PROCESS SIMULATION

DYNAMIC MODELLING & CONTROL

Design, Implementation and Operation

SAMPLER VERSION

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Preface

This manual is based on experience gained by the process and control engineers at P & I Design Ltd, with the full support from Chemstations simulation engineers based in Houston. This experience is based on design and implementation, involving a wide range of projects, in the process fields, including both batch and continuous process plant and terminal storage facilities.

The manual is intended as an introduction to the principles of dynamic simulation. Process simulations are carried out using CHEMCAD™ software by Chemstations, Inc. of Houston. Applications are presented from real situations involving design, testing or operations.

The engineering fundamentals section has been included, as a refresher, to provide a concise and clear presentation of the relevant applied maths and basic fluid flow principles.

Reference is made to many classic texts, industry standards and manufacturers’ data. Information has been mined from individual project reports, technical papers and contributions by specialists working in the instrumentation and control field.

There is a heavy emphasis on the principles of measurement and control as it is considered that a detailed appreciation of this topic is essential for the successful implementation of dynamic simulation. This topic has been covered in Section 3 Process Measurement and Control of the book “Chemical Engineering in Practice” by J.E.Edwards. Some additional principles and features have been considered here.

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 nomenclature being section specific. The references are not a comprehensive list and apologies for unintended omissions.

The Author

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John E.Edwards is the Process Simulation Specialist at P&I Design Ltd based in Teesside, UK. In 1978 he formed P&I Design Ltd to provide a service to the Process and Instrumentation fields. He has over fifty years experience gained whilst working in the process, instrumentation and control system fields.

Acknowledgements

A special thanks to my colleagues at Chemstations, Houston, who have always given support in my process simulation work and the preparation of the articles that make up this book: N.Massey, Ming der Lu, S.Brown, D.Hill, A.Herrick, F.Justice and W.Schmidt, Germany
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. This manual provides a comprehensive review of the fundamentals, definitions and engineering principles for the study of processes encountered in normal practice using dynamic simulation techniques.

Simulators provide process control engineers with a powerful tool to assist in the design, optimisation and operation of processes. Prior to the introduction of process simulators, this activity involved a team of engineers working many man hours and maybe not achieving a definitive result. 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.

Mass and Energy Balances

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 satisfying the mass and energy balances.

The law of conservation of mass, which states that mass can neither be created nor 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 from the time feed is charged and product is removed and for a continuous process inputs and outputs flow continuously. A semi-batch process combines both characteristics.

A distillation unit at steady state must satisfy the overall material balance for each component. Only one product stream can be set independently making the other product stream a dependent variable. If the distillate flow is manipulated, directly or through varying reflux ratio, the bottom outlet flow must be adjusted to maintain the material balance 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 impose 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 First Law of Thermodynamics states energy cannot be created or destroyed. 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, where subscript $H$ refers to stream enthalpy, yields:

$$Q_r + F_n = D_n + B_n + \text{losses}$$

The process design objective is always to minimize the use of energy consistent with achieving the desired product quantity and quality. In this case reflux ratio must be kept to a minimum, subject to satisfying the requirements for the desired separation specification, to optimise the heat input.

For an absorber the gas inlet stream condition and the liquid inlet composition are determined by the upstream process. The liquid flow rate is the only variable to adjust for 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 $G_S$.

$$Y = \frac{y}{1-y} = \frac{p}{p_t-p}$$

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:

$$X = \frac{x}{1-x}$$

Since the inert gas $G_S$ and solvent liquid $L_S$ remain essentially unchanged in the tower giving:

$$G_S(Y_1-Y_2) = L_S(X_1-X_2)$$

The composition of both product streams is dependent on $L/G$. 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.
Simulators

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

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 and composition change, can all be studied. Dynamic simulators can also be used for operational plant troubleshooting, control loop tuning and real time optimisation. Dynamic simulations require more information and are more difficult to set up.

The iterative process can be based on the following Convergence Parameters:

Direct substitution, the value is recalculated each iteration

Wegstein acceleration, the value is recalculated after three iterations, speed up frequency 3

Dominant Eigenvalue (DEM), the value is recalculated after three iterations, speed up frequency 4

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

The Calculation Sequence default mode is Sequential Modular, which starts with the first feed on the left and follows the sequence of streams and the Unit operations are run sequentially.

