time Step for Dynamic Simulation to allow study of model behaviour.

The control valve can be operated in various operating modes which allows the simulations to be driven to the desired condition. These features allow control valve positions to be set manually or automatically from an assigned controller.



## 7.0 Measurement Sensors<sup>(2)</sup>

This section has been included as an introduction to the process engineer who is not familiar with process measurement technology and its application. Correct selection is one of the key parameters in the successful operation of a process plant.

Measurement sensor technology is a key driver in the development of modern industrial processes. The technologies, to measure and transmit process parameters, such as flow, level, temperature and pressure, have developed significantly since the 1960's.

Impulse lines, used to connect instruments to the process, are found less frequently on new installations and are being replaced on existing ones. Where used, they require specialist knowledge during design, installation and maintenance for reliable measurement. Modern techniques have simplified maintenance and enhanced plant performance.

### Data transmission

Transmission technology development has allowed universal application of self-powered two wire 4-20 mA dc signals. This has eliminated power supply and special sensor cabling for magnetic flow meters, thermocouples and resistance bulbs, reducing cost and simplifying installation.

In the 1980's, microprocessors facilitated the transition from signal to information based process automation. Smart transmitters provided bi-directional digital communication and diagnostics capability with HART<sup>®</sup> (Highway Addressable Remote Transducer) protocol. The 4-20 mA and HART digital signals are transmitted over the same wiring, providing a centralised capability to configure, calibrate, characterise and diagnose devices in real time together with reporting capability. Data can be captured from multi-parameter devices without additional hardware, providing predictive maintenance capability.

Development in fieldbus digital communication allows field devices to be connected using a single cable bus structure, reducing cabling, installation time and cost. Fieldbus is a device level network that sacrifices speed for security. There are several protocols available with Modbus<sup>®</sup>, PROFIBUS PA and FOUNDATION<sup>™</sup> being the most common. Modbus<sup>®</sup> was the earliest protocol and has connectivity with Ethernet and other fieldbus protocols. PROFIBUS PA was developed in Europe and with PROFINET has Ethernet connectivity. FOUNDATION<sup>™</sup> fieldbus was developed in North America by ISA, suppliers and users.

Fieldbus technology is more complex and costly, requiring suppliers to provide sensor options to meet the different standards. Fieldbus selection is guided by plant layout, sensor interface capabilities and data management infrastructure. An industry working group is currently developing the capabilities of Electronic Device Description (EDD) technology.

## Flow Measurement

Accurate flow measurement is a key element in process productivity. Various types of flow meters are used, with the orifice plate and differential pressure transmitter predominant prior to 1965. New materials, manufacturing techniques and micro-electronics have resulted in significant developments.

Measurement accuracy is quoted for a given turndown ratio (max/min reading) as % span (max-min reading), % full scale or % actual, with the latter being highest specification for same value. Accuracy is important for stock and custody monitoring, and reproducibility, the ability of the sensor to reproduce its reading, being important for control.

The positive displacement flowmeter, one of the earliest meters, is based on a fixed volume of fluid causing a known mechanical displacement to generate a calibrated pulse. Configurations based on vanes, gears, pistons, or diaphragms are available. Oval gear meters have reduced slippage, achieving accuracies of  $\pm 0.05\%$  rate for  $\mu = 0.2-5$  cps and  $\pm 0.25\%$  rate for  $\mu > 5$  cps over 10:1 turndown. Advancements in accuracy from  $\pm 0.5\%$  rate have been achieved by temperature compensation, multivariable flow computation and HART, making meters suitable for custody transfer. Fluid viscosity affects the pressure drop and presence of solids or entrained air can cause mechanical damage.

The axial turbine flowmeter consists of a rotor, driven at a rate proportional to the fluid velocity, to generate a calibrated pulse. Developments in materials have improved bearing design to extend the application and improve robustness, achieving accuracies of  $\pm 0.5\%$  rate for  $\mu = 0.8-2$  cSt over a 15:1 turndown, depending on size and conditions. Installations require an upstream strainer and straight pipe section with custody transfer requiring upstream flow straighteners. Meter is suitable for bi-directional flow.

The magnetic flowmeter measures the voltage generated by an electrically conducting liquid flowing through a magnetic field, which is proportional to fluid velocity. Fluid contact electrodes can measure liquids with conductivities as low as  $2 \mu\text{S}/\text{cm}$  and with non-contact capacitive signal pick-up electrodes down to  $0.05 \mu\text{S}/\text{cm}$ . Meters can achieve accuracies of  $\pm 0.2\%$  rate over a 10:1 turndown depending on size and conditions and contribute no additional pressure drop. Installation requires minimum 5D upstream straight pipe section and is suitable for bi-directional flow. Preferred method for conducting liquids, including corrosive liquids, slurries, sludges, liquids with abrasive solids.

The vortex shedding flowmeter measures the frequency of vortices formed by a fluid flowing across a bluff non-streamlined body, which is proportional to fluid velocity above the minimum flow condition at which vortex shedding ceases. Typical accuracies claimed for liquids are  $\pm 0.5\%$  rate for Reynolds Number (Re)  $> 20,000$  and for steam/gases  $\pm 1.0\%$  rate for velocity  $< 35$  m/s. Advancement in accuracies are being achieved by compensating for varying Re and process conditions, with reduced bore meters extending the measuring range. Installation requires a minimum 15D upstream and 5D downstream straight pipe section with pressure drop being  $\sim 2$  velocity heads. Preferred method for steam and with integral temperature compensation gives mass flow of saturated steam.

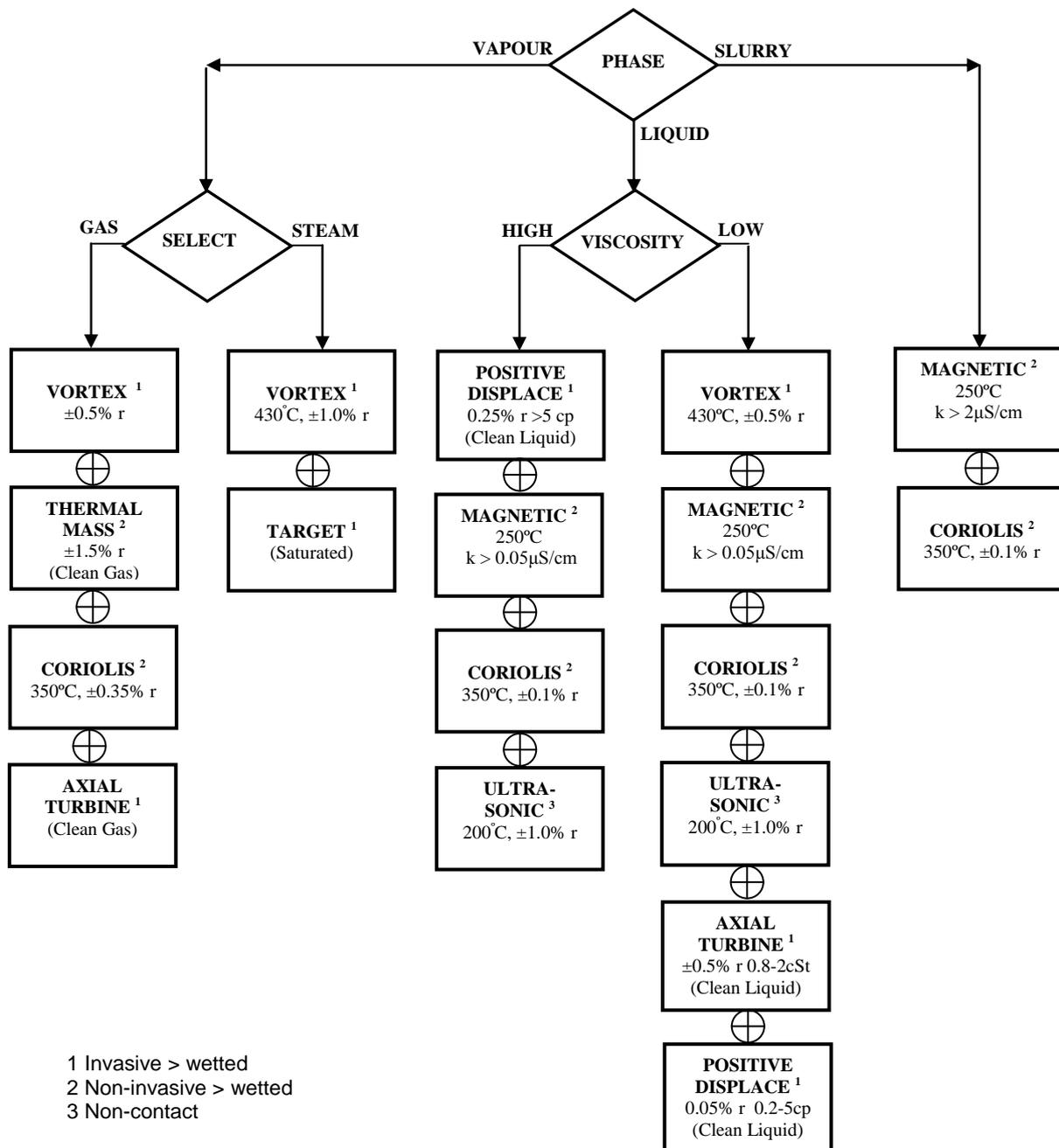
The Coriolis flowmeter measures the twist created by fluid flowing through an oscillating single or dual tube assembly, which is proportional to mass flow and is independent of fluid viscosity and density. This is a "one for all" multi-variable meter and provides density and temperature measurement allowing derivation of other variables such as volume flow, solids content and concentration. Typical accuracies claimed for liquids are  $\pm 0.1\%$  rate and for gases  $\pm 0.35\%$  rate over a 20:1 turndown, and is suitable custody metering. There are no special installation requirements but pressure drops can be significant. If capital cost is not an issue, this is preferred method for non-conducting liquids.

The thermal dispersion flowmeter measures the cooling effect of a gas as it passes over a heated transducer, which is proportional to the mass flow, thermal and flow properties of the gas. Typical accuracies claimed are  $\pm 1.5\%$  reading over a 10:1 turndown. Installation may require up to 20D upstream straight pipe and 5D downstream no additional pressure drop. This is preferred method for pure gases and constant composition gas mixtures.

The ultrasonic “time of flight” flowmeter measures the time difference between the paths of two or more ultrasonic signals beamed in opposite directions. Meters can be clamp on or insertion type. The accuracy is enhanced by characterising the varying velocity profiles due to changes in Re and process conditions. Multi-path chordal insertion meters can achieve accuracies of  $\pm 0.25\%$  rate over a 10:1 turndown whilst clamp on meters claim  $\pm 1.0\%$  rate. Installation may require up to 20D upstream straight pipe without a flow conditioner and 3D downstream. The meters can be used on bi-directional flow and contribute no additional pressure drop. Ultrasonic meters are now gaining acceptance for liquid custody transfer. Time of flight ultrasonic flowmeters are not suitable for use on liquids containing entrained gases or solids.

The following gives an indication of comparative costs with the lowest first:  
 turbine → magnetic → vortex → thermal → ultrasonic → positive displacement → Coriolis.

The chart shows typical applications:



## Liquid Level Measurement

Liquid level measurement is key to reliable and safe process plant operation. Normally flows are held steady whilst levels are allowed to change within limits, requiring reproducibility. Accuracy is important for tanks used for stock and custody control.

The hydrostatic continuous, indirect, level method measures the pressure due to liquid level and density plus over-pressure. The sensor measures the pressure difference between this pressure and a reference pressure, normally atmospheric, so is not preferred for vacuum and pressure service. Instruments can be flanged mounted or rod insertion type, the latter not being recommended for turbulent conditions. Typical accuracies claimed are  $\pm 0.2\%$  reading, and is dependent on process fluid properties and conditions.

The displacer continuous or point level method measures the change in buoyancy via a torque tube or lever arrangement. The continuous measuring range is set by the displacer length immersed in the tank or external cage, which is preferable on noisy applications. The point method uses a float with the range being limited by the length of the float arm.

The nucleonic point or continuous, non-contact, level method measures the signal strength of a radioactive source beamed across a vessel. Independent of fluid properties and has typical ranges of 0.24 to 3.36m. Typical accuracies claimed are  $\pm 2\%$  reading. This is the preferred method for controlling level in flash vessels and reboilers under all temperature and pressure conditions

The radar point or continuous level method measures the travel time of an impulse transmitted and reflected from the liquid surface. Interference echoes resulting from tank internals and agitators are suppressed and signals characterised to give liquid volume. The sensor has no contact with the liquid but is exposed to head space conditions, which do not affect the measurement. Reflectivity requires the liquid dielectric constant ( $\epsilon_R$ ) to be  $\geq 1.4$  (hydrocarbons 1.9-4.0, organic solvents 4.0-10 and conductive liquids  $> 10$ ). The antenna and signal conditions are adjusted to suit the process, with guided radar being used for low  $\epsilon_R$  and turbulent conditions. Method is suitable for custody transfer with accuracy  $\pm 0.5\text{mm}$  being claimed.

The capacitance point or continuous level method is suitable for liquids which can act as dielectrics. The measurement is more sensitive when the difference  $\delta\epsilon_R$  of the liquid and the vapor space or between the two liquids are higher. Special designs, involving coated and twin probes, are used when  $\delta\epsilon_R < 1.0$ , conductivities  $> 100 \mu\text{mho}$ , coating effects or vessel material is non conducting. Typical accuracies claimed are  $\pm 0.25\%$  span and is dependent on fluid properties so is not suitable for changing conditions. Maximum conditions  $200^\circ\text{C}$  at 100 bar and  $400^\circ\text{C}$  at 10 bar.

The ultrasonic point or continuous level measurement is based on the time-of-flight principle. A sensor emits and detects ultrasonic pulses which are reflected from the surface of the liquid. The method is non-invasive, with some types being non-contact, and is not affected by  $\epsilon_R$ , conductivity, density or humidity. Maximum conditions  $150^\circ\text{C}$  at 4 bar.

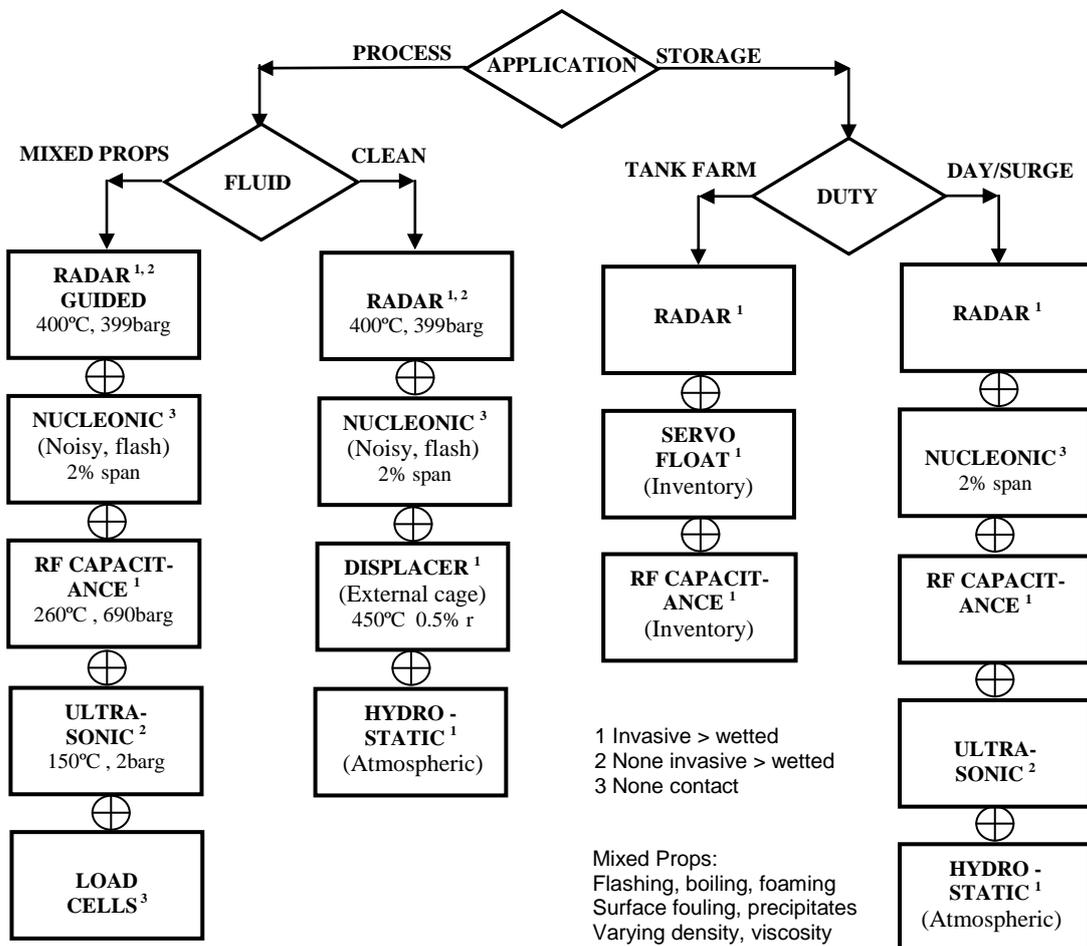
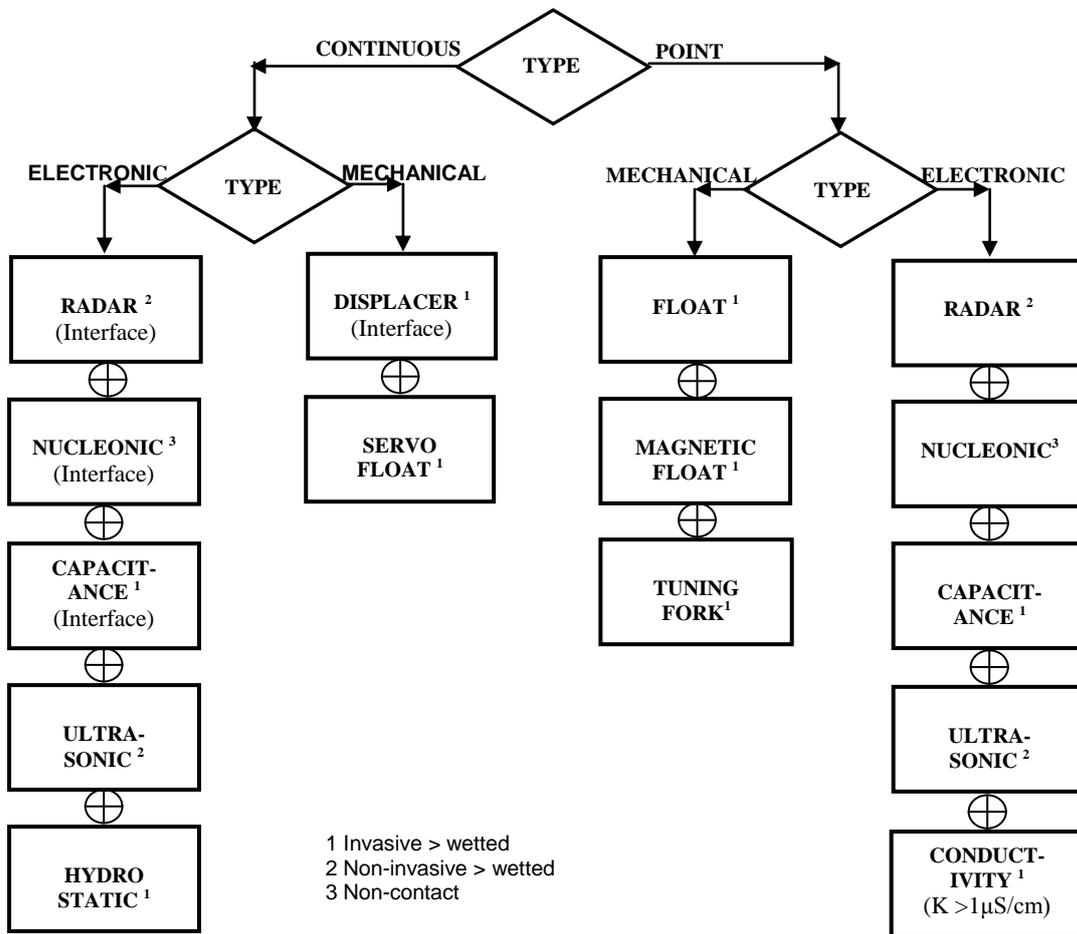
Load cells, based on strain gauge or piezoelectric, measure the weight of the process vessel plus contents. Individual load cell accuracy of 0.03% full scale is achievable but overall performance is dependent on correct installation practices preventing external forces, due to associated piping and equipment. For vessels with jackets, agitation and complex piping it is difficult to obtain an acceptable accuracy. When the container can be totally isolated, as in final dispensing and filling applications, precision weighing can be achieved.