Simultaneous modular mode uses linear algebra to solve sections of the flowsheet simultaneously.

Complex flowsheets involving distillation, recycle loops and controllers may converge faster in this mode. Pressure Nodes require this calculation mode.

Steady state and dynamic process simulation proves the capability to achieve stable and reproducible operating conditions with acceptable product purity, yield and cycle times to satisfy the commercial requirements and the safety and environmental issues for the regulatory authorities.

In summary dynamic simulation allows for the study and identification of the following:

Dynamic pipe networks and emergency relief
Dynamic vessel and agitated batch reactor
Dynamic distillation column
Control system performance and tuning optimization
Equipment failure and hazardous operating conditions
Simulation Procedure

The chart below shows the basic steps involved in setting up a steady simulation.

The steady state mode is used to set up the initial state prior to initiating the dynamic mode. The basic steps in performing a dynamic simulation are shown below:

Create the flowsheet incorporating dynamic unit operations - select components and thermodynamic method - enter feed stream and equipment specifications.

Determine the initial state for a dynamic simulation which involves calculating the flowsheet in steady state and adjusting several parameters - sizing equipment such as control valves, tank geometry and hydraulics of distillation columns.

Set dynamic run parameters such as simulation time, simulation step size, defining Unit Op and stream parameters to be recorded.

Run the simulation in dynamic mode and test control parameter settings. Run time and step size must be selected to ensure consistency with real time behavior. Under “Run – Convergence” the Run One Time Step feature allows study of model behavior.

Interpret the results and optimize the model.
Section 2

Dynamic Simulation Basics

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<th>Description</th>
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<td>D2.02</td>
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<td>D2.03</td>
<td>Indirect Flow Divider 2</td>
</tr>
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2.1 Introduction

The correct sizing and application of control valves is essential for successful dynamic simulations. An incorrectly sized valve will result in dynamic model convergence problems and an unstable condition in the model.

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

- It requires inlet pressure \(P_i\) and outlet pressure \(P_o\) to be specified where \(P_i\) is taken from the inlet stream. \(P_o\) can be specified directly or overwritten indirectly by an assigned UnitOp in the model. A mass balance must be maintained around the control valve. This is achieved by the control valve calculated flow, based on the flowing conditions and pressure drop across the valve, being positioned in the flow sheet correctly or transferred to an upstream UnitOp using the Optional mass flow rate transfer facility. The position rules are summarised:

1. Immediately after a Feed Arrow (Direct Flow Regulation)
2. After a Stream Reference (SREF)
3. Divider (DIVI) (Indirect Flow Regulation)
4. Dynamic Vessel (Indirect Flow Regulation)
5. Dynamic Reactor (Indirect Flow Regulation)
6. Dynamic Column (Indirect Flow Regulation)

The control valve is discussed in more detail in Section 3. For the purposes of this introduction the control valve sizing flow coefficient \(C_v\) is determined using the Equipment Valve Sizing option which will provide a value for the stated stream conditions.

It should be noted that the CHEMCAD valve data base smallest valve \(C_v\) is 9.0. Smaller valve coefficients are determined by separate calculation which can be entered directly or linked to the model using the Excel Data Map facility.

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

If the controller input goes out of the calibrated range the control output continues to change resulting in unreal conditions.

The control valve can be operated in various operating modes which enable the simulations to be forced to start up, shutdown, abnormal and failure conditions. These features also allow control valve positions to be set manually or automatically from an assigned controller.
Case D2.01 Direct Flowrate Regulation

It is assumed that you know how to build a flowsheet and define a job as for a steady state simulation.

The objective is to explain settings of Control Valve (CVAL) and Ramp schedule (RAMP) and a simple dynamic simulation.

Design process flow conditions are 25000kg/h water at 20°C and 3 barg.

The control valve is sized using a downstream pressure of 2 barg.

A schedule is set for the valve position and the flowrate profile over time is monitored using different valve flow characteristics.

Flowsheet

The basis for your simulation is the flowsheet diagram which connects all equipment models using streams to transfer material from one UnitOp to another UnitOp.