The vibrating tuning fork principle is used to detect point liquid level but is unsuitable in viscous and fouling applications. Maximum conditions  $280^\circ\text{C}$  at 100 bar.

The conductivity point level method requires a liquid conductivity  $> 0.1 \mu\text{mho}$  and is frequently used on utility and effluent pump control systems.

The following gives an indication of comparative costs, with the lowest first:

conductivity  $\rightarrow$  capacitance  $\rightarrow$  tuning fork  $\rightarrow$  hydrostatic  $\rightarrow$  displacer  $\rightarrow$  ultrasonic  $\rightarrow$  load cell  $\rightarrow$  radar  $\rightarrow$  nucleonic.



## Appendix I

### Flow Meter Considerations

To model piping systems, involving special items such as flow meters, CHEMCAD provides a facility under the Valve Data entry Window in the Pipe UnitOp for resistance parameters to be entered in various formats. The following guidelines should be considered when selecting flow meter sizes.

#### Magnetic Flow Meter

Velocity Limits for Flow of Fluids through Magnetic Flow Meters (Foxboro Bulletin)				
Service Conditions	Fluid	Reasonable Velocities		Pressure Drop
		m/s	ft/s	kPa / m
General Service and Process Piping	Liquids pumped, non viscous	0.9 to 4.6	3.0 to 15	Line size meter Same ΔP as pipe
	Erosive Slurries	0.9 to 4.6	3 to 6	
	Coating forming liquids	1.8 to 4.6	6 to 16	

#### Mass Flow Meter

Because of the wide turndown capability of Coriolis flowmeters (30:1 to as high as 200:1), the same flow can be measured by two or three different sized flow tubes subject to accuracy requirements. Using the smallest possible meter lowers the initial cost and reduces coating build-up, but increases erosion/corrosion rates and head loss.

Using a meter that is smaller than line size is acceptable if the process fluid is clean with a low viscosity. However on corrosive, viscous, or abrasive slurry services, this practice may cause reduced operational life. Flow tube sizes and corresponding pressure drops, inaccuracies, and flow velocities can be obtained from software provided by the manufacturer.

Different Coriolis meter principles incur different pressure drops, but in general they require more than traditional volumetric meters, which usually operate at less than 10 psi. This higher head loss is due to the reduced tubing diameter and the circuitous path of flow. Head loss can be of concern if the meter is installed in a low-pressure system, or if there is a potential for cavitation or flashing, or if the fluid viscosity is very high.

#### Vortex Shedding Meter

Measurable flow velocities on liquids are in the general range of 0.5 to 9.0 m/s ( 1.5 to 32 ft/s).

On gas or steam the flow velocities are in the range  $\sqrt{\frac{74}{\rho}}$  to 79 m/s (  $\sqrt{\frac{50}{\rho}}$  to 260 ft/s)

Where  $\rho$  fluid density (kg/m<sup>3</sup> or lb/ft<sup>3</sup>)

Process fluid viscosity requires the Reynolds Number to be greater than 20000

Linear performance is achieved for Reynolds Number in the range 20000 to 7.0 E06

## Appendix I

### Flow Meter Considerations

#### Differential Head Flowmeters

The differential pressure measured and unrecovered pressure loss across a square edge concentric orifice plate is dependent on the pressure tap location; as shown in the diagrams below. It can be seen that full flow taps ( $2\frac{1}{2}D$  and  $8D$ ) measures the permanent pressure loss and should be used for restriction orifice calculations.

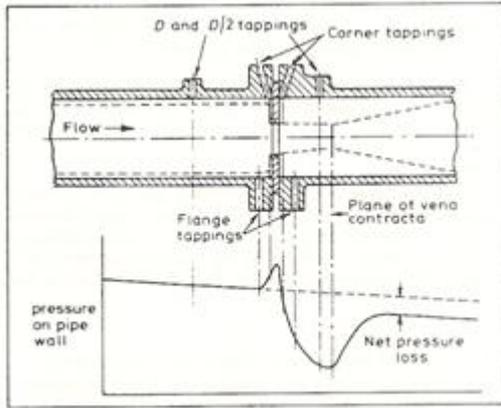
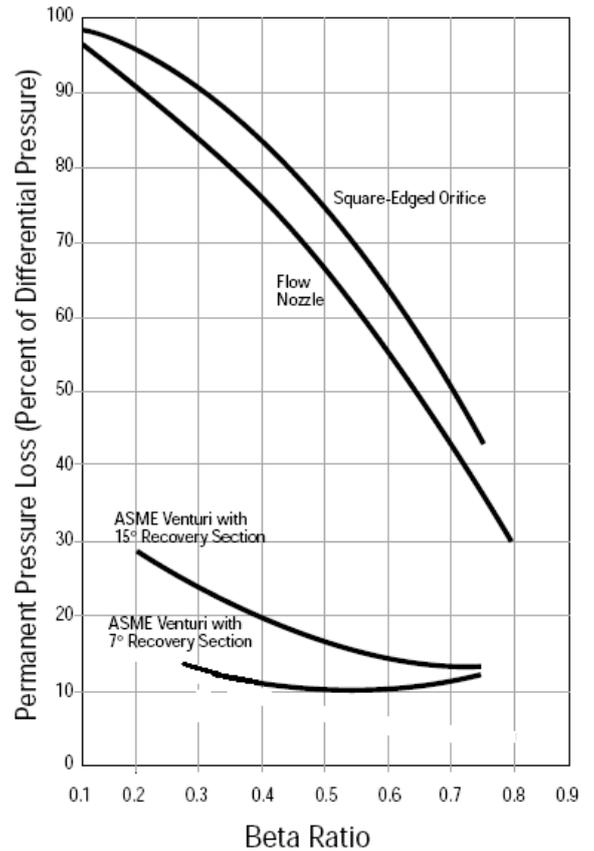


Figure 1—Section of square-edged orifice plate showing variation of pressure along the pipe wall (by courtesy of BSI)



For liquids

$$Q = K d^2 C \sqrt{\frac{h}{\rho_f}}$$

$$W = K d^2 C \sqrt{h \rho}$$

For gases

$$W = K d^2 C \sqrt{\frac{h p_f M}{T_f}}$$

The diagram below shows the dependency of flow coefficient  $C$  on  $Re$  and  $d/D$  ( $\beta$ ).  $d/D$  ( $\beta$ ) ratios  $\leq 0.6$  are preferred. For  $\beta > 0.6$  viscosity effects are magnified combined with increased sensitivity to upstream piping configurations.

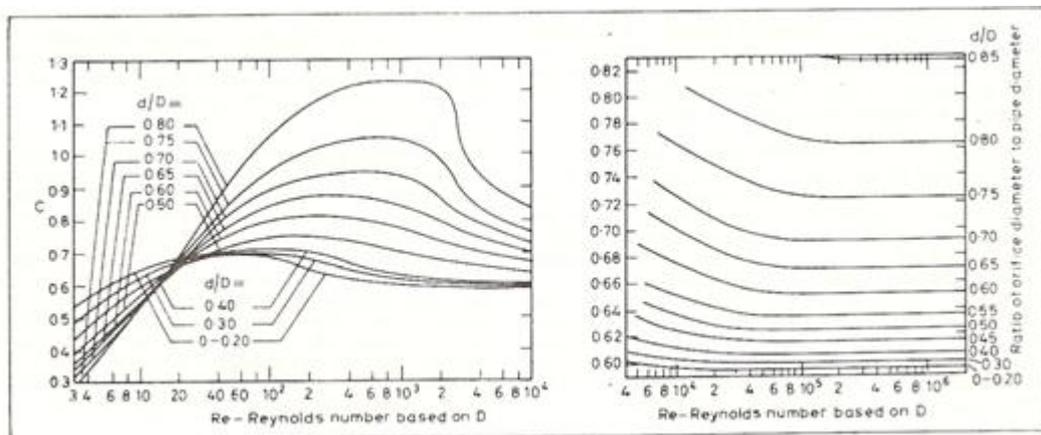


Figure 2—Flow coefficient  $C$  for square edged orifices (by courtesy of Crane Co)

## ***Section 3***

### ***Control Systems Simulation Cases***

In this section are presented cases to facilitate an understanding of the CHEMCAD dynamic simulation and its capabilities in studying control systems

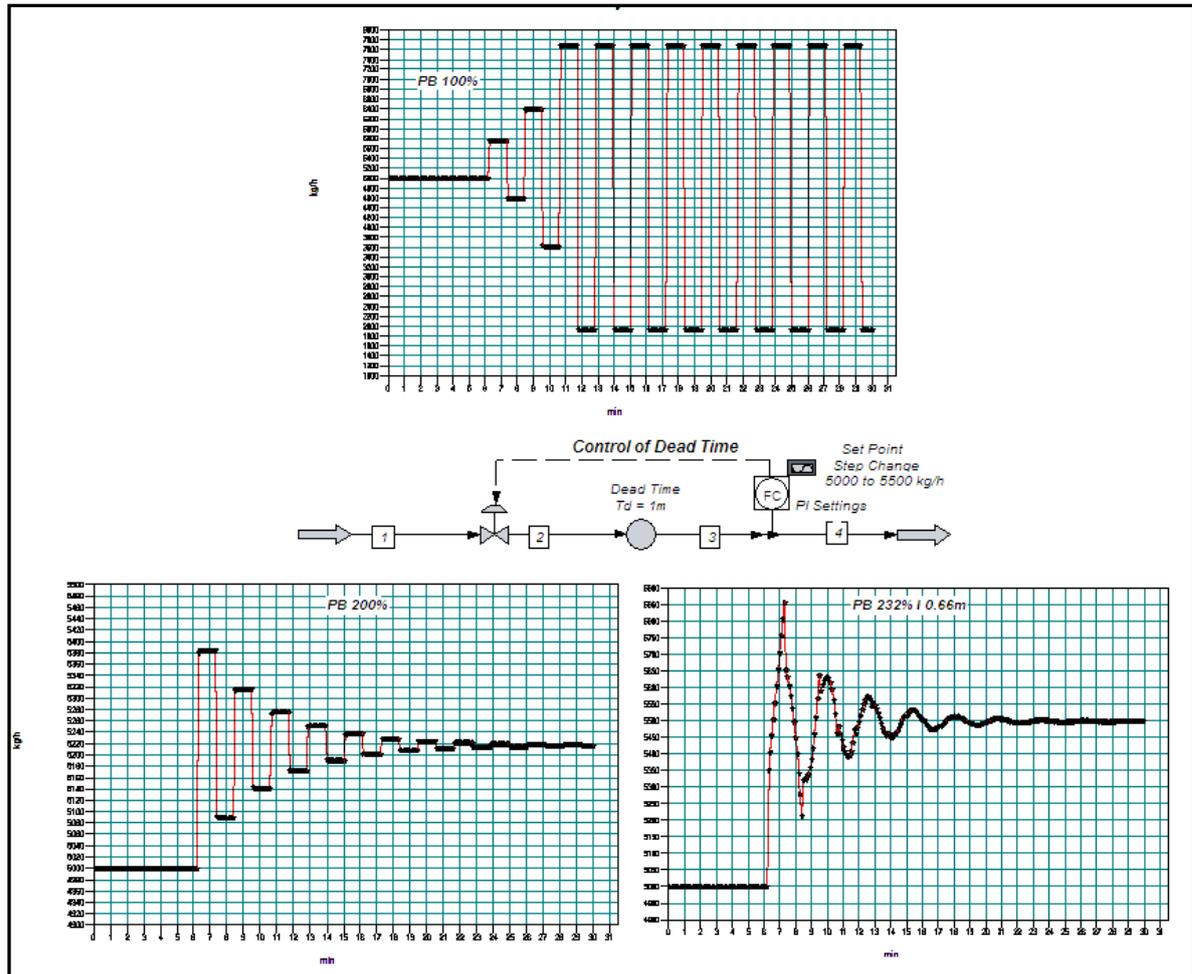
The reference "Process Control Systems" by F.G.Shinskey Chapters 1 and 2 form the basis of the cases presented.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
3.01	Control of Dead Time
3.02	Control of Capacity - Tank Level
3.03	Two Capacity – Tank Displacer Level
3.04	Tank Balancing
3.05	Tank Level Controller Tuning
3.06	Gas Pressure Control
3.07	Flow Control with Level Cut-back
3.08	Level Control Training Simulator

### Case 3.01 Control of Dead Time<sup>(1, p6)</sup>

Dead time (transport lag or distance-velocity lag) is the interval after the application of a control device output change for which no process (measurement) response is observable. It occurs when mass or energy is transported along a path length with velocity constituting the delay.



For a 1m dead time the natural period is fixed at 2m and a proportional band of 200% will give  $\frac{1}{4}$  amplitude damping. Dead time is a difficult element to control and process design should concentrate on minimising or eliminating if practical.

## Section 4

# Thermodynamics

### Contents

- 1.0 Introduction**
- 2.0 Thermodynamic Fundamentals**
  - 2.1 Thermodynamic Energies
  - 2.2 Gibbs Phase Rule
  - 2.3 Enthalpy
  - 2.4 Thermodynamics of Real Processes
- 3.0 System Phases**
  - 3.1 Single Phase Gas
  - 3.2 Liquid Phase
  - 3.3 Vapour liquid equilibrium
- 4.0 Chemical Reactions**
  - 4.1 Reaction Chemistry
  - 4.2 Reaction Chemistry Applied
- 5.0 Summary**

### Appendices

- I Enthalpy Calculations in CHEMCAD
- II Thermodynamic Model Synopsis – Vapor Liquid Equilibrium
- III Thermodynamic Model Selection – Application Tables
- IV K Model – Henry's Law Review
- V Inert Gases and Infinitely Dilute Solutions
- VI Post Combustion Carbon Capture Thermodynamics
- VII Thermodynamic Guidance Note
- VIII Prediction of Physical Properties
- IX Refinery Thermodynamics
- X Petroleum Products Test Methods

### References

1. C.C. Coffin, J.Chemical Education 23, 584-588 (1946), "A Presentation of the Thermodynamic Functions".
2. R.M. Felder and R.W. Rousseau, "Elementary Principles of Chemical Processes", 2<sup>nd</sup> Edition, John Wiley and Sons.
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## 1.0 Introduction

The selection of a suitable thermodynamic model for the prediction of the enthalpy – H value and the phase equilibrium – K value is fundamental to process modelling. An inappropriate model selection will result in convergence problems and erroneous results. Simulations are only valid when the appropriate thermodynamic model is being used. The selection process is based on a detailed knowledge of thermodynamics and practical experience. Most simulators are provided with Thermodynamic Wizards to aid selection which should be used with caution.

The selection process is guided by considering the following:-

- Process species and compositions.
- Pressure and temperature operating ranges.
- System phases involved.
- Nature of the fluids.
- Availability of data.

There are four categories of thermodynamic models:-

- Equations-of-State (E-o-S)
- Activity coefficient ( $\gamma$ )
- Empirical
- Special system specific

This paper is not intended to be a rigorous analysis of the methods available or in their selection but is offered as an “aide memoire” to the practicing engineer who is looking for rapid, realistic results from his process models.

The study of complex systems invariably involves extensive research and considerable investment in manpower effort by specialists. There are extensive sources of physical property data available from organisations such as DECHEMA [www.dechema.de](http://www.dechema.de), DIPPR [www.iche.org/dippr/](http://www.iche.org/dippr/), TÜV NEL Ltd [www.pfds.co.uk](http://www.pfds.co.uk) amongst others.

This paper presents selection methods developed in discussions with engineers in the field. The validity of the thermodynamic models being used should be tested against known data whenever possible.

## 2.0 Thermodynamic Fundamentals

### 2.1 Thermodynamic Energies<sup>(1)</sup>

The thermodynamic fundamentals of fluid states in relation to energies and phase behaviour needs to be thoroughly understood.

Four thermodynamic variables determine six thermodynamic energies:

Intensive variables	Extensive variables (capacity)
Pressure ( <b>P</b> )	Volume ( <b>V</b> )
Temperature ( <b>T</b> )	Entropy ( <b>S</b> )

We define thermodynamic energy as follows:

$$\text{Energy} = \text{Intensive variable} \times \text{Extensive variable}$$

**P or TV or S**

**TS** represents internal bound energy isothermally unavailable.

**PV** represents external free energy.

Helmholtz Free Energy (**F**) is Internal Energy available for work and is part of the Internal Energy (**U**).

We have the following energy relationships:

Internal Energy	<b>U = T S + F</b>
Gibbs Free Energy	<b>G = F + P V</b>
Enthalpy	<b>H = T S + F + P V</b>
	<b>H = U + P V</b>

When considering chemical reactions we have:

$$\text{Chemical Energy} = \text{Chemical Potential Factor} \times \text{Capacity Factor}$$

$$dU = (\mu_i - \mu_i^0) dn_i$$

Where

**dn<sub>i</sub>** is change in species i moles

**μ<sub>i</sub>** is chemical potential species i

$$dU = T dS - P dV + \sum_i \mu_i dn_i$$

For equilibrium

$$\sum_i \mu_i dn_i = 0$$

Other equilibrium conditions **dF = 0 (constV & T)** **dG = 0 (constP & T)**

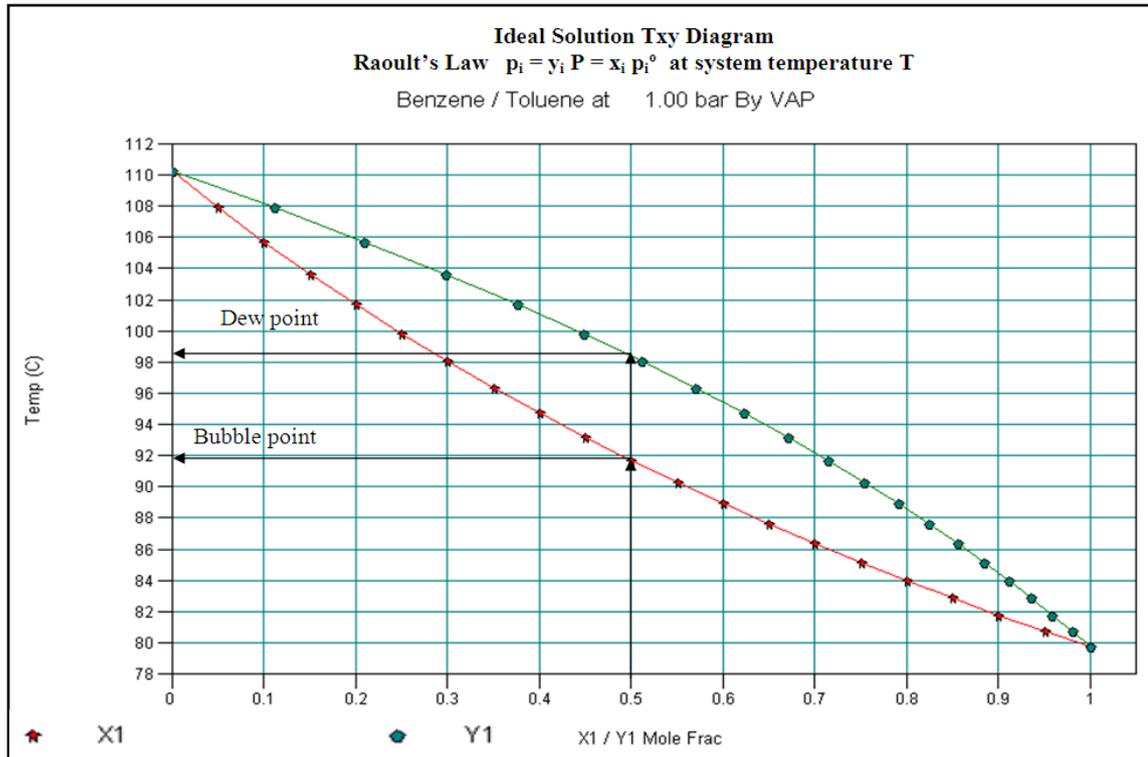
$$dU = 0 \text{ (constS \& V)} \quad dH = 0 \text{ (constS \& P)}$$

It can be shown that

$$G = \sum_i \mu_i n_i$$



The figure shows the Txy diagram for Benzene/Toluene, a near ideal mixture. The bubble point for a given composition is read directly from the liquid curve and the dew point is read directly from the vapour curve.



The bubble point of a mixture is determined by trial and error from value of  $T_{bp}$  that satisfies:

$$P = \sum x_i p_i^*(T_{bp})$$

The dew point of a mixture is determined by trial and error from value of  $T_{dp}$  that satisfies:

$$\sum \left( \frac{y_i P}{p_i^*(T_{dp})} \right) = 1$$

### 2.3 Enthalpy

Enthalpy is the sum of the internal energy  $U$  and the external free energy  $PV$  where:

$$H = U + P V$$

The heat supplied is given by:

$$dQ = dU + P dV$$

The sign convention should be noted and is  $+$  for heat added and  $dU$  gain in internal energy

$$dU = C_v dT$$

The specific heat at constant pressure  $C_p$  is related to heat input:

$$dQ = C_p dT$$

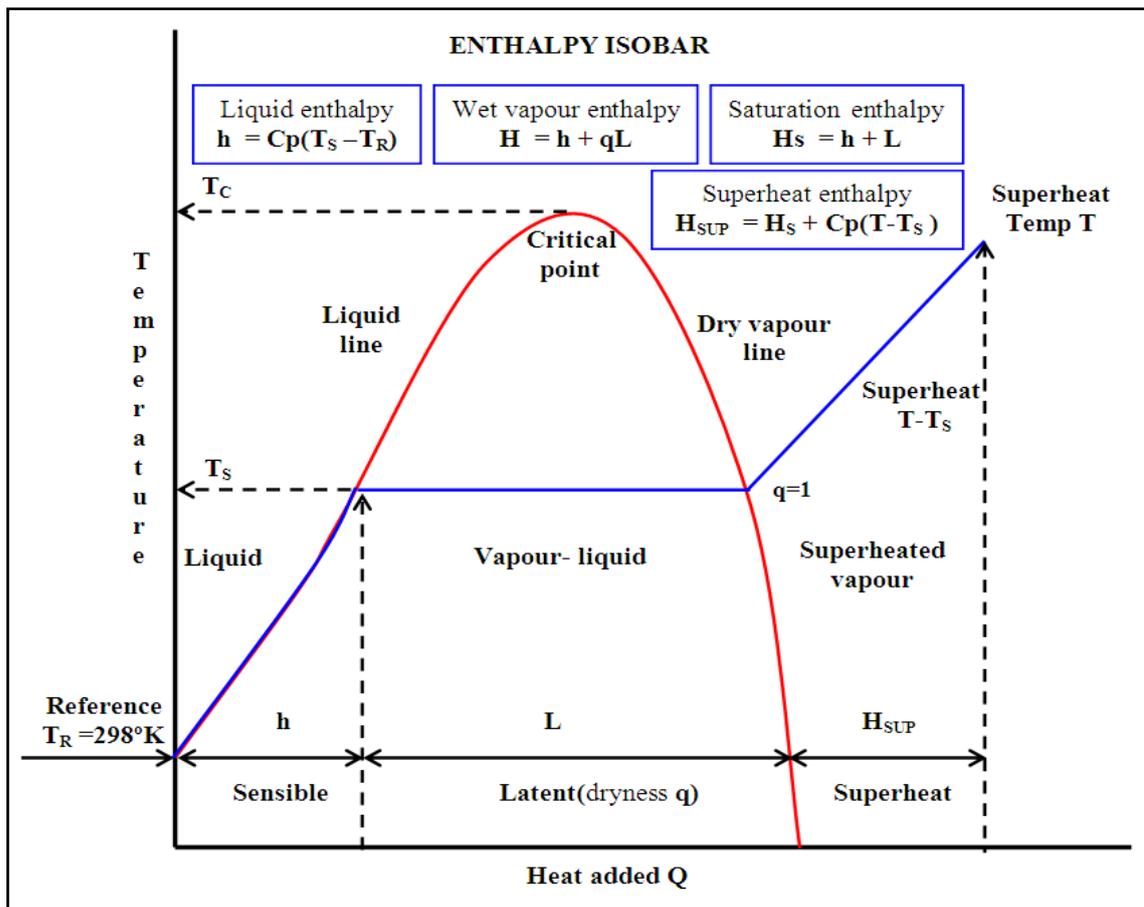
The adiabatic index or specific ratio  $\gamma$  is defined:

$$\gamma = \frac{C_p}{C_v}$$

It can be shown that the following relationship holds

$$C_p - C_v = R$$

The heating of a liquid at constant pressure e.g. water is considered in the figure below. The figure shows the relationships between the enthalpies in the different phases namely the sensible heat in the liquid phase, the latent heat of vaporisation during the vapour liquid equilibrium phase and the superheat in the gas phase.



Enthalpy is calculated using Latent Heat (LATE) in the liquid and vle phases and E-o-S (SRK) in the superheated or gas phase.

Appendix I reviews the calculation methods adopted in CHEMCAD. A standard reference state of 298°K for the liquid heat of formation is used providing the advantage that the pressure has no influence on the liquid  $C_p$ . It is worth noting that if water is the only component, the simulation enthalpies will match steam table values.

The enthalpy method used will depend on the K-value method selected as detailed in Appendix II. CHEMCAD forces the following H-values from K-value selected.

Equilibrium-K	Enthalpy-H
Peng Robinson (PR)	PR
Grayson-Streed-Choa-Seeder(GS)	Lee Kessler (LK)
ESSO	LK
Benedict-Webb-Rubin-Starling (BWRS)	BWRS
AMINE	AMINE

Special methods are used for:

Enthalpy of water steam tables (empirical)  
Acid gas absorption by DEA and MEA  
Solid components

## 2.4 Thermodynamics of Real Processes<sup>(7)</sup>

To establish if a real process is possible we need to consider:

$$\Delta G = \Delta H - T \Delta S$$

The values for  $\Delta H$  are determined from the heats of formation of the components and for  $\Delta S$  from thermodynamic property tables. Superscript <sup>0</sup> indicates materials present in standard state at 298°K.

For isothermal processes at low temperature the  $\Delta H$  term is dominant. At absolute zero  $\Delta S$  and  $T$  are zero so  $\Delta G = \Delta H$ . The relationship shows  $\Delta S$  becoming of increasing importance as the temperature increases.

### Adsorption Processes

The enthalpy change is  $\Delta H = \Delta G + T\Delta S$  with  $\Delta G$  being necessarily negative.

All adsorptions with negative entropy change, which comprise all physical and the great majority of chemical adsorptions, are exothermic.

### Evaporation Processes

When a liquid boils the vapour pressure is equal to the atmospheric pressure and the vapour is in equilibrium with the liquid. If there is no superheat the process is reversible and  $\Delta G = 0$  and the entropy change can be calculated:

$$\Delta S = \frac{\Delta H_{\text{vaporisation}}}{T_B}$$

Entropies of vaporisation, at these conditions, have values near 88 J/mol°K, and substitution in the above gives Trouton's rule. However in the case of water, due to significant hydrogen bonding, the entropy change on evaporation is larger at 108.8 J/mol°K.

### Endothermic Chemical Processes

The link between Gibbs Free Energy and the reaction equilibrium constant  $K$  is represented by the equation

$$\Delta G = -RT \log K$$

A reaction will proceed provided  $\Delta G$  is negative. The reaction temperature can alter the sign and therefore the process feasibility.

### Chemical Equilibrium

For a reaction at equilibrium (all reactions can be considered equilibrium since no reaction goes to completion) there is no net reaction in either direction and we have:

$$\Delta G = 0$$

In CHEMCAD the Gibbs reactor is based on the principal that at chemical equilibrium the total Gibbs free energy of the system is at its minimum value. The Gibbs reactor can be used in the study of combustion processes including adjustment of air to fuel ratios and calculation of the heats of reaction.

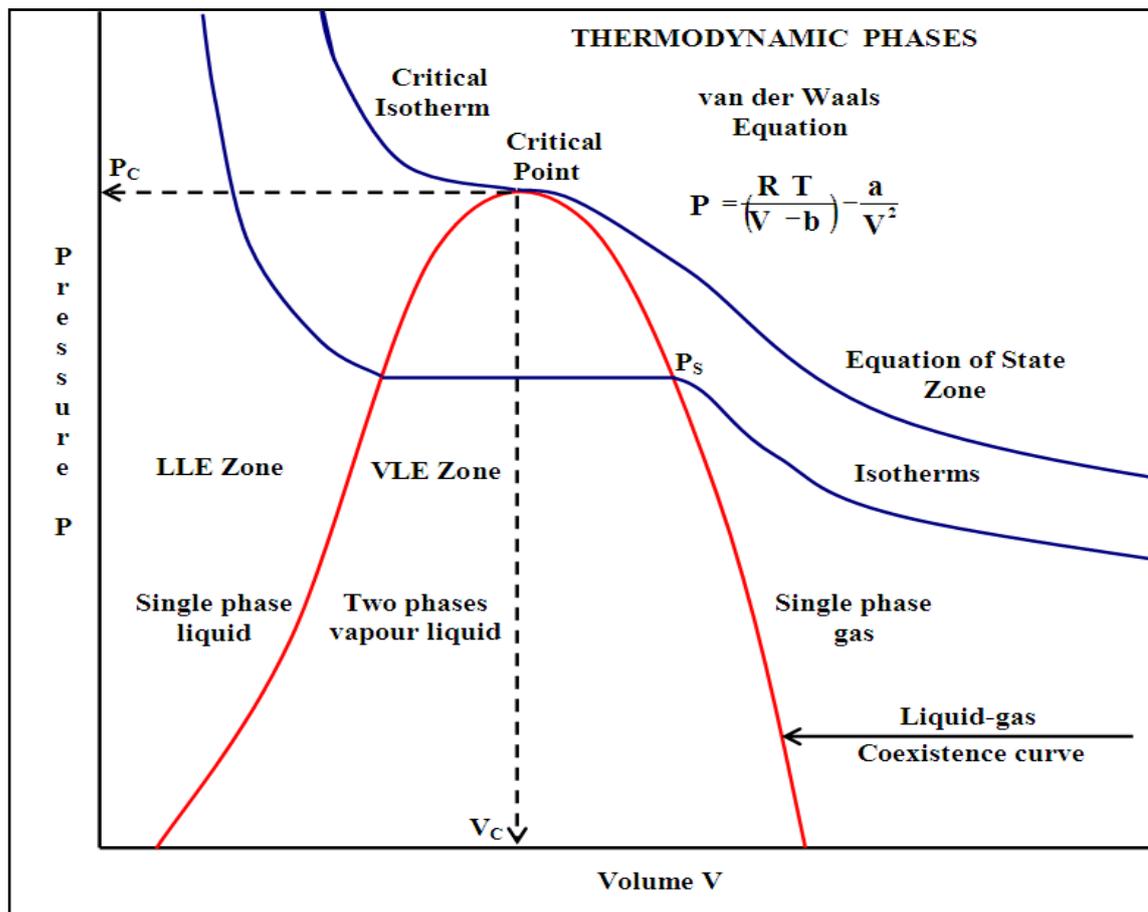
### 3.0 System Phases

There are three phase states namely solid, liquid and gas. Processes comprise either single phase or multiphase systems with separation processes involving at least two phases.

Processes involving solids such as filtration and crystallisation, solid – liquid systems and drying, solid – gas system are special cases and receive no further consideration here.

The primary area of interest for thermodynamic model selection involves two phases. Liquid – liquid systems, such as extraction and extractive distillation, where liquid – liquid equilibrium (LLE) is considered and vapour liquid systems, such as distillation, stripping and absorption, where vapour – liquid equilibrium (VLE) is considered.

The figure below shows the inter-relationships between the system phases for a series of isotherms based on the Equation of State (E-o-S) due to van-der-Waal. This figure provides the first indication of the validity of making a thermodynamic model selection for the K-value on the basis of the system phases namely single phase gas by E-o-S and VLE by activity coefficient.



Simulator thermodynamic settings include the Global Phase Option which can be set for Vapor/Liquid/Solid or Vapor/Liquid/Liquid/Solid. When carrying out azeotropic distillation or solvent extraction the Vapor/Liquid/Liquid/Solid option should be selected.

## Section 4

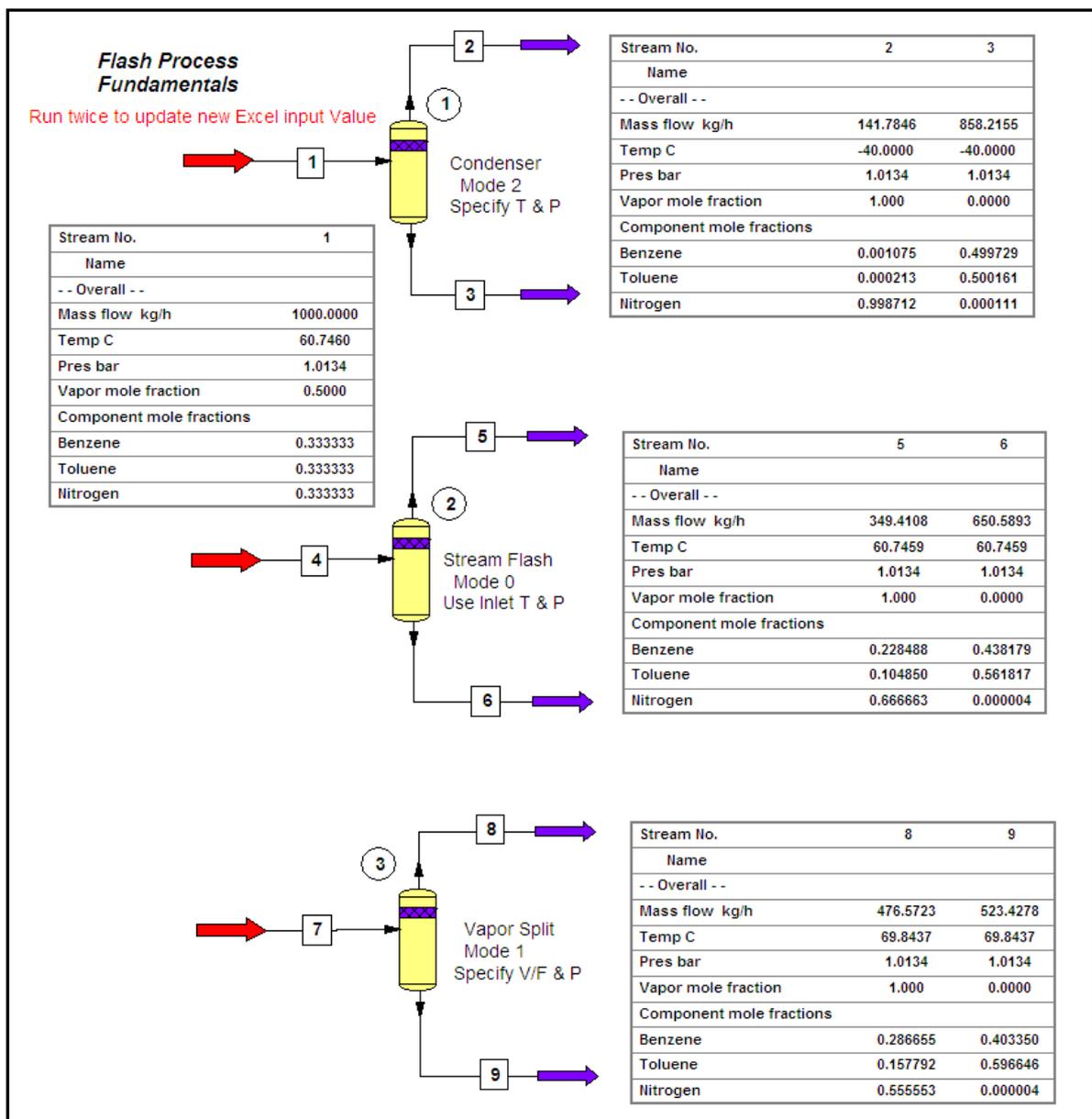
### Thermodynamics Simulation Cases

In this section are presented cases to facilitate an understanding of the CHEMCAD steady state simulation particularly in relation to the Flash UnitOp. For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

Case/File Name	Description
4.01	Flash Process Fundamentals

This case introduces the Flash UnitOp showing its application as a condenser with or without sub-cooling, a vapour liquid separator by flashing at inlet stream condition and achieving a vapour to feed ratio split at a specified pressure. The feed mixture contains benzene, toluene and nitrogen in at equal 0.33 mole fractions.

The model is connected to an Excel spreadsheet, shown, by using the simulator DataMap facility.



## **Section 5**

# ***Fluid Flow and Pipe Networks***

### **Contents**

- 1.0 Introduction to Piping Networks
- 2.0 Piping Calculation and Design Methods
  - Energy Equation and Momentum
  - Friction Factor
  - Isothermal Flow
  - Darcy Weisbach
  - Hazen-Williams
  - Fritzsche
  - Two Phase Flow
  - Baker Two Phase Flow Method
  - Beggs and Brill Two Phase Flow Method
  - 3K-Darby Method Resistance Method
  - Heat Loss in Piping Systems
  - Net Positive Suction Head
  - Piping Design Considerations
  - Instrumentation Considerations
- 3.0 Description of Valves and Fittings

### **Appendices**

- I Losses due to Valves, Pipe Fittings and Special Components
- II Flow Meter Considerations
- III General Information

### **References**

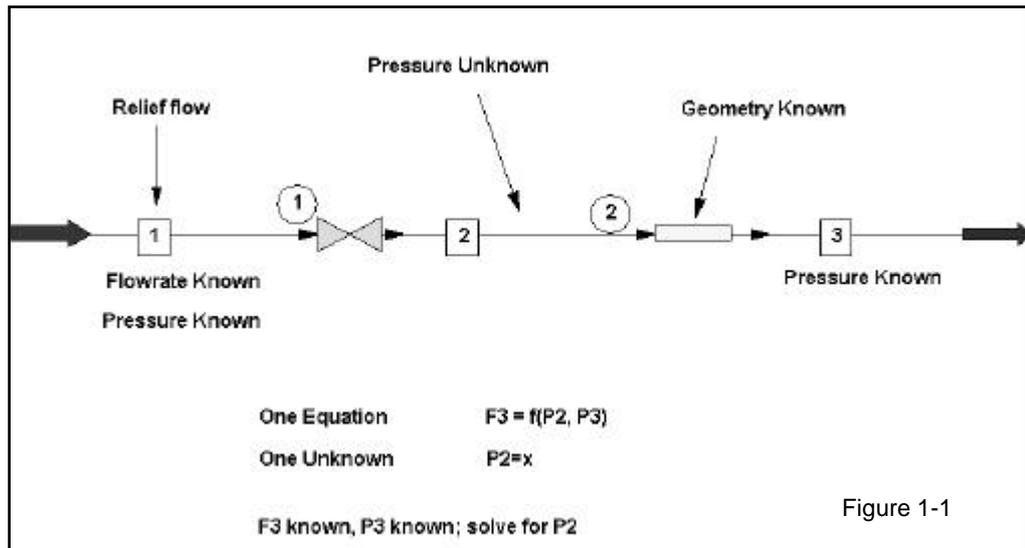
- D.J.Deutsch and J.David "Chemical Engineering; Process Piping Systems" McGraw-Hill,1980.
- J.P.Brill and H.D.Beggs, "Two-Phase Flow in Pipes" 4<sup>th</sup> edition,1978.
- R.Darby,"Chemical Engineering Fluid Mechanics", Marcel-Dekker, ISBN No 0-8247-0444-4.
- G.R.Kent, "Preliminary Pipeline Sizing", Chemical Engineering; September,1978.
- Crane Co., "Flow of Fluids Through Valves, Fittings, and Pipes", Technical Paper No. 410, 1991.

## 1.0 Introduction to Pipe Networks

A pipe network represents the flow of fluids through pipes, valves and fittings. If sufficient variables, flowrates and pressures are specified, the unknown variables may be calculated.