Set Engineering Units

Format Menu → Engineering Units → Alt SI → Save Default

All newly created jobs will now use “Alt SI” Engineering Units until you change the system of units again.

Go to Options and References and set the vapour reference temperature and pressure to required standard. The default references for temperature units in °F or °R is 60°F and when in °C is 0°C and for pressure is 14.696 psia or 1.01325 bar.

Select Components and Define Thermodynamics

1. Thermophysical → Select Components

Components searches can be done on the basis of word strings, molecular formula, CAS number or CHEMCAD component number. If word string does not locate your component select Next to go to a higher component in the list, e.g. methanol to ethanol.

Select Water in “Search” field.

Click Add button or press [Enter] key. Click OK button.

2. Thermophysical → Thermodynamic Settings → Define K and H values

Select the Global K and H options. Note that Global applies to all UnitOps in the flowsheet. Some flowsheets will require individual UnitOps to have their own K and H values set using the “Set local thermodynamics” option.

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<td>Latent Heat</td>
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Specify Inlet Stream

It is required to size the control valve to pass 25000 kg/h of water at a pressure drop of 1 bar. Specify the Inlet Stream 1 as follows:

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<th>Parameter</th>
<th>Value</th>
<th>Units</th>
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<tr>
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<td>20</td>
<td>°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>4</td>
<td>bara</td>
</tr>
<tr>
<td>Flowrate</td>
<td>25000</td>
<td>kg/h</td>
</tr>
<tr>
<td>Composition</td>
<td>Water</td>
<td>wf 1.0</td>
</tr>
</tbody>
</table>

Right-click Stream 1 and select Edit Stream from drop down menu

Enter the following and click OK

Control Valve Sizing

Sizing results can be displayed in Word or Excel.

Go to Tools → Options → Preferences → Report Viewer and select Excel which allows data to be manipulated if required.

Select Sizing → Control Valve from main menu. If Stream 1 has been selected, you will see a dialog box as shown below. If the stream has not been selected then select the desired stream. Enter 3 bar as the downstream pressure and click OK.
Case D2.02 Indirect Flow Regulation

When CVAL is located within a flowsheet, it has to be able to pass its calculated flow, determined from fluid state, valve size, pressure drop, characteristic, and position, to a suitable UnitOp to control the flow. American football (or Rugby) is a good analogy with the Control Valve, as the passer and the Divider, as the receiver.

The process stream flow is 50000 kg/h water at 15°C and 4 barg. This flowsheet is the arrangement for simulating a 3-way diverting control valve.

The control valve passes its calculated flow to Divider UnitOp 1 resulting in the remaining flow splitting to Stream 3. The linear control valve $C_v = 75$ is obtained from using the sizing option with a downstream pressure of 4 bar. The operating mode is “Fix flow rate adjust valve position” and the rangeability is set at 10. The UnitOps are configured as shown:

A common problem with this combination is for the control valve to be oversized resulting in its calculated value being greater than the Divider stream inlet flow. An error warning will appear at the end of the Run. This could have been the result of a transient condition and may have no effect on the simulation result but should be avoided if possible.
The controller UnitOp 3 is configured as shown:

![PID Controller Image]

A detailed review of Process Control principles is covered in Section 3. The key points for configuring a controller and control valve combination are:

**Measurement**
The measurement from process is normally a 4 to 20 mA dc signal representing the calibrated range of process variable with 4 mA = 0 kg/h (use 1E-06, never use 0) and 20 mA = 50000 kg/h.
Elevated ranges can be used 4 mA = 10000 kg/h or suppressed zero ranges e.g. 4 mA = -50ºC.
The measurement and its units are defined in the Measured Object. The measurement function, on modern systems, is normally linear as any signal conditioning is carried out elsewhere.

**Controller**
The set point value is the desired process value in the measurement units specified.
The controller action defines the controller output (OP) response to Set Point (SP) ± Measurement (MV) errors. For Reverse Action: If MV > SP the OP decreases and if MV < SP the OP increases. For Direct Action: If MV > SP the OP increases and if MV < SP the OP decreases.
Incorrect selection will result in Positive Feedback with MV continually increasing or decreasing.

**Control Valve**
The control valve failure action is determined by the process e.g. heating valve fail closed and cooling valve fail 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). An incorrect match of controller action and valve action gives positive feedback.