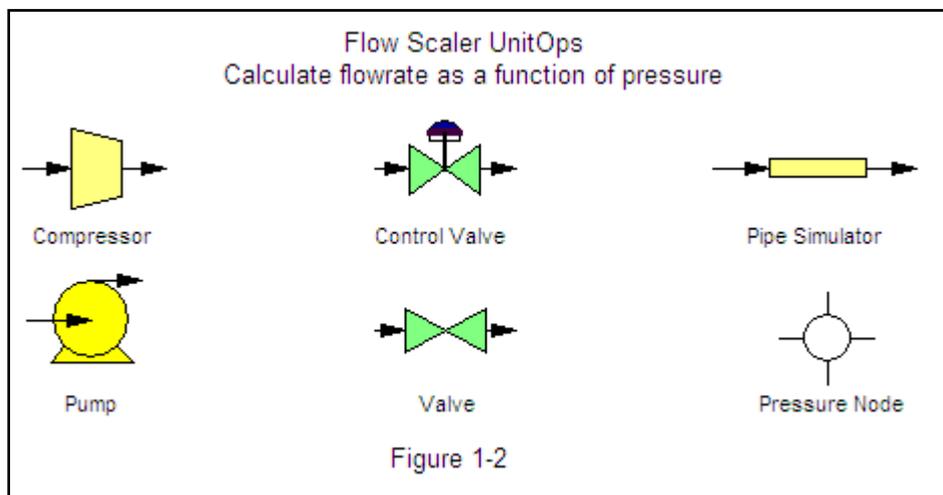
The flowrate through a component may be calculated as a function of the inlet and outlet pressures, giving three variables. If two of the three variables are specified the third is dependent. Specification of pressure at various junctions in a pipe network diagram allows the system to be described as a system of dependent equations.

The pipe network model allows for the simultaneous solution, if sufficient constraints are specified, to converge on the unknown pressures and flowrates. A simple flow system is shown in the Figure 1-1.



The known variables are the geometry of the pipe, pressure out of pipe, and flowrate through pipe. A single equation can be used to solve for the pressure into the pipe as a function of the known variables.

Fluid mechanics enables the calculation of fluid flowrate through a pipe, valve or nozzle as a function of the inlet and outlet pressures, the pressure drop. Performance curves allow the calculation of fluid flow through a compressor or pump as a function of the inlet and outlet pressures. Figure 1-2 shows equipment that calculate flowrate as a function of pressures. These UnitOps are referred to as flow scaling UnitOps.



## Fluid Mechanics

Static pressure at the base of a vertical column of fluid is given by:

$$p = H \rho$$

The Continuity equation for incompressible fluid flow is given by:

$$q = a_1 v_1 = a_2 v_2 \quad \longrightarrow \quad d_1^2 v_1 = d_2^2 v_2 \quad \longrightarrow \quad \frac{d_1^2}{d_2^2} = \frac{v_2}{v_1} = \beta$$

A Conservation of Energy equation due to Bernoulli, assuming no work, is given by:

$$\frac{p_1}{w} + \frac{v_1^2}{2g} + z_1 = \frac{p_2}{w} + \frac{v_2^2}{2g} + z_2 + \sum h_L$$

- p** pressure (lb/ft<sup>2</sup>)
- H** height of column of fluid (ft)
- ρ** fluid density - specific weight of fluid (lb/ft<sup>3</sup>)
- q** flow rate
- a** area of flow section (ft<sup>2</sup>, m<sup>2</sup>)
- d** circular pipe diameter (ft, m)
- v** velocity of fluid (ft/s, m/s)
- g** gravitational constant (32.2 ft/s<sup>2</sup> or 9.81 m/s<sup>2</sup>)
- z** potential energy or static head (ft, m)
- h<sub>L</sub>** losses due to friction or work done
- 1, 2** state 1 to state 2, below 1 refers to smaller diameter and 2 to larger diameter

The flow through a pipe section is determined from the general form of the Darcy Weisbach equation:

$$q = k \sqrt{\frac{\Delta P \rho d^5}{f L}}$$

The flow through a control valve is determined from an equation of the general form:

$$q = k C_v \sqrt{\frac{\Delta P}{\rho}}$$

The flow through an orifice plate is determined from an equation of the general form:

$$q = k d^2 C \sqrt{\frac{h}{\rho}}$$

- ΔP** pressure drop
- h** orifice plate differential pressure
- f** pipe friction factor
- k** constant
- C<sub>v</sub>** valve sizing coefficient
- C** orifice discharge coefficient

## Section 5

### *Pipe Network Simulation Cases*

In this section are presented cases to facilitate an understanding of the CHEMCAD simulator and its capabilities in handling the design and simulation of pipe networks.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
5.01	Specifying pipe size changes and fittings
5.02	Control valve sizing, flow balancing
5.03	Piping design
5.04	Pipe and orifice sizing, pump curve, flow split
5.05	Cooling water distribution balancing
5.06	Gravity flow between reservoirs
5.07	Piping Flow Split (Olson Example 10-3)
5.08	Complex pipe network
5.09	Valve sizing - liquid
5.10	Valve sizing – compressible fluid
5.11	Orifice sizing – liquids, gases and steam

## Case 5.01 Pipe size changes and fittings

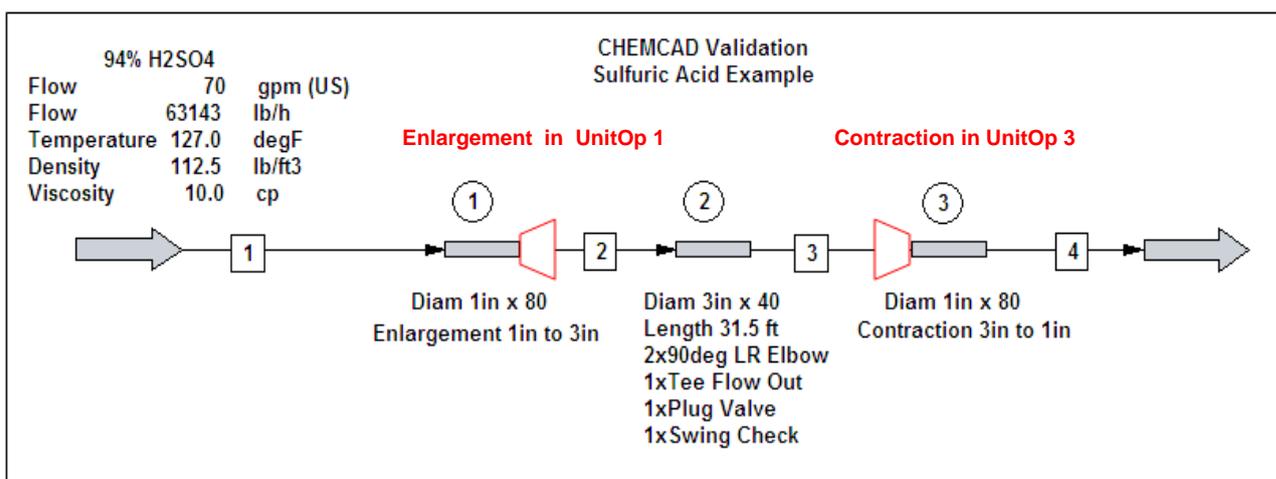
This validation case study has been based on the flow of 94% Sulphuric Acid through a 3 in x Schedule 40 carbon steel pipe from an example given in [www.cheresources.com/eqlength.shtml](http://www.cheresources.com/eqlength.shtml). The process conditions are shown below:

Process Data	Units	Example Data	CHEMCAD
Mass Flow Rate	lb/h	63143	
Volumetric Flow rate	gpm (US)	70	70
Density	lb / ft <sup>3</sup>	112.47	112.47 (Pipe Props)
Specific Gravity	dimensionless	1.802	
Viscosity	cps	10	10 (Pipe Props)
Temperature	°F	127	127
Pipe ID	in	3.068	3.068
Velocity	ft / s	3.04	3.036
Reynold's Number	dimensionless	12998	12998.9
Darcy Friction Factor	f (pipe)	0.02985	0.03000
Friction Factor at Turbulence	f <sub>t</sub>	0.018	Not declared
Straight Pipe	ft	31.5	31.5

The pipe section has 2 x 90° elbows, 1 x flow-out branch Tee, 1 x swing check valve, 1 x plug valve, and 1 x 3 in to 1 in expansion. The contraction has been added to the model for testing purposes.

### Simulation Model

For practice you can build the model or use the model called "Sulfuric Acid" in the electronic media supplied. It is strongly recommended that you work with a copy of this job. The model flowsheet is shown that represents the piping layout .



### Configuration

The key aspect of this problem is the handling of the enlargement and contraction. The fitting must be located in the 1 in pipe section with separate Pipe UnitOps 1 and 3 included to allow for this. Locating the enlargement and contraction in Pipe UnitOp 3 gives incorrect results. Refer to Appendix I for a detailed assessment of this theory.

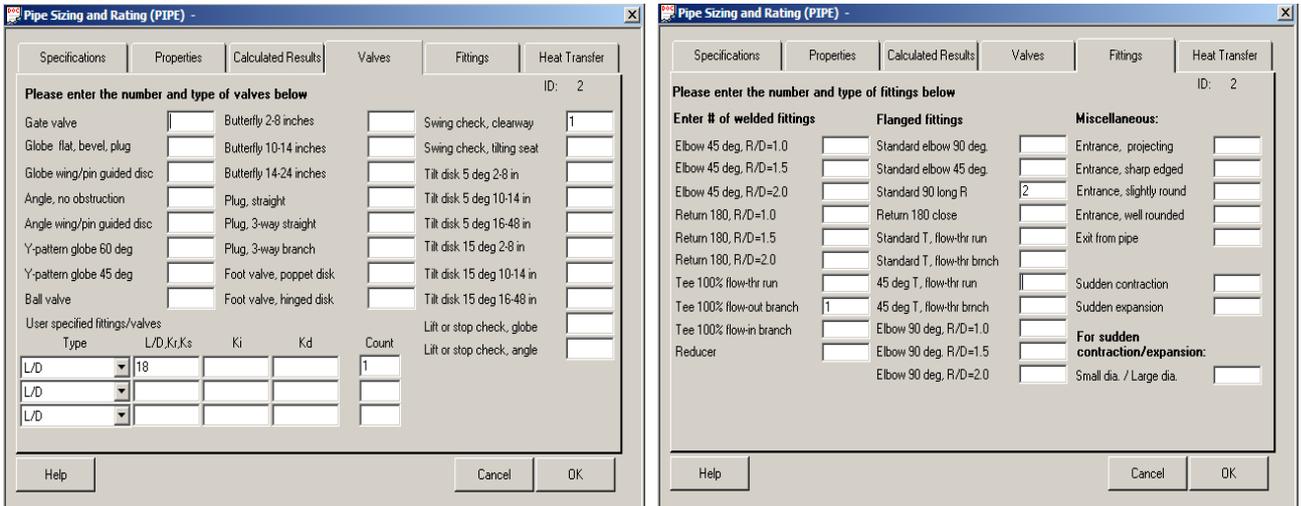
The plug valve L/D has been entered as a user value as the CHEMCAD library value did not match the example data. The Pipe Section data entry for the 3 in pipe is shown following. The Churchill friction factor has been selected due to the application being in the transition flow region. CHEMCAD library has been used for pipe roughness factor.

Friction factor model

Enter one of the following:

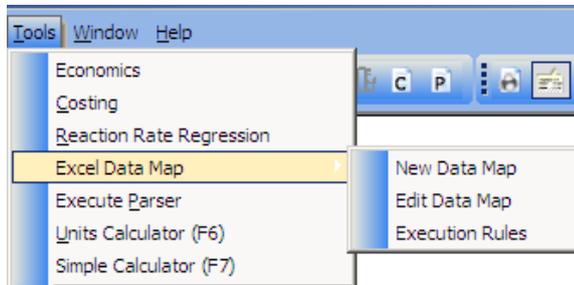
Roughness factor  ft

Pipe Material



### Simulation with Excel

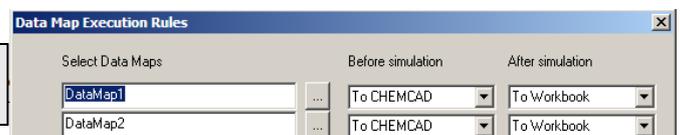
The model is controlled directly from an Excel spreadsheet Sulfuric Acid. This is linked to the model using the CHEMCAD Data Mapping Tool which is accessed from the main Toolbar. The Data Map operation is controlled by the Execution Rules.



The control spreadsheet is selected with Browse. The Data Map is shown in which the desired Stream or UnitOp is selected, with the required parameter, and assigned an Excel cell in the control spreadsheet.

Map Rule	CC Obj Type	CC Obj ID	Par ID	Component	WrkSht Cel...	Weight
To Workshe...	UnitOp	1	Calc. Velocity	<None>	F9	1.00000
To Workshe...	UnitOp	1	Fric factr liq	<None>	F10	1.00000
To Workshe...	UnitOp	2	Calc. Velocity	<None>	F13	1.00000
To Workshe...	UnitOp	2	Reynolds # liq	<None>	F14	1.00000
To Workshe...	UnitOp	2	Fric factr liq	<None>	F15	1.00000

The execution rules, as set below, transfers input data to CHEMCAD at the start of the simulation and returns results at the end of the simulation.



## Results

Fitting resistance coefficients are shown in the table together with CHEMCAD derived  $L_{eq}$  values.

Fittings	$L_{eq}/D$	$L_{eq}$	$L_{eq}$ (CHEMCAD)	$K = f_t (L/D)$	Quantity	Total $L_{eq}$
90° Long Radius Elbow	20	5.1	5.1	0.36	2	10.23
Tee Flow-out branch	60	15.3	14.8	1.08	1	15.34
Swing Check Valve	50	12.8	12.9	0.9	1	12.78
Plug Valve	18	4.6	4.6 <sup>(1)</sup>	0.324	1	4.6
3in x 1in Reducer	None	822.7	492.6 <sup>(2)</sup>	57.92	1	822.7
Total						865.6

### Notes

(1) User value fitting coefficient entered into CHEMCAD

(2) The value quoted is calculated using  $f_{pipe}$ , if  $f_t$  is used value is 821.6. Refer to control Excel worksheet for further details.

The spreadsheet studies the handling of the enlargement fitting by different methods. It can be seen that there is agreement between the different methods with the main issue being whether to use  $f_t$  or  $f_{pipe}$  to calculate  $L_{eq}$ .

Validation of CHEMCAD in handling pipe diameter changes.										
Example 96% Sulfuric Acid		CHEMCAD	Fittings 1 in x 80 by 3 in x 40 Enlargement				CHEMCAD			
Data		Results	Calculations using pipe conditions f				Results			
D1	0.0798 ft		Inlet Pipe				Inlet Pipe			
L1	0.5 ft									
v1	31.21 ft/s	3120	K1	$2.6 \sin(\theta/2) [1 - \beta^2]^2$	0.543	K1(fr) $f_{144}$	8.30	ft fluid		
f1		0.0270	Friction Loss (hf)1	$(hf) [(\rho/\rho_{144})]$	6.48	psi				
D2	0.2557 ft		Equivalent Length Method Inlet Pipe				Example Calculations using ft			
L2	31.5 ft		L1/D1	$K1/H1$	20.304	K1/fr	30.48			
v2	3.04 ft/s	3.036	(Leq)1	$(L/D)1D1$	1.62	ft	(L/D)1D1	2.43	2.405	ft
Re No	12998	12998.9	Friction Loss (hf)1	$(fL/v^2 2gD)1$	8.300	ft fluid	$(fL/v^2 2gD)1$	12.32		
f2	0.02985	0.0300		$(hf) [(\rho/\rho_{144})]$	6.48	psi	$(hf) [(\rho/\rho_{144})]$	9.62	9.64	psi
r	0.018		Outlet Pipe							
$\Delta P_{H00ft}$	1.308 psi	1.32	K2	$K1\beta^4$	57.84					
p	112.47 lb/ft <sup>3</sup>		Friction Loss (hf)2	$K2 (v^2/2g)$	8.28	ft fluid				
psi/100ft	1.307			$(hf) [(\rho/\rho_{144})]$	6.47	psi				
$\theta$	30 deg		Equivalent Length Method Outlet Pipe				Example Calculations using ft			
d	3.0684 in		L2/D2	$K2/H2$	1926.29	K2/fr	3213.12			
w	63143 lb/h		(Leq)2	$(L/D)2D2$	492.55	ft	(L/D)2D2	821.60		
			Friction Loss (hf)2	$(fL/v^2 2gD)2$	8.25	ft fluid	$(fL/v^2 2gD)2$	13.76		
				$(hf) [(\rho/\rho_{144})]$	6.44	psi	$(hf) [(\rho/\rho_{144})]$	10.75		
g	32.2 ft/s <sup>2</sup>		Pressure Loss				Enlargement located in larger diameter pipe			
			Basis	1.32 psi/100ft	6.48	psi	Total Leq	38.4	ft	
			K value method		6.82	psi	Leq( $\Delta p/100ft$ )	0.505	psi	
							Calculated	From psi/100ft	0.505	psi
							Calculated	$(fL/v^2 2gD)2$	0.642	ft fluid
							Friction Loss (hf)2	$(hf) [(\rho/\rho_{144})]$	0.501	psi
Formulae used for K1 and K2			Note consistency of results throughout on inlet and outlet using the Crane method with pipe f							
$h_L = \frac{v^2}{2g} \left( \frac{1}{\beta^4} - 1 \right) + K_1 \frac{v^2}{2g}$			Also consistent results using $\Delta P_{H00ft}$ method							
$h_L = \frac{K_2}{\beta^4} \frac{v^2}{2g} + K_2 \frac{v^2}{2g}$			CHEMCAD calculates correctly <b>only when</b> enlargement or contraction is placed in smaller diameter pipe UnitOp							
Formula used for calculating $\Delta P_{H00ft}$			CHEMCAD calculates equivalent length of fittings using prevailing pipe friction factor and not ft							
Set L=100										
$\Delta P = 0.00000336 \frac{f L W^2}{\rho d^5}$			Fittings 1 in x 80 by 3 in x 40 Contraction							
			K1	$0.5(1-\beta^2)$	0.451					
			Friction Loss (hf)1	$K1(v^2/2g)$	6.827	ft fluid			5.34	psi
				$(hf) [(\rho/\rho_{144})]$	5.332	psi				
			L1/D1	$K1/H1$	16.702					
			(Leq)1	$(L/D)1D1$	1.33	ft			1.33	ft
			Entrance to Pipe							
			K1	0.5	0.5					
			Friction Loss (hf)1	$K1(v^2/2g)$	7.564	ft fluid			5.91	psi
				$(hf) [(\rho/\rho_{144})]$	5.91	psi				
			L1/D1	$K1/H1$	18.50					
			(Leq)1	$(L/D)1D1$	1.48	ft			1.47	ft
			Exit from Pipe							
			K1	1	1					
			Friction Loss (hf)1	$K1(v^2/2g)$	15.13	ft fluid			11.8	psi
				$(hf) [(\rho/\rho_{144})]$	11.82	psi				
			L1/D1	$K1/H1$	37.01					
			(Leq)1	$(L/D)1D1$	2.95	ft			2.95	ft

CHEMCAD predicts a line pressure drop of 12.61 psi as compared to the example line pressure drop of 11.734 using the total equivalent length method. CHEMCAD physical property predictions for 94% Sulfuric Acid did not agree with the example values. CHEMCAD has a feature in the Pipe UnitOp to allow the user to enter different physical properties to the Stream values and this was used.

## Section 6

# Emergency Relief Sizing

### Contents

- 1.0 Introduction
- 2.0 Relief Sizing Fundamentals
  - 2.1 Vessel Models
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- 3.0 Definitions and Assumptions
  - 3.1 % overpressure
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    - 4.5.3 Omega Method for Two Phase Vapour Liquid Flow
    - 4.5.4 Henry Fauske's Homogeneous Non-equilibrium HNE Model
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- 5.0 Nomenclature

### Appendices

- I CHEMCAD Relief Sizing Tool Design Note Two Phase Flow
- II CHEMCAD Relief Sizing Tool User Notes
- III General Guidance Notes
- IV Blowdown Tank Sizing

### References

1. J. Wilday and J. Etchells, "Workbook for Chemical Reactor Relief System Sizing" HSE Contract Research Report 136/1998.
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## 1.0 Introduction

To achieve safe operation of chemical processes, particularly when involving exothermic reactions, requires a combination of preventative and protective measures.