**Controller Tuning**
Tuning parameters for noisy control loops as shown here e.g. liquid flow, liquid pressure and level use wide proportional bands (PB%) as controller gain is 100/PB and rely on short Integral Times to drive MV to SP. Never use Derivative on noisy signals as it operates on rate of change of error.

![Indirect Flow Regulation Stream Divert Control Graph]
3.1 Fundamentals
3.2 Orifice Plate Flowmeters
3.3 Control Valves
3.4 Control Valve Actuators
3.5 Control Valve and Actuator Construction
3.6 Control Valve CHEMCAD Calibration

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References
3.1 Fundamentals

In 1967 Shinskey presented a novel approach to the understanding of process characteristics and the associated control systems by studying the problem in the time domain and the application of basic mass and energy balances.

The basic principle of control system design is to achieve mass and energy balances regardless of the process. Control loop interaction should be avoided or at the best minimised for stable control.

Each process parameter exhibits unique properties that determine the control strategy to be applied.

Flow and liquid pressure periods are fast and noisy with no dead time, requiring a low gain response with reset adjustment to maintain a desired value.

Gas pressure exhibits a high capacity with no dead time, requiring a high gain response which is adequate to maintain a desired value. This is considered to be the easiest parameter to control.

Liquid level period can be fast or slow and sometimes noisy (boiling) with capacity, requiring medium gain and sometimes with reset adjustment to maintain a desired value.

Temperature period can be medium or slow with capacity and dead time, requiring variable gain, reset adjustment and anticipatory response.

Control systems should not be used to overcome shortcomings in plant design. To avoid this, the process plant design and the control philosophy should be considered throughout the design process. For example, if a processing unit takes a long time to achieve stable and optimal operating conditions the feeds should be held constant by the use of surge tanks in which the level is allowed to float between acceptable limits.

Processes can be batch, semi-continuous or continuous with the selection depending on many factors. Batch processes are used in the manufacture of a wide variety of fine and speciality chemicals and are inherently transient in nature and as such can present unique control problems.

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 settings Proportional, Integral and Derivative (PID). The output signal is connected to a regulating device, such as a control valve or variable speed drive. A typical single loop is shown:

![Single Loop Control Diagram]

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

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 and 20 mA = 50000 kg/h. An elevated zero can be used where 4 mA = 10000 kg/h or a suppressed zero 4 mA = -50°C.
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 are Length and for mass flow is Mole/Mass.

The controller set point value is the desired process value in the same units as specified for the measurement. Controller Action determines the controller output (OP) in response to the error between Set Point (SP) ± Measured Variable (MV). Negative feedback control is required which behaves as follows:

For Reverse Action: If MV > SP the OP ↓ and if MV < SP the OP ↑
For Direct Action: If MV > SP the OP ↑ and if MV < SP the OP ↓

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

Control Valve failure action is determined by the process e.g. a heating valve usually fails closed and a 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). An incorrect match of controller action and valve action will result in Positive Feedback.

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. In this case, short Integral Action Times (T_i) are used to eliminate SP±MV error. Derivative is never used on noisy signals as T_d operates on rate of change of error de/dt where rapid changes in error will result in large rapid changes in controller output leading to control valve slamming and damage.

Single loop control systems have limited application with more advanced systems requiring multiple loop configurations. The more common of these multiple loop systems are shown below:

Heating and cooling valves are frequently used in split range such that the cooling valve is fully open at 0% controller output and the heating valve is fully open at 100% controller output. Split range control valve operation and function is discussed in more detail in Section 5.
**Cascade Control**

The output of one controller, the primary or master, manipulates the set point of another controller, the secondary or slave. Each controller has a separate measurement and the secondary controller manipulates the control device. The principle advantages of this configuration are:

Process upsets in the secondary loop are corrected before they can influence the primary measurement and lags existing in the secondary loop are reduced, improving speed of response. Also the secondary loop provides exact manipulation of the mass or energy balance by the primary controller.

The secondary loop process variable must respond faster than the primary loop process variable. The simplest example of a cascade loop is a control valve fitted with a positioner.

A temperature loop is frequently cascaded to a flow loop. In this case the flow measurement must be linearised by square root extraction, if required, to provide acceptable control.