Preventative measures minimise the occurrence of an event and include:-

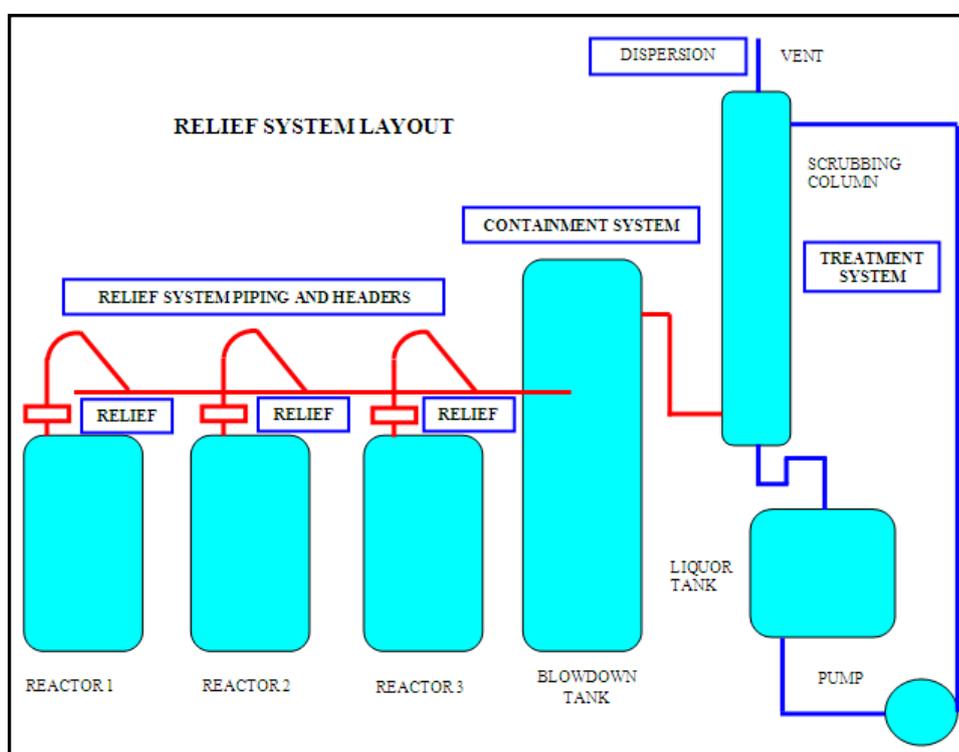
- Automatic control systems including the use of independent hardwired alarm and trip systems based on Safety Integrity Level (SIL) analysis.
- Provision for appropriate manual intervention.

Protective measures mitigate the consequences of a runaway reaction and include:-

- Emergency pressure relief.
- Crash cooling.
- Reaction inhibition.
- Drown out.

This paper reviews the techniques associated with the design of emergency pressure relief and blowdown systems. An emergency relief system comprises the following key components:-

- Primary pressure relief device.
- Relief system piping and headers.
- Containment system.
- Treatment system.
- Atmospheric dispersion.



Specific design techniques are required for each component of the system and process modelling of the total integrated system will demonstrate the adequacy of the total design.

The pressure relief device is either a relief valve, a bursting disc or a combination of both. On chemical reactors the bursting (rupture) disc is the most favoured due to being able to handle the following conditions:-

- Rapid pressure rise with full relief area available, except when vacuum support used.
- Toxic fluids where no leakage past a safety valve is permitted.
- Corrosive fluids that may cause progressive deterioration of a safety valve.
- Fluids that may deposit solids or build ups that interfere with safety valve operation.

The major disadvantages of bursting discs are :-

- Require a larger allowance between the operating pressure and the set pressure.
- If the operating pressure and the set pressures are too close, the disc can fail prematurely due to pressure pulsations.
- Loss of containment of reactor contents on operation i.e. valve does not reseal, unless used in conjunction with a safety valve.

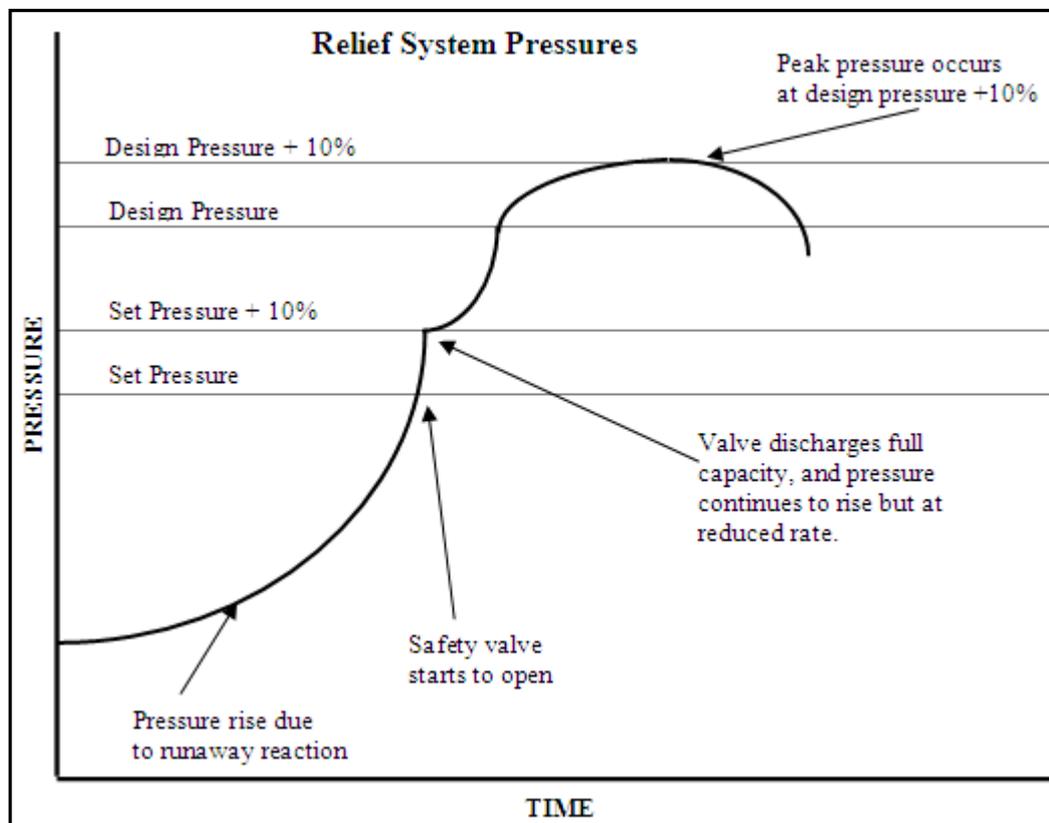
To mitigate against the loss of containment due to operation of a bursting disc sized for the worst case scenario the installation of a smaller bursting disc/relief valve combination in parallel set at a lower relief pressure can be considered. This smaller system operates in the event of nuisance pressure build ups, due to maloperation, without total loss of containment. This technique has the disadvantage, due to the poor set pressure tolerance of bursting discs typically  $\pm 10\%$ , of significantly increasing the set pressure of the main bursting disc to ensure the smaller disc operates first. This may lead to an undesirable situation particularly when protecting for exothermic runaway events.

The relief pressure at which the relief device is fully open should be set at the lowest pressure practicable consistent with preventing nuisance operations for the following reasons :-

- For most exothermic runaway reactions, the reaction rate and heat release rate increases exponentially with temperature. For a vapour pressure system, a low relief pressure means a low relief temperature and hence a relatively low rate of heat release. The relief area required is directly proportional to the rate of heat release by the reaction.
- For a relief system venting a two-phase mixture, pressure relief acts to remove reactants from the reactor. A low relief pressure allows a greater margin between the relief pressure and maximum permitted pressure, and advantage is taken of this by the sizing methods to yield a smaller relief area.

The requirements for the design of the relief system sizing can be summarised:-

- The equipment design pressure plus permitted accumulation is not exceeded.
- The pressure relief system is as small as possible consistent with the above clause. A small relief system minimises cost, disposal requirements and the potential rate at which material could be discharged to the environment.



### Relief System Piping and Headers

The flow capacity of a bursting disc is determined by the disc diameter and the discharge coefficient. However the system capacity can be limited by the discharge piping system. Key features of the relief system piping design can be summarised:-

- Branch pipe from reactor to the header to be not less than the outlet diameter of relief device
- Branch pipe to enter main header as a 45 degree T, flow through branch
- All 90° bends to have maximum R/D consistent with layout constraints
- Main header to slope towards the blowdown drum and enter tangentially
- Consideration to be given to nitrogen inerting to prevent explosive mixtures
- Provision of adequate inspection and test facilities to ensure headers are clear

### Containment System

In many instances the discharge stream from an emergency relief system is a two phase vapour liquid mixture. The stream is routed to a blowdown/knock out drum designed to disentrain the liquid from the vapour to allow discharge to atmosphere or for downstream treatment. The justification for the blowdown drum is:-

- Prevents release of hot, toxic and corrosive liquid resulting in potential safety hazards and environmental damage.
- Prevents release of flammable droplets leading to vapour cloud explosion.
- Allows downstream treatment of toxic vapours for treatment in a wet scrubber, flare or incinerator.

There are many designs of blowdown drum depending upon the circumstances but key features include:-

- Tangential inlet into a vessel of sufficient diameter to effect good vapour – liquid separation.
- Total volume sufficient to hold the estimated carryover, typically two times the volume of the largest reactor connected to the relief system.
- Adequate instrumentation monitoring for level and pressure detection.
- Appropriate facilities for drainage and material handling.
- Appropriate facilities for quenching reaction mixtures.

Sizing of the blowdown drum is carried out in accordance with API 521. The basic design method<sup>(3)</sup> involves the calculation of the allowable vapour velocities for the components under consideration which allows the vapour flow area to be set. A drum diameter can then be determined on the basis that the vapour flow area occupies half of the drum area.

The drum volume allowed for the disentrained liquid is based on the following criteria:-

- For non-foaming systems the volume should be equal to the maximum working volume of the largest reactor connected to the system.
- For foaming systems the volume should be a minimum of 1.5 times the maximum working volume of the largest reactor connected to the system.
- As a general rule in multi-purpose batch plants the minimum blowdown drum volume should be equal to 2 times the maximum working volume of the largest reactor connected to the system.

The benefits of a pressure relief system are:-

- Different and independent failure modes to the preventative measures.
- Provides relatively passive means of protection.
- Provides adequate protection if all other systems fail.

The emergency pressure relief system is considered the ultimate protection. The primary basis of safety for overpressure protection is based on prevention involving management control procedures and instrument protective systems.

Emergency pressure relief may not be appropriate due to economical, environmental or technical considerations. In such cases, appropriate preventative measures must be relied on.

The design of emergency relief systems for exothermic batch reactors requires a thorough understanding of the reaction conditions including:-

- The credible maloperations and system failures that might occur during reaction.
- The kinetics of the reaction under runaway conditions.
- Whether the reaction pressure is from vapour, gas or both.
- The flow regimes in the vessel and relief system during relief.
- The design and layout of the relief system.

Emergency Relief System (ERS) design has been covered extensively by the Design Institute for Emergency Relief Systems (DIERS)<sup>(2)</sup> of the American Institute of Chemical Engineers (AIChE), the American Petroleum Institute Standards (API)<sup>(3,4,5)</sup>, the UK Health and Safety Executive (HSE)<sup>(1)</sup> and work by Leung<sup>(10)</sup>, Fauske<sup>(7)</sup>, Huff, Etchells, Wilday and many others.

The practising engineer is required to provide safe, practical and timely solutions to ERS design problems without having the opportunity to study the topic in depth. This technical note attempts to provide a comprehensive review of ERS fundamentals, definitions and design principles to allow the solution of cases encountered in normal practice. For more complex cases or when in doubt reference should be made to an appropriate authority or specialist in the field.

CHEMCAD Relief Sizing Tool, supported by a component data base with comprehensive thermodynamics, is used for this Section. The extensive features of the sizing tool cover most situations encountered in practice and are summarised below

- Batch or continuous process applications
- Reactive or non reactive systems
- Relief device: conventional relief valve, balanced relief valve, bursting disc or relief valve and bursting disc in combination
- Relief device: set pressure and allowable overpressure
- Design or rating for pressure vessel or atmospheric vessel
- Vessel model options: churn turbulent, bubbly or homogeneous equilibrium
- Single phase vent flow: liquid, gas / vapour or steam flow
- Prediction of two phase flow onset with relief sizing using Leung's method
- Two phase vent flow model options: homogeneous equilibrium (HEM), equilibrium rate (ERM) and Henry Fauske's homogeneous non-equilibrium (HNE)
- Heat model code options: API 520/521, NFPA 30, OSHA 1919.106 or API 2000
- Heat model options: specify heat rate, tempered runaway reaction, non-tempered runaway and additional heat input
- Vessel geometry: cylindrical/spherical, vertical/horizontal
- Vessel end type: ellipsoidal, spherical, conical or flat
- Vessel parameters: diameter, tan-tan height and design pressure
- Vessel operating liquid level
- Vessel void volume calculated from geometry and liquid level or specify
- Height of bottom tan line from grade where fire can be sustained
- Options for fire fighting protection available and insulation factor
- Relief device stagnant or flowing input stream composition and condition set from CHEMCAD component database with appropriate thermodynamic options applied
- Relief device inlet and outlet diameter and length specified and pressure drop calculated and checked for design code compliance

## Section 6

### *Emergency Relief Sizing Simulation Cases*

<b>Case/File Name</b>	<b>Description</b>
6.01	Liquid Relief Sizing, API 520 Part 1, 3.8.2 page 53
6.02	Vapour Relief Sizing, API 520 Part 1, 3.6.2.2 page 44
6.03	Steam Relief Sizing, API 520 Part 1, 3.7.2 page 51
6.04	Diers Example Appendix II-E (page 113)
6.05	Diers Example Appendix II-E (page 113)
6.06	Diers Final Report Appendix D (page 181)
6.07	Diers Non - Tempered Relief Example 15 (page 438)
6.08	Diers Non - Tempered Relief Example 15 (page 438)
6.09	Diers Tempered Relief Example 11 (page 432)
6.10	Diers Tempered Relief Example 11 (page 432)
6.11	Diers Test-T3A (Vessel page174 Test Data page 198)
6.12	Diers Two Phase Rigorous Design Case
6.13	Relief Vent Piping Manifold
6.14	Flare Header Design

**Case 6.01**  
**Liquid Relief Sizing** (API 520 Part 1 section 3.8.2 page 53)

API 520 Part 1 3.8.2 page 53 FLUID Crude Oil					
Set Pressure (psig)	Back Pressure (psig)	Accumulation %	Viscosity Saybolt Universal sec	Specific Gravity	Flow gpm
250	0 to 50	10	2000	0.9	1800

Using the sizing equation for liquid service in US customary units

$$A = \frac{Q}{38 K_d K_w K_c K_v} \sqrt{\frac{G}{p_1 - p_2}}$$

- Where  $p_1 = 250 \times 1.1 = 275$  psig  
 $p_2 = 50$  psig  
 $K_d = 0.65$   
 $K_w = 0.975$  for balanced bellows valve with variable back pressure  
 $K_c = 1.0$  since no rupture disc  
 $K_v = 1.0$  viscosity correction factor  
 $G = 0.9$

Substitution gives  $A=4.752$  in<sup>2</sup>, nozzle P selected with orifice area 6.38 in<sup>2</sup>  
 Applying viscosity correction factor  $K_v = 0.964$  gives an area of 4.930 in<sup>2</sup>  
 Dowtherm A was used to simulate fluid conditions with user viscosity of 397.8 cps entered.



Stream No.	1
Stream Name	
Temp F	375.0000*
Pres psia	264.7000*
Enth MMBtu/h	-0.0077588
Vapor mole fraction	0.00000
Total lbmol/h	1.0000
Total lb/h	166.0000
Total std L ft3/hr	2.4948
Total std V scfh	379.48
Flowrates in lb/h	
Dowtherm A	166.0000

- Calculated nozzle area ft2 = 0.032284 (4.6489 in2)**  
**Selected valve type: 4P6**  
**Actual nozzle area ft2 = 0.044306**  
**The following calculation is base on vent area 0.044306 ft2.**  
**Calculated vent rate lb/h = 1.1113e+006**  
**Device inlet density lb/ft3 = 57.279**  
**Nozzle inlet vapor vol. fraction = 0**

Calculated area= 0.032284 ft<sup>2</sup> (4.649 in<sup>2</sup>) compared with 0.03424 ft<sup>2</sup> (4.930 in<sup>2</sup>) Selected nozzle P with orifice area 0.0443 ft<sup>2</sup> (6.38 in<sup>2</sup>) Viscosity correction factor  $K_v$  was calculated correctly at 0.964. Note that the capacity correction factor  $K_p$  is not applied when capacity certification.

## **Section 7**

# ***Heat Transfer > Heat Exchanger Design and Rating***

### **Contents**

- 1.0 Introduction**
- 2.0 Fundamentals**
  - 2.1 Basic Theory
  - 2.2 Heat Transfer Model Selection
- 3.0 Design Guidelines**

### **Appendices**

- I Thermal Design Models Synopsis
- II Sizing Procedure
- III CC THERM Guidelines
- IV TEMA Heat Exchanger Layout Designation
- V Typical Overall Heat Transfer Coefficients
- VI Typical Resistance Fouling Coefficients
- VII LMTD Correction Factor  $F_t$
- VIII Wolverine Tube General Details
- IX Midland Wire Cordage Turbulator Details
- X Tube Dimensional Data
- XI Shell Tube Count Data

### **References**

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## 1.0 Introduction

Shell and tube heat exchangers are used extensively throughout the process industry and as such a basic understanding of their design, construction and performance is important to the practising engineer.

The objective of this section is to provide a concise review of the key issues involved in their thermal design without having to refer to the extensive literature available on this topic.

The optimum thermal design of a shell and tube heat exchanger involves the consideration of many interacting design parameters which can be summarised as follows:

### Process

Process fluid assignments to shell side or tube side.  
Selection of stream temperature specifications.  
Setting shell side and tube side pressure drop design limits.  
Setting shell side and tube side velocity limits.  
Selection of heat transfer models and fouling coefficients for shell side and tube side.

### Mechanical

Selection of heat exchanger TEMA layout and number of passes.  
Specification of tube parameters - size, layout, pitch and material.  
Setting upper and lower design limits on tube length.  
Specification of shell side parameters – materials, baffle cut, baffle spacing and clearances.  
Setting upper and lower design limits on shell diameter, baffle cut and baffle spacing.

There are several design and rating packages available, including Aspen BJAC, HTFS and CCTHERM, which enable the designer to study the effects of the many interacting design parameters and achieve an optimum thermal design.

It must be stressed that software convergence and optimisation routines will not necessarily achieve a practical and economic design without the designer forcing parameters in an intuitive way. It is recommended that the design be checked by running the model in the rating mode.

In the Attachments a Design Aid is presented which includes key information for data entry and a shortcut calculation method in Excel to allow an independent check to be made on the results from software calculations.