Liquid level loop can only be cascaded to flow loop involving boiling or condensing processes. Steam boiler drum three element level control in which the boiler feedwater flow set point is set equal to the steam flow and the level controller trims the boiler feedwater flow controller in cascade to maintain a material balance is shown:

\[ W_F = W_S + m_L + 0.5 \]

A primary temperature loop, with dead time and slow response is frequently cascaded to a faster acting temperature loop installed on the utility system. An example of this is a batch reactor contents temperature cascaded to either the jacket inlet or outlet temperature as shown below:

---

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Ratio Control

Ratio control is frequently used in ingredient control where any number of streams can be set in ratio to one independent stream which is set according to production requirements. This type of system is used in gasoline blending, bio-fuel additive control and composition control in many industries. The diagram shows two additives being mixed with a single independent stream, note that the flow signals from orifice plate applications have been linearised.

Consider a biodiesel methyl ester (ME) additive blending system.

\[ \frac{D}{E} = \frac{D_E + E}{V} \]

Where:
- \( D_E \): Diesel in Methyl Ester Flow (m³/h)
- \( E \): Methyl Ester Flow (m³/h)
- \( V \): Methyl Ester Volume Fraction
- \( D_S \): Diesel Flow from Ship (m³/h)
- \( V_P \): Bio-diesel Product Volume Fraction

We have:
\[ V_E = \frac{E}{E + D_E} \quad \text{and} \quad V_P = \frac{E}{E + D_E + D_S} \]

Rearranging gives:
\[ D_E = \frac{E \left( 1 - V_E \right)}{V} \quad \text{and substituting for } D_E \quad \text{leads to the following:} \]
\[ E = \frac{V_P D_S}{\left( 1 - V_P/V_E \right)} \]
\[ \frac{D_E + E}{D_S} = \frac{1}{V_E/V_P - 1} \]

The blender flow ratio will be set by entering the ME blend (\( V_E \)) and Final Product blend (\( V_P \)). The ME blend flow (\( E + D_E \)) required for a “wild” Ship Discharge flow (\( D_S \)) is calculated. The flow ratio control system will manipulate the ME flow control valve to achieve the desired ratio.
Auto Select Control

This multiple loop configuration is used in the situations where two or more variables must not pass specified limits due to economy, efficiency or safety.

Pipe line transfer systems require the maximum flow to be delivered subject to satisfactory operating conditions being maintained at the prime mover, be it a pump or compressor. If a selected parameter, such as suction pressure, goes below a set limit the suction pressure controller output overrides the flow controller output via a signal selector and will control the flow.

If a processing unit is to be operated at a maximum allowable measurement parameter across the unit, where several measuring points are provided, a high selector is used to select the highest measurement for input to the controller. An example of this would be to control at the highest temperature in a fixed bed reactor.

The diagram shows an auto select control system, where it is required to provide a preset steady flow to a downstream processing unit, provided there is an adequate level in the upstream surge tank. If the level cannot be maintained the flow to the downstream unit will be cut back to maintain the surge tank level.

![Auto-select level control system](image-url)
3.2 Orifice Plate Flowmeters \(^{(5)}\)

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 (2½D and 8D) measures the permanent pressure loss and should be used for restriction orifice calculations.

The fundamental relationships for orifice plates are:

For liquids:

\[
Q = K \ d^2 C \ \sqrt{\frac{h}{\rho_f}} \quad W = K \ d^2 C \ \sqrt{\frac{h}{\rho}}
\]

For gases

\[
W = K \ d^2 C \ \sqrt{\frac{h \ p_f \ M}{T_f}}
\]
Sizing Methods (5)


The equation for non-viscous liquid flow is given by:

\[ S = \frac{W_{m}}{N D^{2} F_{a} F_{m} G_{f} \sqrt{h_{m}}} \]

Where:

- \( W_{m} \): maximum rate of flow (lb/h)
- \( D \): inside pipe diameter (in)
- \( F_{a} \): ratio of area of device bore at flowing temperature to that at 68ºF
- \( F_{m} \): manometer correction factor (=1 for diaphragm transmitters)
- \( N \): constant for units adjustment (N=2835 for lb/h)
- \( G_{f} \): specific gravity of liquid at flowing temperature, water at 60ºF=1.0
- \( h_{m} \): maximum differential pressure (in wg)

\[ F_{a} = 1 + 2\alpha (t_{f} - 68) \]