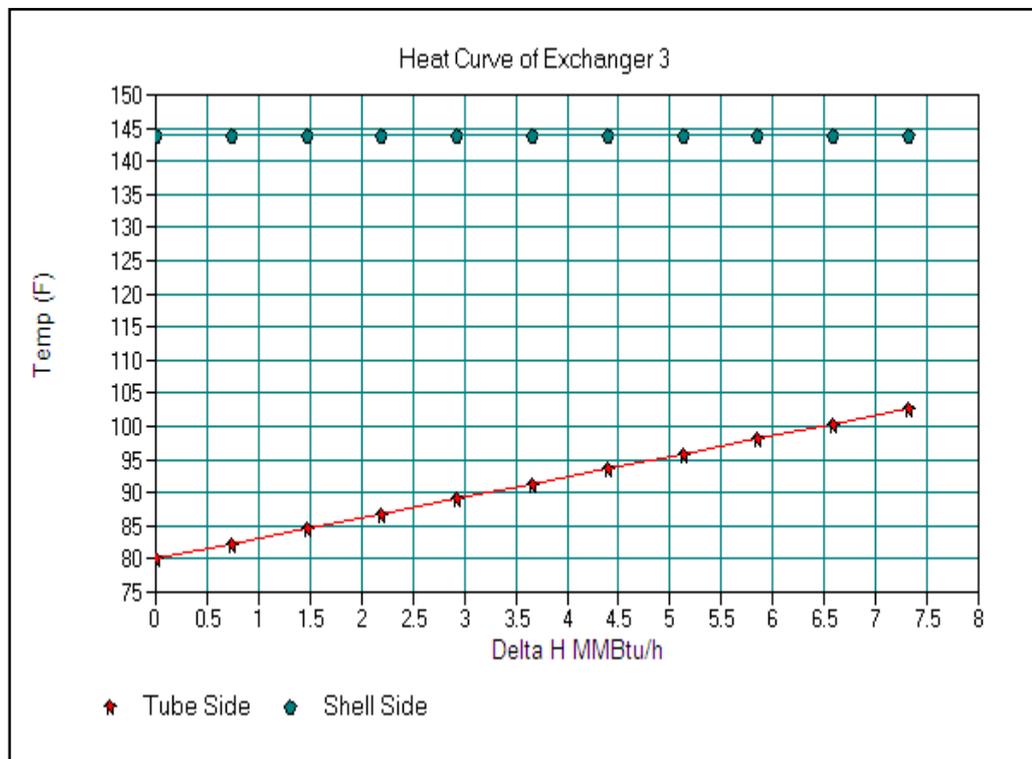
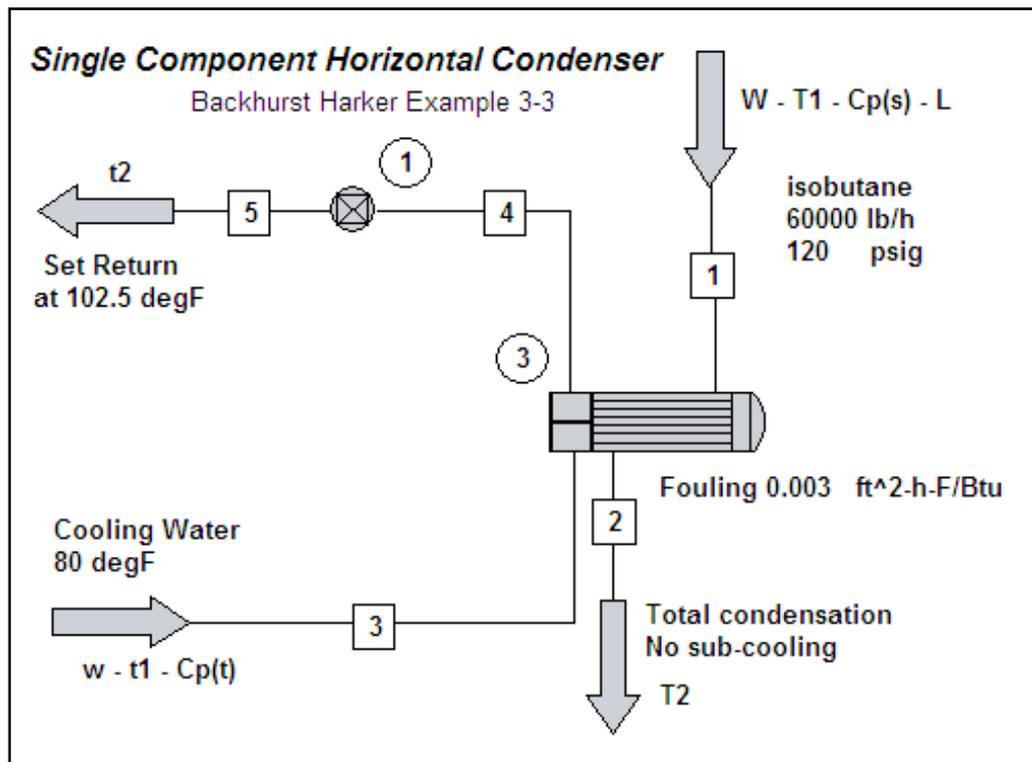
Detailed mechanical design and construction involving tube sheet layouts, thicknesses, clearances, tube supports and thermal expansion are not considered but the thermal design must be consistent with the practical requirements.

Source references are not indicated in the main text as this paper should be considered as a general guidance note for common applications and is not intended to cover specialist or critical applications. Sources for this paper have been acknowledged where possible.

The symbols, where appropriate, are defined in the main text. The equations presented require the use of a consistent set of units unless stated otherwise.

## 2.0 Fundamentals

The basic layout for a countercurrent shell and tube heat exchanger together with the associated heat curve for a condensing process are shown below:-



## 2.1 Basic Theory

The fundamental equations for heat transfer across a surface are given by:

$$Q = U A \Delta T_{lm} = w C_{p(t)}(t_2 - t_1) = W C_{p(s)}(T_1 - T_2) \quad \text{or} \quad W L$$

Where **Q** heat transferred per unit time (kJ/h, Btu/h)  
**U** the overall heat transfer coefficient (kJ/h-m<sup>2</sup> °C, Btu/h-ft<sup>2</sup>-°F)  
**A** heat-transfer area (m<sup>2</sup>, ft<sup>2</sup>)  
**Δt<sub>lm</sub>** log mean temperature difference (°C, °F)  
**C<sub>p(t)</sub>** liquid specific heat tube side,  
**C<sub>p(s)</sub>** liquid specific heat shell side (kJ/kg-°K, Btu/lb-°F)  
**w** tube side flow **W** shell side flow (kg/h, lb/h)

The log mean temperature difference ΔT<sub>lm</sub> (LMTD) for countercurrent flow is given by:

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \left( \frac{T_1 - t_2}{T_2 - t_1} \right)}$$

Where **T<sub>1</sub>** inlet shell side fluid temperature  
**T<sub>2</sub>** outlet shell side fluid temperature  
**t<sub>1</sub>** inlet tube side temperature  
**t<sub>2</sub>** outlet tube-side temperature

In design, a correction factor is applied to the LMTD to allow for the departure from true countercurrent flow to determine the true temperature difference.

$$\Delta T_m = F_t \Delta T_{lm}$$

The correction factor is a function of the fluid temperatures and the number of tube and shell passes and is correlated as a function of two dimensionless temperature ratios

$$R = \frac{(T_1 - T_2)}{(t_2 - t_1)} \quad S = \frac{(t_2 - t_1)}{(T_1 - t_1)}$$

Kern developed a relationship applicable to any heat exchanger with an even number of passes and generated temperature correction factor plots; plots for other arrangements are available in the TEMA standards.

The correction factor **F<sub>t</sub>** for a 1-2 heat exchanger which has 1 shell pass and 2 or more even number of tube passes can be determined from the chart in the Appendix VIII and is given by:

$$F_t = \frac{(R^2 + 1)^{0.5} \ln [(1 - S)/(1 - RS)]}{(R - 1) \ln [(2 - S(R + 1 - (R^2 + 1)^{0.5})) / (2 - S(R + 1 - \sqrt{R^2 + 1}))]}$$

The overall heat transfer coefficient **U** is the sum of several individual resistances as follows:

$$\frac{1}{U} = \frac{1}{h_i} + \frac{1}{h_{fi}} + \frac{1}{k/x} + \frac{1}{h_o} + \frac{1}{h_{fo}}$$

The combined fouling coefficient **h<sub>f</sub>** can be defined as follows:

$$h_f = \frac{h_{fi} h_{fo}}{h_{fi} + h_{fo}}$$

The individual heat transfer coefficients depend on the nature of the heat transfer process, the stream properties and the heat transfer surface arrangements. The heat exchanger layout depends on the heat transfer area (HTA) so an initial estimate is required based on a trial value of the OHTC.

CHEMCAD is used to establish the steady state mass and energy balances across the heat exchanger and typical values of the OHTC are shown in the Attachments. A quick calculation method XLTHERM is also available to assist this procedure. The fouling factors chosen can have a significant effect on the design and again typical values are shown in the Appendices.

## Section 7

### Heat Exchanger Simulation Cases

This section reviews the sizing methods for shell and tube heat exchanger design using CC-THERM. It must be emphasised that convergence and optimisation routines will not necessarily achieve a practical and economic design without the designer forcing parameters in an intuitive way. It is recommended that the design is supported by short-cut design methods and finally checked/optimised by running the model in the rating mode.

The optimum thermal design of a shell and tube heat exchanger involves the consideration of many interacting design parameters which can be summarised as follows:

#### Process

1. Process fluid assignments to shell side or tube side.
2. Selection of stream temperature specifications.
3. Setting shell side and tube side pressure drop design limits.
4. Setting shell side and tube side velocity limits.
5. Selection of heat transfer models and fouling coefficients for shell side and tube side.

#### Mechanical

1. Selection of heat exchanger TEMA layout and number of passes.
2. Specification of tube parameters - size, layout, pitch and material.
3. Setting upper and lower design limits on tube length.
4. Specification of shell side parameters – materials, baffle cut, baffle spacing and clearances.
5. Setting upper and lower design limits on shell diameter, baffle cut and baffle spacing.

For process design using a simulation program the following preliminary conservative estimates are given for pressure drops due to friction. An additional pressure change occurs if the exchanger is placed vertically.

Initial Process Design Pressure Drop Estimates		
Process Description	Pressure Drop (psi)	Pressure (kPa)
Liquid streams with no phase change	10	70
Vapor streams with no phase change	2	14
Condensing streams	2	14
Boiling streams	1	7

The following initial guidelines can assist in arriving at an economic design.

1. Set shell-side velocity  $\geq 4$  ft/s subject to any pressure drop constraints. Shell-side pressure drop can be reduced by increasing the baffle pitch spacing for example by doubling the pitch the velocity will halve which will reduce the pressure drop by  $\approx (\frac{1}{2})^2$ .
2. The shell-side is normally the limiting heat transfer coefficient. It is preferable to have the shell-side taking the maximum number of tubes possible to eliminate stagnant zones.
3. Set tube-side velocity  $> 4$  ft/s subject to any pressure drop constraints. Forcing the tube-side velocity down increases the number of tubes.
4. Use  $\frac{3}{4}$  in or 1 in BWG tube as preference.
5. TEMA (Section B-2-1) prefers tube lengths 8/10/12/16/20 but does not exclude shorter lengths.
6. Typical safety margins in range  $\geq 15\%$  not forgetting that the fouling factor provides an additional safety margin.

Case/File Name	Description
7.01	Single Component Horizontal Condenser
7.02	Horizontal Vacuum Condenser
7.03	Multiple Component Horizontal Condenser
7.04	Liquid – Liquid Heat Exchanger
7.05	Heat Exchanger temperature Control
7.05a	Heat Exchanger 3 way Valve Control

## Section 8

# Mass Transfer > Absorption and Stripping

### Contents

- 1.0 Introduction**
- 2.0 Fundamentals**
  - 2.1 Molality, Molarity, Mole Fraction and Mole Ratio
  - 2.2 ppm(w), ppm(v), mg/m<sup>3</sup>, Mole Fraction and Weight Fraction
  - 2.3 Worked Example on Unit Conversions
  - 2.4 Mass Balance
  - 2.5 Simplified Mass Transfer Theory
- 3.0 Thermodynamics**
  - 3.1 Physical Property Predictions
  - 3.2 K Models
  - 3.3 Vapour Liquid Equilibrium (VLE)
- 4.0 Gas Absorption**
  - 4.1 SCDS Column in CHEMCAD
  - 4.2 CO<sub>2</sub> Absorption in 30% MEA-Water Solution Regular VLE Model
  - 4.3 CO<sub>2</sub> Absorption in 30% MEA-Water Solution Mass Transfer Model
  - 4.4 CO<sub>2</sub> Absorption in Selexol
  - 4.5 HCl Absorption in Water Mass Transfer Model
- 5.0 Liquid Stripping**
  - 5.1 Air Stripping of Trichloroethylene

### Appendices

- I Fast Chemical Reaction Systems
- II Design Note on Enhancement Factor
- III Column Simulation Convergence
- IV Nomenclature
- V Guidance Notes

### References

1. R.E.Treybal, "Mass-Transfer Operations", McGraw-Hill, 3<sup>rd</sup> Edition, 1984.
2. I. Smallwood, "Solvent Recovery Handbook", Edward Arnold, 1993.
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13. K.Y.Li and K.J.Hslao, "VOC strippers: how many trays", Hydrocarbon Processing, February 1990.
14. H.Kister, "Distillation Design", McGraw-Hill, ISBN 0-07-034909-6.

## 1.0 Introduction

This workbook reviews the simulation of gas absorption and liquid stripping processes using CHEMCAD software. It discusses thermodynamic considerations and the basic chemical engineering relationships for vapour liquid equilibrium, mass and energy balances.

Methods are discussed for interpreting vapour liquid equilibrium data, design procedures and determining satisfactory operating condition. Simulations are developed for gas absorption, with and without chemical reaction, and liquid stripping processes. Particular emphasis is given to the absorption and desorption of CO<sub>2</sub> in alkanolamines due to its application to carbon capture technology.

Gas absorption is used extensively throughout the process industries to achieve a variety of process objectives:

- Gas purification processes such as acid gas treating or sweetening
- Water removal and drying of gas streams
- Removal of reactant off-gases from batch chemical reactions
- Removal of volatile organic compounds from inert gas streams
- Removal of malodorous compounds from inert gas streams

Liquid stripping is used extensively throughout the process industries to achieve a variety of process objectives:

- Air stripping for removal of CO<sub>2</sub> from water
- Air stripping for removal of volatile organic compounds from drinking water
- Regeneration of amine solution to remove CO<sub>2</sub>
- Steam stripping to remove volatile compounds

Gas absorption and liquid stripping can be difficult processes to simulate because:

- Complex thermodynamics and mass transfer based on physical or chemical solvents
- Prediction of real performance due to mal-distribution and stage efficiency prediction
- Feed conditions, temperature and composition, can significantly affect performance
- Column temperature and pressure profile can significantly affect performance

CHEMCAD has two basic vapour liquid equilibrium or mass transfer models:

SCDS            Simultaneous correction distillation with rigorous VLE calculations, particularly suited to activity coefficient models. Applicable for steady state or dynamic models and reactive distillation.

TOWER           Rigorous VLE calculations, particularly suited to equation of state models. Uses the Inside-Out algorithm Applicable for steady state or dynamic models.

In addition, special modules are available which are used to maintain mass balances and control feed, recycle and make-up streams.

1. Component Separator enables component fractions to be split from a stream.
2. Controllers can force a Stream to copy / scale another Stream flow and composition.
3. Stream Reference can fix a recycle flow at a constant value.
4. RAMP controller can change stream parameters and switch streams on or off on a time basis.

## ***Section 8***

### ***Mass Transfer > Absorption and Stripping***

In this section are listed the cases referred to in the main section.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
8.01	CO <sub>2</sub> Absorption VLE and Mass Transfer Models
8.02	CO <sub>2</sub> Absorption in Selexol
8.03	HCl Absorption in Water
8.04	Air Stripping of TCE

## **Section 9**

### ***Mass Transfer > Continuous Distillation***

#### **Contents**

- 1.0 Introduction**
- 2.0 Fundamentals**
  - 2.1 Mass Balance
  - 2.2 Separation Criteria
  - 2.3 Theoretical Stages
  - 2.4 Reflux Ratio
  - 2.5 Heat Duty
  - 2.6 Pressure
- 3.0 Thermodynamics**
  - 3.1 Activity Coefficients
  - 3.2 Thermodynamic Model Selection
  - 3.3 Column Convergence
- 4.0 Vapour Liquid Equilibrium**
  - 4.1 Bubble Point and Dew Point
  - 4.2 TPxy Plots
  - 4.3 Residue Curve Mapping
  - 4.4 Azeotrope Finders
- 5.0 Simple Distillation**
- 6.0 Heterogeneous Azeotrope Distillation**

#### **References**

1. F.G. Shinskey, "Process Control Systems", McGraw-Hill, 1967.
2. Smallwood, "Solvent Recovery Handbook", Edward Arnold, 1993.
3. J.R. Backhurst, J.H. Harker and J.E. Porter, "Problems in Heat and Mass Transfer", pages 190 – 197, Edward Arnold, 1985.
4. R.M.Felder and R.W. Rousseau, "Elementary Principles of Chemical Processes", Wiley, 2<sup>nd</sup> Edition, 1986.
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7. R.E.Rooks, "Draw Insights on Distillation", Chemical Processing, Article 2006/071, Dow.
8. E.C.Carlson, "Don't Gamble with Physical Properties for Simulation", Chemical Engineering Progress, October, 1996.
9. R.H. Perry and D. Green, "Chemical Engineers' Handbook", 6<sup>th</sup> Edition, 13-82 to 13-90, McGraw-Hill, 1984.

## 1.0 Introduction

This workbook reviews the simulation of distillation processes using CHEMCAD software. It discusses thermodynamic model selection considerations and the basic chemical engineering relationships for vapour liquid equilibrium, mass and energy balances.

Methods are discussed for identifying azeotropes and to determine the feasibility of distillation for a given application. Simulations are developed for simple distillation and the more complex heterogeneous azeotrope distillation .

Distillation is used extensively throughout the process industries to achieve a variety of processing objectives:

- Removal of impurities / unwanted components from reaction mixes.
- Water removal and drying.
- Solvent change between reaction stages on multistage syntheses.
- Concentration prior to crystallisation.
- Heat removal control for reactions at reflux.
- Solvent recovery.

Distillation is probably the most difficult process to simulate and control because:

- Separation is a multi-variable process
- Distillation units are frequently subject to process upsets from upstream units.
- Feed conditions, temperature and vapour fraction, have a dramatic effect on performance
- Column pressure variations, likewise, affect performance
- Control loops are interactive rendering stable control impossible if incorrect selection

CHEMCAD has five basic distillation models:

BATCH	Batch distillation based on rigorous Vapor Liquid Equilibrium (VLE) or Mass Transfer models. Simultaneous correction used by SCDS or Inside-Out algorithm used by Tower are available.
SHOR	Short Cut method due to Fenske-Underwood–Gilliland for constant molar bottoms flow.
SCDS	Simultaneous correction distillation with rigorous VLE calculations, particularly suited to activity coefficient models. Applicable for steady state or dynamic models and reactive distillation.
TOWER	Rigorous VLE calculations, particularly suited to equation of state models. Uses the Inside-Out algorithm Applicable for steady state or dynamic models.
TOWER+	Rigorous VLE calculations Allows specification of pump-arounds, side strippers, and side exchangers Useful for modeling fractionating columns Uses the TOWER algorithm as basis

In addition, special modules are available which are used to maintain mass balances, satisfy reaction stoichiometry and control feed, recycle and make-up streams.

5. Component Separator enables component fractions to be split from a stream.
6. Controllers can force a Stream to copy / scale another Stream flow and composition.
7. Stream Reference can fix a recycle flow at a constant value.
8. RAMP controller can change stream parameters and switch streams on or off on a time basis.