Where

- \( \alpha \): coefficient of thermal expansion orifice material (in/in °F)
  - Typical value for 18/8 SS is 9.5E-06 and for Monel is 7.0E-06
- \( t_{f} \): flowing temperature (°F)

The orifice resistance coefficient is given by:

\[ K_{r} = \frac{1 - \beta^{2}}{C^{2} \beta^{4}} \quad C = \frac{C_{d}}{(1 - \beta^{4})^{0.5}} \]

Where:

- \( C \): orifice flow coefficient
- \( d \): orifice bore
- \( \beta \): \( d/D \) (For better measurement try and keep in the range 0.3 to 0.6)

The equation for viscous liquid flow is given by:

\[ S = \frac{W_{m}}{N D^{2} F_{a} F_{m} F_{c} G_{f} \sqrt{h_{m}}} \]

The application of the viscosity correction factor \( F_{c} \) for plant operational measurements and control is rarely justified. Viscosity limits for 1% calculation tolerance vary in the range of 1 to 8 cps depending on the \( \beta \) ratio, keeping <0.6, and pipe size. \( F_{c} \) can vary in the range of 1.0 to 1.09.
Case D3.01 Orifice Sizing - Liquids Gases and Steam

The CHEMCAD model Orifice Sizing is set up with streams suitably configured for liquids, steam, vapors and gases. Dummy streams are used to determine liquid vapour pressure and steam saturation temperature. Data Maps are defined to interface with the relevant sheet LIQUID, STEAM or VAPOUR of the Flow Meter Sizing spreadsheet.

An orifice plate is sized by selecting Sizing – Orifice on the main Toolbar. Sizing is carried using the stream properties of the selected stream. The data entry Window is as follows:

Results

Sizing Spreadsheets have been created to analyze the CHEMCAD model calculation results and to obtain Physical Property Data to allow validation of orifice sizing results. In all cases agreement was found to be within -0.75% accuracy. Sizing parameters and thermal expansion factors are calculated using the relevant equations and values for d/D and Y were determined manually from the appropriate tables in L.K.Spink.
The spreadsheet for liquid orifice plate sizing is shown below:

<table>
<thead>
<tr>
<th>Orifice Plate Sizing</th>
<th>Liquid</th>
<th>CHEMAGI ORIFICE SIZING TOOL RESULTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process Fluid</td>
<td>Water</td>
<td></td>
</tr>
<tr>
<td>Design Mass Flow</td>
<td>$W_m$</td>
<td>10000.0</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T_1$</td>
<td>208.60</td>
</tr>
<tr>
<td>Exit Pressure</td>
<td>$P_r$</td>
<td>70</td>
</tr>
<tr>
<td>Liquid Density</td>
<td>$\rho$</td>
<td>60.050</td>
</tr>
<tr>
<td>Liquid Viscosity</td>
<td>$\mu$</td>
<td>0.383</td>
</tr>
<tr>
<td>Vapor pressure at flowing conditions</td>
<td>$p_{vapor}$</td>
<td>11.53</td>
</tr>
<tr>
<td>Water differential pressure</td>
<td>$h_w$</td>
<td>100.0</td>
</tr>
<tr>
<td>Liquid specific gravity</td>
<td>$G_l$</td>
<td>0.950</td>
</tr>
<tr>
<td>Calculated pipe velocity</td>
<td>$v$</td>
<td>6.50</td>
</tr>
<tr>
<td>Pipe internal diameter</td>
<td>$D$</td>
<td>2.067</td>
</tr>
<tr>
<td>Material thermal expansion</td>
<td>$\alpha$</td>
<td>0.5641</td>
</tr>
<tr>
<td>Thermal expansion factor</td>
<td>$F_\alpha$</td>
<td>1.0025E+00</td>
</tr>
</tbody>
</table>

Source for Sizing: K.S. Smith Tables 12 and 13

Pressure taps: Flange

The spreadsheet for steam orifice plate sizing is shown below:

<table>
<thead>
<tr>
<th>Orifice Plate Sizing</th>
<th>Steam</th>
<th>CHEMAGI ORIFICE SIZING TOOL RESULTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process Fluid</td>
<td>Water</td>
<td></td>
</tr>
<tr>
<td>Design Mass Flow</td>
<td>$W_m$</td>
<td>10000.0</td>
</tr>
<tr>
<td>Temperature</td>
<td>$T_1$</td>
<td>208.60</td>
</tr>
<tr>
<td>Exit Pressure</td>
<td>$P_r$</td>
<td>70</td>
</tr>
<tr>
<td>Compressibility</td>
<td>$Z_0$</td>
<td>0.998</td>
</tr>
<tr>
<td>Isentropic Coefficient</td>
<td>$k$</td>
<td>1.333</td>
</tr>
<tr>
<td>Density fraction</td>
<td>$\gamma$</td>
<td>1.000</td>
</tr>
<tr>
<td>Specific weight</td>
<td>$m$</td>
<td>0.457</td>
</tr>
<tr>
<td>Meter differential pressure</td>
<td>$h_m$</td>
<td>200.0</td>
</tr>
<tr>
<td>Reynolds number correction</td>
<td>$F_r$</td>
<td>10.73×$10^4$</td>
</tr>
<tr>
<td>Expansion Factor</td>
<td>$Y$</td>
<td>0.8894</td>
</tr>
<tr>
<td>Pipe internal diameter</td>
<td>$D$</td>
<td>3.067</td>
</tr>
<tr>
<td>Pipe velocity</td>
<td>$v$</td>
<td>2.80</td>
</tr>
<tr>
<td>Material thermal expansion</td>
<td>$a$</td>
<td>9.605E-09</td>
</tr>
<tr>
<td>Thermal expansion factor</td>
<td>$F_\alpha$</td>
<td>1.007E+00</td>
</tr>
<tr>
<td>Pressure taps:</td>
<td>Flange</td>
<td></td>
</tr>
</tbody>
</table>

The data copied and pasted from CHEMAGI orifice sizing tool result

Y from alignment chart in Data with initial $d/D$

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3.3 Control Valves

The selection of a control valve, with an appropriate operating characteristic, valve size and actuator power, is essential for satisfactory control loop performance in dynamic simulations.


Control valve pressure drop needs to be at a reasonable % of total system pressure drop to provide good control. If too low, i.e. valve oversized, the control valve opening will be small leading to unstable control; if too high flow could be limited leading to throughput concerns. As a general "rule of thumb" control valves, fitted with full size trims, are usually sized to be less than the line size of diameter D, typically ½D. This results in valves being fitted between pipe reducers. Line size valves, fitted with reduced trims, simplify installation but with a potential increase in installation cost.

The control valve must be sized to cover the anticipated maximum and minimum operating limits of the process. Valve rangeability, maximum flow to minimum flow ratio, of 50:1 is normal. The maximum flowing quantity should be set at 15% to 50% above the maximum flow required by the process. An initial estimate would be to set a full size trim valve at half the line size. Line sized valves, fitted with reduced trims, can avoid the use of piping reducers which create an additional pressure drop. This simplifies the piping design and installation but these benefits need to be offset against the increased valve cost.

The gain of a valve is the rated flow under nominal process conditions at full stroke. The flow characteristic is the relationship between the flow through the valve and the % rated stem travel as it is varied from 0 to 100%. An equal % characteristic produces a change in flow by a certain % of present flow for a given increment in stem position and compensates for gain variations elsewhere in the control loop. An equal % characteristic has an interesting feature in that changing the valve size does not affect the loop gain, which is directly proportional to flow, making valve sizing less critical.

The liquid flow through a valve is a function of the available pressure, size and opening:

\[ F = C_v \frac{\Delta P}{\rho} \]

Where:

- \( C_v \) flow coefficient of the valve
- \( \Delta P \) pressure drop across valve
- \( \rho \) specific gravity of flowing liquid

The consequences of an undersized valve are self-apparent. An oversized valve will only operate over part of its travel, requiring a wider proportional band, which results in poor control and at worst case no control.