## ***Section 9***

### ***Mass Transfer > Continuous Distillation***

In this section are listed the cases referred to in the main section.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
9.01	Minimum Boiling Point Azeotrope Finder
9.02	Maximum Boiling Point Azeotrope Finder
9.03	EtOH – Water Distillation
9.04a	Heterogeneous Azeotrope Distillation
9.04b	Heterogeneous Azeotrope Distillation

## **Section 10**

### ***Mass Transfer > Batch Distillation***

- 1.0 Introduction**
  
- 2.0 Process Characteristics**
  - 2.1 Thermodynamics
  - 2.2 Operational Constraints
  - 2.3 Mass and Energy Balances
  
- 3.0 Process Modelling**
  - 3.1 Parameter Specification
  - 3.2 General Considerations
  - 3.3 Column Testing Model
  - 3.4 Simple Batch Distillation
  
- 4.0 Dynamic Batch Distillation**

#### **Appendices**

- I Nomenclature**

#### **References**

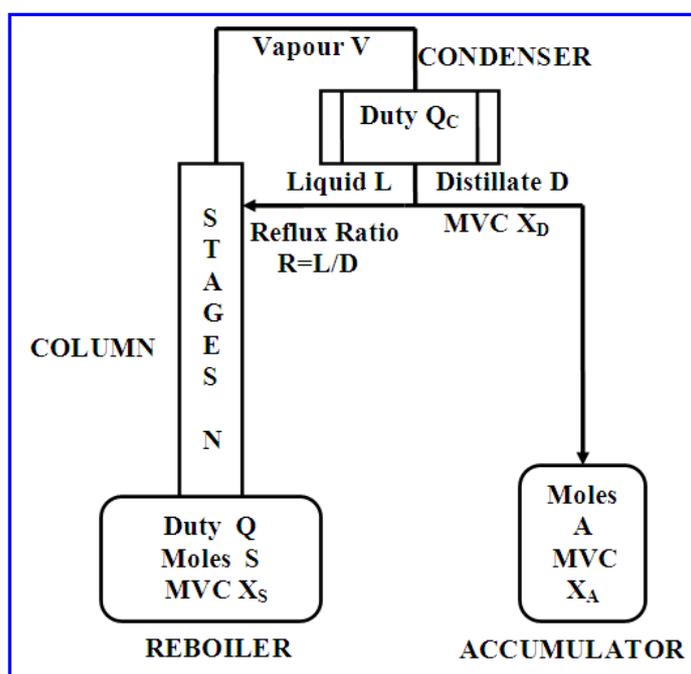
1. R.H. Perry and D. Green, "Chemical Engineers' Handbook", 6<sup>th</sup> Edition, 13-82 to 13-90, McGraw-Hill, 1984.
2. I. Smallwood, "Solvent Recovery Handbook", Edward Arnold, 1993.
3. F.G. Shinskey, "Process Control Systems", pages 484 – 489, McGraw-Hill, 1988.
4. U.M. Diwekar, "Batch Distillation", Taylor & Francis, 1996.
5. J.R. Backhurst, J.H. Harker and J.E. Porter, "Problems in Heat and Mass Transfer", pages 190 – 197, Edward Arnold, 1985.

## 1.0 Introduction

Batch distillation techniques are used extensively in the Fine Chemicals and Pharmaceutical Industries to achieve a variety of processing objectives. These include:-

- Removal of impurities/unwanted components from reaction mixes.
- Water removal and drying.
- Solvent change between reaction stages on multistage syntheses.
- Concentration prior to crystallisation.
- Heat removal control for reactions at reflux.
- Solvent recovery.

The simplest form of batch distillation involves a single separation stage (represented by the act of evaporation) which is used where a large difference in volatility exists between the components to be separated. Such a distillation does not need a fractionating column between the batch still (normally a stirred jacketed reactor) and the condenser. Simple batch distillation (sometimes referred to as pot to pot) provides only one theoretical plate of separation.



When the difference in volatility between the components to be separated is small or when operating over narrow composition ranges a rectification section is required between the still and the condenser. Overhead facilities are also required to provide control of reflux ratio and layer separation when handling heterogeneous azeotropes.

In operation the system is brought to steady state under total reflux which is taken as the start condition for simulation. Overheads are continuously withdrawn in accordance with the reflux control strategy. Cuts are taken by switching to different receivers, following a time or overhead composition strategy, at which point simulation conditions may be changed whilst starting from the current condition.

Batch distillation with rectification can be operated as follows:

- **Constant reflux ratio, varying overhead composition.**  
Distillation is continued until the desired composition is achieved in the still or the distillate receiver as required.
- **Constant overhead composition, varying reflux ratio.**  
As the distillation proceeds the still is depleted of the lighter component with the reflux ratio continually increasing. The stage is terminated at a maximum economic reflux ratio or achieving the desired still composition. This technique can be extended to a multi-component mixture.
- **Cyclical total reflux.**  
The unit is operated at total reflux until equilibrium is established and then distillate is withdrawn as total draw off for a short period of time before returning to total reflux. This technique is useful when required to separate a light end with a low overhead composition.
- **Minimum time, varying reflux ratio.**  
This provides the most cost effective mode of operation consistent with achieving the desired separation.

The distillation is normally operated at atmospheric pressure, however reduced pressure operation is sometimes required to achieve the desired separation, to reduce operating temperature for economic reasons, or when processing temperature sensitive materials.

For multipurpose operation careful consideration is required when selecting column internals to achieve acceptable column loadings and operational turndown.

The boil up rate achievable with stirred jacketed reactors is dependent upon many factors associated with heat transfer and is discussed in Section 10.

## ***Section 10***

### ***Batch Distillation > Simulation Cases***

<b>Case/File Name</b>	<b>Description</b>
10.01	Batch Distillation – No Heat Transfer
10.02	Batch Distillation with Dynamic Reactor and Column
10.03	Batch Distillation with Control System

## ***Section 11***

### ***Batch Processes > Reaction***

#### **Contents**

- 1.0 Introduction**
- 2.0 Thermal Design Fundamentals**
  - 2.1 Heat Transfer
  - 2.2 Thermal Lag
  - 2.3 Reaction Chemistry
- 3.0 Process Design Considerations**
  - 3.1 Jacket Service Fluid Selection
  - 3.2 Reactor Parameters
  - 3.3 Reactor Heat Transfer
  - 3.4 Jacket / Coil Services Heat Exchangers
- 4.0 Performance Characteristics**
  - 4.1 Jacket / Coil Services
  - 4.2 Temperature Control
  - 4.3 Jacket / Coil Services Configurations
    - 4.3.1 Direct Jacket Heat / Direct Cool
    - 4.3.2 Indirect Jacket Heat / Direct Heat
    - 4.3.3 Indirect Jacket Heat / Indirect Cool

#### **Appendices**

- I Condensed Heat Transfer Data

#### **References**

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2. J. Wilday and J. Etchells, "Workbook for Chemical Reactor Relief System Sizing", HSE Contract Research Report 136/1998.
3. J.G. Ziegler and N.B. Nichols, "Optimum Settings for Automatic Controllers", Transactions of the American Society of Mechanical Engineers, Volume 42, pages 759-768, 1942.
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## **1.0 Introduction**

Batch processes are used extensively in the manufacture of relatively small volume products with relatively high value. These processes are frequently carried out in production facilities intended for multi-purpose use.

The achievement of stable and reproducible operating conditions is important in order to achieve the required product purity, yield and cycle times to satisfy the commercial requirements and relevant regulatory authorities.

Batch processes are inherently transient in nature and the capability to demonstrate dynamically the adequacy of the equipment design and performance provides a powerful design tool. Dynamic modelling can prevent costly mistakes prior to start up. Once a process model signature has been validated against real plant performance the dynamic model can be used as a diagnostic tool to identify operating problems.

This Section reviews the basic characteristics of batch reactors and the techniques for dynamic modelling the process and control systems.

## ***Section 11***

### ***Batch Processes > Reaction > Simulation Cases***

<b>Case/File Name</b>	<b>Description</b>
11.01	Reactor Indirect Heating Direct Cooling
11.02	Reactor Indirect Heating Indirect Cooling
11.03	Reactor Jacket Circulation Hydraulics
11.04	Cryogenic Reactor System
11.05	Batch Reactor Kinetics

## ***Section 12***

### ***Environmental Emission and Control***

This section reviews the methods and correlations that are used for depicting process emissions to the environment.

All the models have been implemented using Excel and are marketed as ENVIROKIT. These models have been used extensively in the process industries since 2003 to prepare submissions to the regulatory authorities.

ENVIROKIT can be obtained by contacting the author at [jee@pidesign.co.uk](mailto:jee@pidesign.co.uk)

The models presented here are:

1. Atmospheric Dispersion from Stack
2. Fast Chemical Reaction Scrubbing
3. Stack Height Determination
4. Atmospheric Dispersion from Pools
5. VOC Emissions from Process Vessels
6. Blowdown Drum Sizing
7. Carbon Adsorber Column
8. Fugitive Emission Auditing

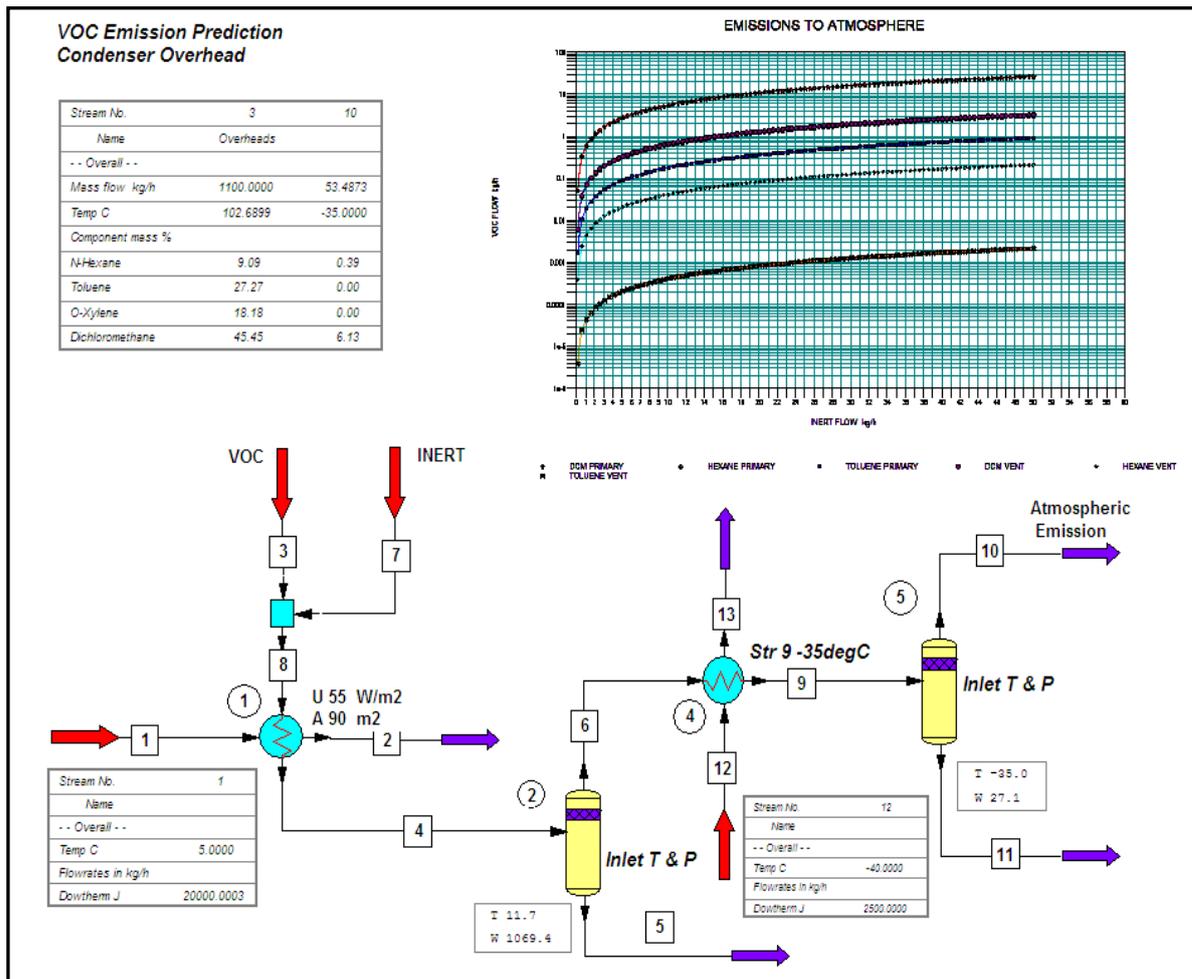
## Section 12

### Environmental Emission Control Simulation Cases

In this section are presented cases to facilitate an understanding of the CHEMCAD steady state simulation. For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

Case/File Name	Description
12.01	VOC Emission Prediction Condenser Overhead

This case models VOC emissions from a batch reactor condenser being inerted with nitrogen. A sensitivity study demonstrates that the nitrogen flow, if required at all, should be minimized.



## Section 13

# Hydrocarbon Processing

### Contents

- 1.0 Oil Refinery - Overview**
- 2.0 Thermodynamics**
  - 2.1 Global K and H Models
  - 2.2 True Boiling Point Curves
- 3.0 Crude Distillation**
  - 3.1 Process Description
  - 3.2 Simulation Considerations
  - 3.3 CHEMCAD Simulation Case Study
- 4.0 Vacuum Distillation**
- 5.0 Gas Sweetening**
  - 5.1 Process Description
  - 5.2 Simulation Considerations
  - 5.3 CHEMCAD Simulation Case Study

### Appendices

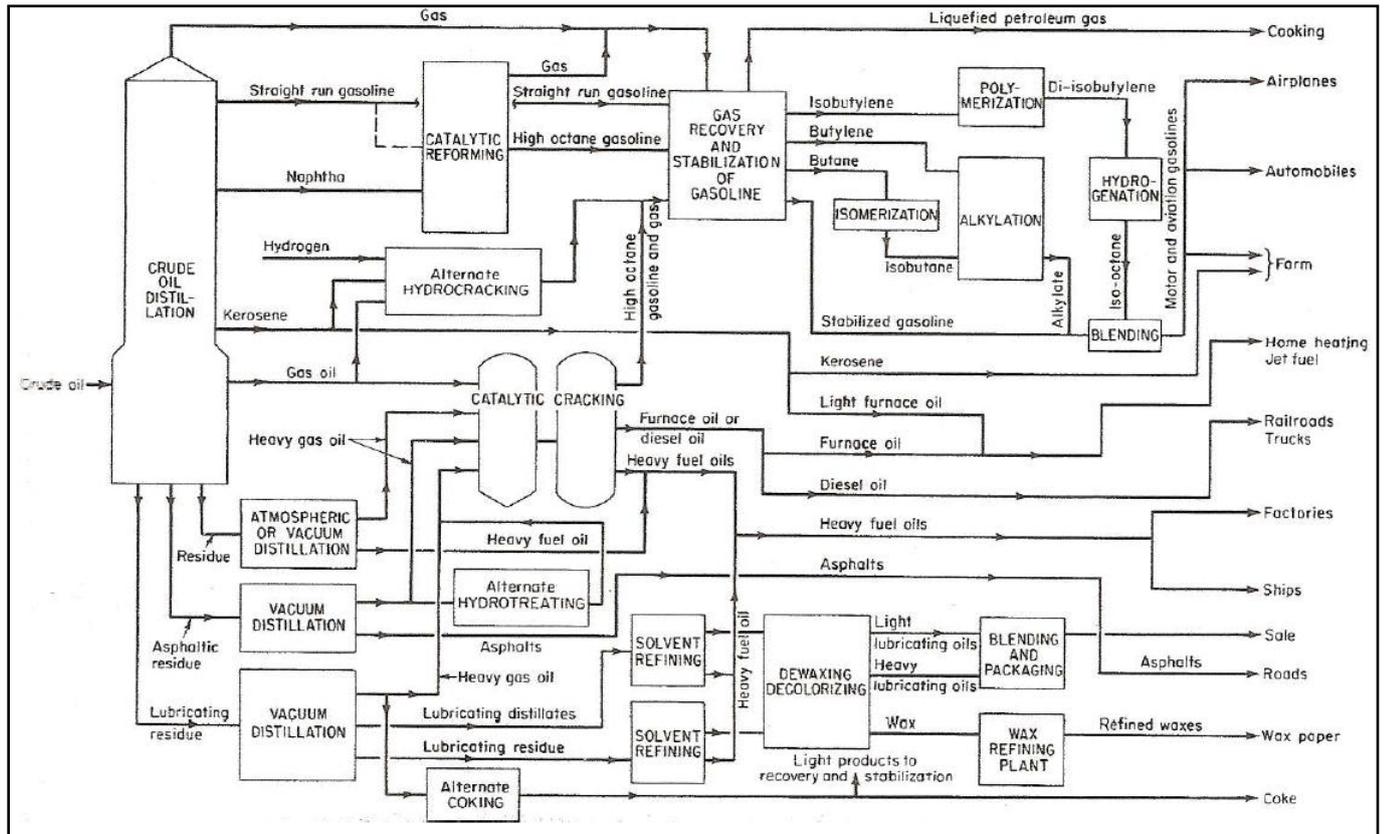
- I Petroleum Product Test Methods
- II Mass Balance Considerations
- III Column Simulation Convergence

### References

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- 3 G.A. Morris and J.Jackson, "Absorption Towers", Butterworths Scientific Publications (The British Library Reference WQ6 7604)
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- 10 G.L.Kaes, "Refinery Process Modeling", Athens Printing Company, 1<sup>st</sup> Edition, March 2000.
- 11 W.L.Nelson, "Petroleum Refinery Engineering", 4<sup>th</sup> Edition, McGraw Hill, 1958.
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## 1.0 Oil Refinery – Overview <sup>7</sup>

Most refinery products are mixtures separated on the basis of boiling point ranges. The block diagram, by API, shows the overall relationship between the refining processes and refined products.



This workbook studies the simulation of atmospheric crude distillation, vacuum distillation and sour gas amine treatment using CHEMCAD software. A basic introduction to process modelling of distillation, absorption and stripping processes is covered in the references <sup>1,2</sup>.

The applicable thermodynamics are reviewed with special reference to the generation and application of pseudocomponent curves.

Crude petroleum consists of thousands of chemical species. The main species are hydrocarbons but there are significant amounts of compounds containing nitrogen (0-0.6%), sulphur (0-6%) and oxygen (0-3.5%). The main groups are:

Aliphatics or open chain hydrocarbons

n-paraffin series or alkanes ( $C_nH_{2n+2}$ )

This series contains the largest fraction of most crudes. Most straight run (distilled directly from the crude) gasolines are predominately n-paraffins. The light ends primarily consist of propane ( $C_3H_8$ ), n-butane ( $C_4H_{10}$ ) together with water which are defined as pure components.

iso-paraffin series or iso-alkanes ( $C_nH_{2n+2}$ )

i-butane ( $C_4H_{10}$ ) is present in the light ends but these compounds are mainly formed by catalytic reforming, alkylation or polymerization.

Olefin or alkene series ( $C_nH_{2n}$ )

This series is generally absent from crudes and are formed by cracking (making smaller molecules from larger molecules). They tend to polymerize and oxidize making them useful in forming ethylene, propylene and butylene.

## Ring compounds

### Naphthene series or cycloalkanes ( $C_nH_{2n}$ )

These compounds are the second most abundant series of compounds in most crudes. The lower members of this group are good fuels and the higher members are predominant in gas oil and lubricating oils separated from all types of crude.

### Aromatic series

Only small amounts of this series occur in most common crudes but have high antiknock value and stability. Many aromatics are formed by refining processes including benzene, toluene, ethyl benzene and xylene.

### Lesser Components

Sulfur has several undesirable effects including its poisonous properties, objectionable odour, corrosion, and air pollution. Sulfur compounds are removed and frequently recovered as elemental sulfur in the Klaus process.

Nitrogen compounds cause fewer problems and are frequently ignored.

Trace metals including Fe, Mo, Na, Ni and V are strong catalyst poisons and cause problems with the catalytic cracking and finishing processes and methods are used to eliminate them.

Salt, which is present normally as an emulsion in most crudes, is removed to prevent corrosion. Mechanical or electrical desalting is preliminary to most crude processing.

Atmospheric and vacuum distillation produce the different fractions as detailed in the table below.

Crude Petroleum Fractional Distillation							
Temperature	<30°C	40-70 °C	70-120°C	120-150 °C	150-300 °C	>350 °C	Residue
Description	Gaseous Hydrocarbon	Gas oil	Naptha	Benzene	Kerosene	Heavy oils	Asphalt or Bitumen
Density		0.65	0.72	0.76	0.8		
~Composition	$C_3H_8$ , $C_4H_{10}$	$C_5H_{12}$ , $C_6H_{14}$	$C_6H_{14}$ , $C_7H_{16}$ $C_8H_{18}$	$C_8H_{18}$ , $C_9H_{20}$	$C_{10}H_{22}$ , $C_{11}H_{24}$ $C_{12}H_{26}$ to $C_{18}H_{36}$	$C_{18}H_{38}$ to $C_{28}H_{58}$	
Applications	Gas fuel or enrichment	General solvent, aviation spirit	Solvent for oils, fats & varnishes	Solvent for oils, fats & varnishes	Home heating Jet fuel	Diesel, fuel oils	Roads, Wax paper
		Gasoline, contains $C_6H_{14}$ , $C_7H_{16}$ , $C_8H_{18}$				40-180 °C	

Further fractionation of the 70 to 150°C cut is required to obtain the naptha and benzene cuts.

Vacuum distillation of the topped crude is required to obtain Light Vacuum Gas Oil(LGVO) and Heavy Vacuum Gas Oil(HVGO)

When the difference in volatility between components is small a solvent of low volatility is added to depress the volatility of one of the components. This process is known as extractive distillation. Butenes are separated from butanes using this method with furfural as the extractant.

When a high volatility entrainer is used the process is known as azeotropic distillation. Anhydrous alcohol is formed from 95% aqueous solution using benzene to free the azeotrope and high purity toluene is separated using methyl ethyl ketone as the entrainer.

## ***Section 13***

### ***Hydrocarbon Processing Simulation Cases***

In this section are listed the cases referred to in the main section.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
13.01	Crude Unit Distillation
13.02	Vacuum Distillation
13.03	Gas Sweetening

## Section 14

# Carbon Capture and Storage

### Contents

- 1 Introduction
- 2 Thermodynamics
- 3 Pre-combustion SELEXOL<sup>®</sup> Process
- 4 Post-combustion Flue Gas Desulfurization
- 5 Post-combustion Carbon Capture
- 6 CO<sub>2</sub> Compression and Transport

### Appendices

- I General Process Data
- II Physical Property Data – Selexol and Genosorb
- III Physical Property Data – MEA, DEA and MDEA
- IV Physical Property Data - Carbon Dioxide
- V Heuristics for Process Equipment Design

### Acknowledgements

The author would like to acknowledge the support of Mott MacDonald, (Brighton, UK) in the preparation of this section

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## Links

- L1 <http://www.co2captureandstorage.info/>  
IEA data
- L2 <http://www.netl.doe.gov/technologies/index.html>  
DOE reports
- L3 [http://www.amines.com/mdea\\_comp.htm](http://www.amines.com/mdea_comp.htm)  
Amine data
- L4 <http://www.ieagreen.org.uk/reports.html>  
IEA reports
- L5 <http://www.glymes.com/businesses/glymes/internet.nsf/directname/home>  
Clariant data
- L6 [http://www.co2captureandstorage.info/networks/capture\\_workshops.htm](http://www.co2captureandstorage.info/networks/capture_workshops.htm)  
Networks
- L7 <http://www.netl.doe.gov/publications/>  
DOE conferences
- L8 <http://www.gasification.org/Docs/Workshops/2007/Indianapolis/03Ciferno%20Pre%20and%20Post%20Combustion%20CO2%20Capture%20Summary.pdf>
- NETL Data
- L9 <http://www.dow.com/gastreating/solution/index.htm>  
Dow data source
- L10 <http://www.co2storage.org.uk/>  
Storage issues
- L11 <http://www.rite.or.jp/English/lab/chemical/090622results-e/csiro2009-e.pdf>  
CSRIO and RITE Symposium, May 2009, Amines for Post-combustion Carbon Capture
- L12 [http://www.dow.com/gastreating/solution/pa\\_ascor.htm](http://www.dow.com/gastreating/solution/pa_ascor.htm)

## 1.0 Introduction<sup>1, L 2</sup>

The worldwide focus on clean power generation and carbon capture has increased the importance of the associated technologies, which involve two distinct approaches, namely pre-combustion and post-combustion carbon capture.

In pre-combustion CO<sub>2</sub> capture, fuel is gasified by applying heat under pressure in the presence of steam and air and/or oxygen to form synthetic gas (Syngas). CO<sub>2</sub> is then captured from the Syngas, before being mixed with air in a combustion turbine, resulting in the CO<sub>2</sub> being relatively concentrated and at a high pressure.

In post-combustion CO<sub>2</sub> capture, mainly, pulverized coal is burnt in air to raise steam. CO<sub>2</sub> is exhausted in the flue gas at atmospheric pressure and concentrations of 10-15% v/v. This process is more challenging due to the low pressure and dilute CO<sub>2</sub> concentration resulting in a high volume of gas having to be treated. Also trace impurities in the flue gas tend to reduce the effectiveness of the CO<sub>2</sub> absorbing processes and compressing the captured CO<sub>2</sub> from atmospheric pressure to pipeline pressure represents a large parasitic load.

Another post-combustion capture technology, oxy-combustion, involves combustion of the fuel with near pure oxygen resulting in a flue gas stream of higher CO<sub>2</sub> concentration. This technology relates more to combustion, and is not discussed further in this paper.

When CO<sub>2</sub> is captured, power station generating efficiency is significantly reduced. Therefore a power cycle with a high thermal efficiency is essential to ensure an acceptable outcome. Power cycle efficiency is continually being improved by increasing the steam temperature and pressure; this development is limited by the availability of suitable alloys.

Operation	Year	Pressure	Temperature	Efficiency
		bar	°C	%
Subcritical	1960 - 1970	166	540	38 to 42
Supercritical	1970 - 1990	240	566	44
Ultra supercritical	1990 - present	310	600	49

Ultra supercritical (USC), once through utility (OTU) operation is considered to be the best option for "Clean Coal Technology". USC operation reduces the CO<sub>2</sub> emissions and therefore improves the economics of carbon capture and sequestration (CCS).

Pre-combustion and post-combustion CCS methods are similar, in that both require significant power for blowers, pumps and compressors. Studies are indicating parasitic power in the range 15 to 25% with the technology, plant layout, pressure drop, compressor operation, transportation and sequestration configurations each having a significant affect. Crucial to CCS economics is the optimization of the heat integration circuits and the minimization of CO<sub>2</sub> stripping steam to reduce the impact on power plant parasitic power.

CO<sub>2</sub> is present at much higher concentrations in Syngas than in post-combustion flue gas, so CO<sub>2</sub> capture should be less expensive for pre-combustion than for post-combustion capture. However, there are few gasification plants in full-scale operation, and capital costs are higher than for conventional pulverized coal plants.

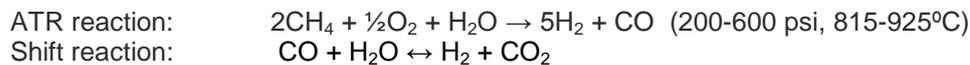
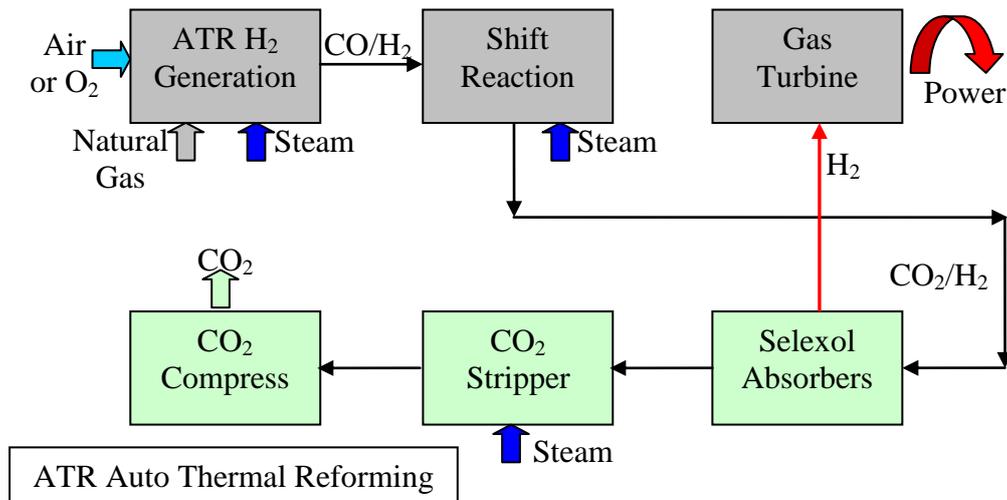
Process simulators are playing an increasingly important role in finding the optimum economic solutions. CHEMCAD is being used in modeling pre-combustion and post-combustion processes and has developed thermodynamics specifically for the pre-combustion and compression technologies.

## Pre-combustion Carbon Capture

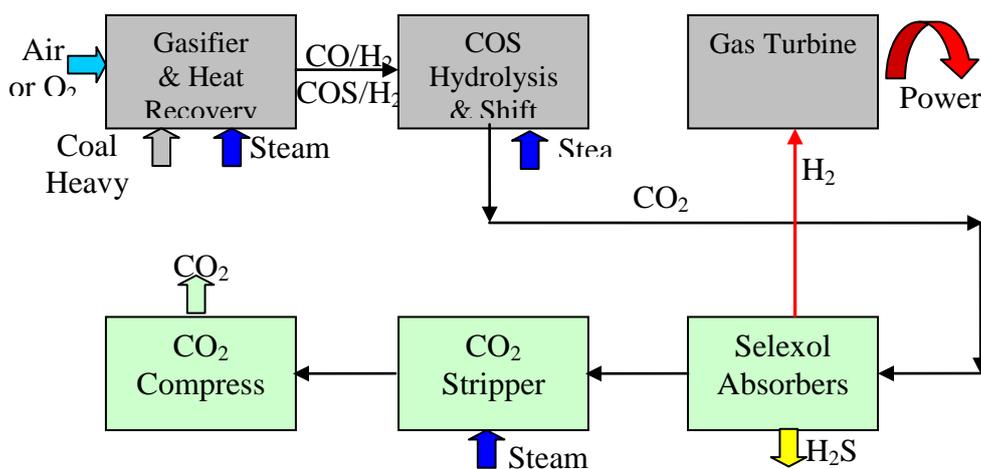
In pre-combustion CC, the fuel will be either natural gas or gasified hydrocarbon feedstock. If natural gas, it is converted into CO and H<sub>2</sub> by auto thermal reforming (ATR) and then CO is converted into CO<sub>2</sub> by the shift reaction. If hydrocarbon (coal or heavy oil), it is gasified in the presence of steam and air or oxygen at a high temperature and pressure, followed by the shift reaction to form CO<sub>2</sub>, H<sub>2</sub>, COS and other gaseous compounds, depending on the hydrocarbon make-up. Appendix I

A key part of this technology is the removal of CO<sub>2</sub> and H<sub>2</sub>S (if present) from the Syngas by absorption in a physical solvent. The captured CO<sub>2</sub> can then be processed or compressed and sequestered in a suitable reservoir. Proven technology includes the Selexol<sup>®</sup> process that uses a solvent, which is a mixture of dimethyl ethers of polyethylene glycol. Dow Chemical Company retains the gas processing expertise, which is offered under license. Clariant GmbH offer an equivalent solvent, available from their Genosorb range. Appendix II

### Syngas Plant Combined Cycle with Carbon Capture



### Integrated Gasification Combined Cycle(IGCC) with Carbon Capture

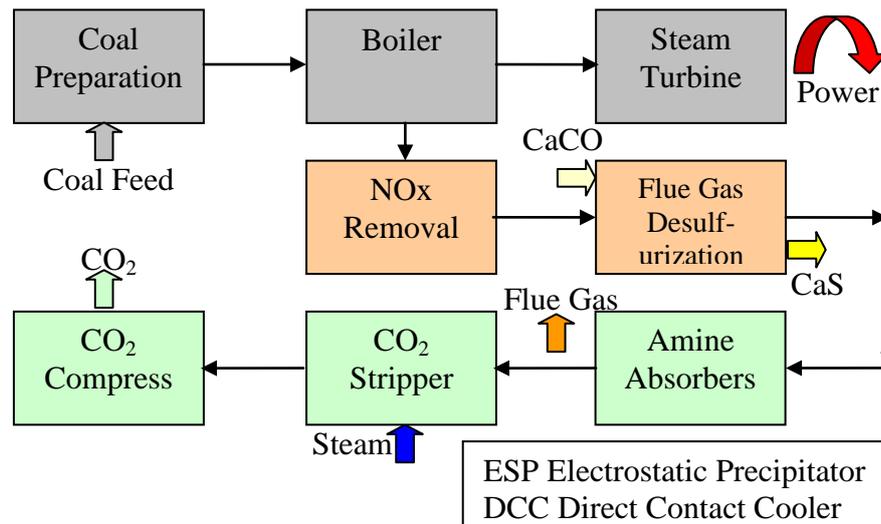


## Post-combustion Carbon Capture

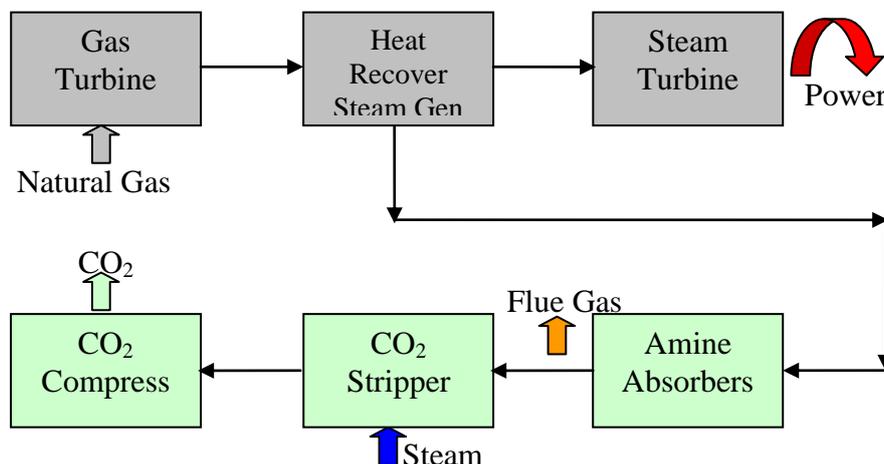
The typical fuel is either natural gas or pulverized coal. <sup>Appendix I</sup> When natural gas, it is combusted in a gas turbine and when coal it is combusted in a steam boiler. Alternative fuels, such as biomass and wood chippings, are now starting to be used.

Key parts of this technology are Flue Gas Desulphurisation (FGD) to remove SO<sub>2</sub>(if present) by spray scrubbing with limestone, particulate removal by Electrostatic Precipitator (ESP), direct contact cooling (DCC) with circulating water and reactive absorption of CO<sub>2</sub> using inhibited amine blends. <sup>Appendix III</sup> The captured CO<sub>2</sub> is then desorbed from the rich amine by steam stripping and then compressed for transfer and sequestration in a suitable reservoir.

### *Pulverised Coal Fired with Carbon Capture*



### *Natural Gas Fired Combined Cycle with Carbon Capture*



A CCGT set has a gas turbine-generator, a waste heat boiler followed by a steam turbine-generator. The combined cycle power plant (CCPP) fuel is usually natural gas, although fuel oil or Syngas are being used. The CCPP can have single-shaft or multi-shaft configurations. The single-shaft has one gas turbine, one steam turbine, one generator and one Heat Recovery Steam Generator (HRSG). The multi-shaft has one or more gas turbine-generators and HRSG's that supply steam to a separate single steam turbine-generator.

## ***Section 14***

### ***Carbon Capture and Storage Simulation Cases***

In this section are listed the cases referred to in the main section.

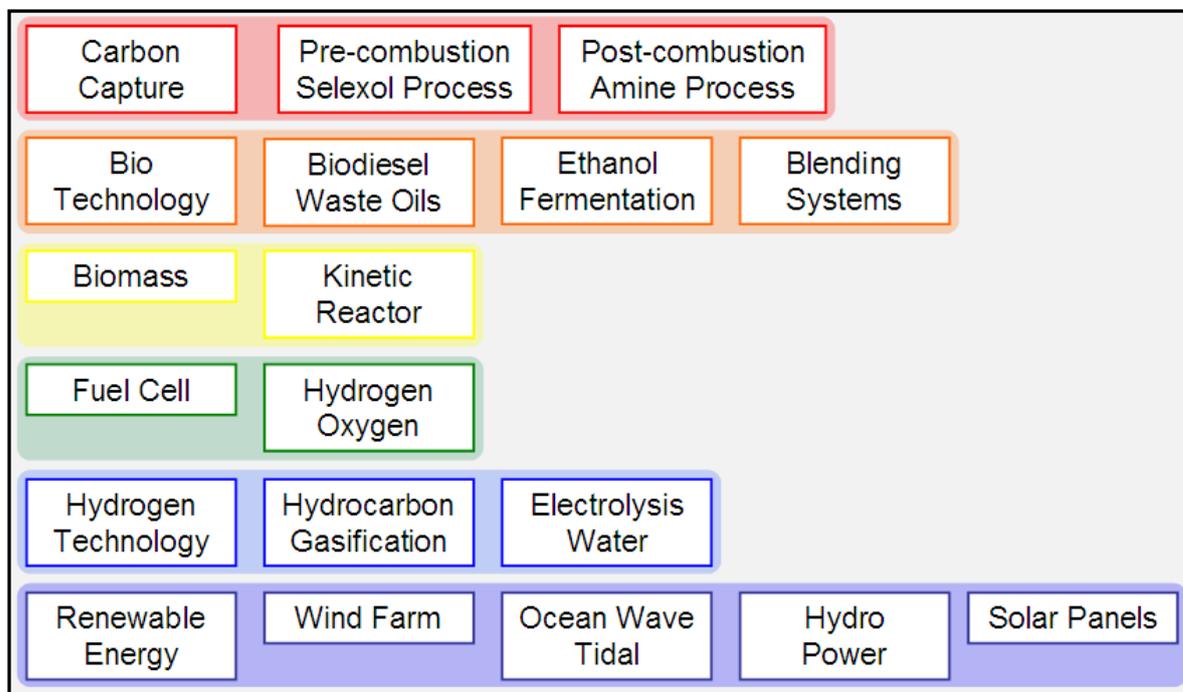
For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
14.01	Pre-combustion Selexol Multiple Flash Regeneration
14.02	Pre-combustion Selexol Combined Flash and Thermal Regeneration
14.03	Pre-combustion Selexol Selective H <sub>2</sub> S and CO <sub>2</sub> Removal
14.04	Post-combustion Flue Gas Desulfurization
14.05	Post-combustion Amine Absorption and Stripping
14.06	CO <sub>2</sub> Compression and Transport

## Section 15

### Emerging Markets

The process industry is continually evolving to encompass a diverse range of activities in what can be referred to as emerging markets. Process simulation is proving to be an important element in the development and optimization of the processes involved. The scope of this variety is shown in the following chart.



Process simulators are being used extensively in all the above areas, with the exception of the renewable energy sector.

The economic and scale up challenges in the Carbon Capture sector are already being studied with, to date, only relatively small demonstration units being operated. However these units are enabling simulations to be validated to provide greater confidence when scaling up to full scale plants. Post-combustion carbon capture provides the biggest challenge because industrial experience with CO<sub>2</sub> absorption and desorption with amine based solvents is at elevated pressure whereas this application is at around atmospheric pressure. The previous Section 14 has considered some of these issues.

For biodiesel production there are three basic methods available, namely:

- Base catalyzed transesterification
- Acid catalyzed esterification
- Enzymatic catalysis.

Each reaction has associated optimal operating parameters (T & P) and conversion, although much of the available literature emphasizes the base catalyzed route because it is claimed to be the most economical.

The reaction progresses in three reversible steps

- Triglyceride reacts with the alcohol to form a diglyceride and a fatty acid ester,
- Diglyceride reacts with the alcohol to form a monoglyceride and a fatty acid ester
- Monoglyceride reacts with the alcohol to form glycerin and a fatty acid ester.

## ***Section 15***

### ***Emerging Markets Simulation Cases***

In this section are cases are shown indicating the wide range of applications that can be simulated.

For practice you can build the models or use the models provided as downloads from electronic media available. It is strongly recommended that you work with a copy of the jobs.

<b>Case/File Name</b>	<b>Description</b>
15.01	Base Catalyzed Biodiesel Process
15.02	Hexane Extraction Biodiesel Process
15.03	Hydrogen Oxygen Fuel Cell
15.04	Hydrogen Production by Electrolysis

## ***Section 16***

# ***General Engineering Data***

### **Contents**

- 1 Dished End Dimensions
- 2 Commercial Steel Pipe Dimensions
- 3 Stainless Steel Pipe Dimensions

### **Reference**

Crane Co., "Flow of Fluids Through Valves, Fittings, and Pipes", Technical Paper No. 410, 1991.