The selection of the valve pressure drop, for design, needs to consider the maximum and minimum inlet and outlet pressures that will be experienced. In many cases, the process will set the inlet and outlet pressures and the valve must be sized accordingly. However for liquid transfers using centrifugal pumps a valve pressure drop of ~30% of total system pressure, at full flow, will give reasonable control. For valves installed in extremely long or high pressure drop lines at least 15% up to 25% of system pressure drop should be taken.

If the pressure in the valve vena contracta drops below the liquid vapour pressure, bubbles will form and limit flow through the valve. If the outlet pressure remains below the vapour pressure the bubbles remain, and the liquid is said to have flashed. If the outlet pressure rises above the vapour pressure the bubbles will implode, producing cavitation, which sounds as if sand is flowing through the valve. Flashing and cavitation can cause severe damage to the valve and even pipework and should be avoided if possible by increasing the inlet pressure or selecting a valve type that has a larger critical flow factor, \( C_r \). A change in flow direction by installing a streamlined angle valve will achieve a significant increase in \( C_r \).
Control Valve Sizing *(4)*

CHEMCAD provides facilities for the sizing of globe type control valves. The methods are based on “Control Valve Sizing” by Masoneilan Company, 6th Edition, which is entirely compatible with ISA SP39.1, “Control Valve Sizing Equations for Incompressible Fluids”.

**Liquid**

The fundamental equations are presented as follows:

The valve coefficient (Cv) metric equations for non-viscous liquid flow are given by:

For sub-critical flow where \( \Delta P < C_t^2(\Delta P_s) \)

\[
C_v = 1.16 q \frac{G_f}{\Delta P}
\]

Where:
- \( q \) liquid flow rate (m\textsuperscript{3} / h)
- \( C_t \) critical flow factor from manufacturers’ data
- \( G_f \) specific gravity of liquid at flowing temperature, water at 15ºC = 1.0
- \( \Delta P \) actual pressure drop (bar)

For critical flow where \( \Delta P \geq C_t^2(\Delta P_s) \)

\[
C_v = \frac{1.16 q}{C_t} \frac{G_f}{\Delta P_s}
\]

\[
\Delta P_s = P_1 - 0.96 - 0.28 \left( \frac{P_s}{P_v} \right) P_v
\]

Where:
- \( P_1 \) upstream pressure (bar)
- \( P_2 \) downstream pressure (bar)
- \( P_v \) fluid vapour pressure at flowing temperature (bar)
- \( P_c \) critical pressure (bar)
- \( \mu \) fluid viscosity (cps)

Laminar flow can result at high viscosity or when the valve \( \Delta P \) or \( C_v \) is small. Calculate turbulent flow \( C_v \) and laminar flow \( C_v \) and use the larger value as the required \( C_v \).

For laminar flow we have:

\[
C_v = 0.032 \left( \frac{\mu q}{\Delta P} \right)^{0.667}
\]
Case D3.04 Tank Level Control Inlet

This case introduces the concept of a control loop and the influence of control valve and controller specifications. The influence of the controller tuning parameters on performance is investigated.

Process

At initial state, a vessel, at a constant pressure of 2 barg, has a liquid level of 2 m. It is supplied with water at a rate of 4000 kg/h and has a constant liquid outflow demand of 4000 kg/h. A sensor is measuring liquid level in the vessel, and a controller tries to maintain a constant liquid level of 2 m in the vessel by regulating a control valve on the inlet feed.

After 10 minutes, the demand for water falls linearly to zero over 5 minutes and then there is no demand for 5 minutes. This is followed by a sudden demand of 16000 kg/h of water which continues for the next 5 minutes. Finally, the demand falls down to original 4000 kg/h and remains for 15 minutes.

The Flowsheet

Thermodynamics, K Ideal Vapor pressure and H Latent heat

Parameter Definition

The vessel is sized using retention and surge times.
Set Stream 3 to T = 20 ºC, P = 3 bar, F = 25000 kg/h and run DVSL.

Go to Sizing → Vessel. Design Pressure is
Set design pressure at 10 bar whilst retain all other defaults.

The vessel design parameters are transferred to the dynamic vessel automatically.

Adjust diameter to 1.2 m for standard dished end dimensions and height to 4.8 m.
Right click dynamic vessel and select Edit Unit Op Data and enter data.

Note that vessel outlet stream is set at a constant value of 4000 kg/h. The dynamic vessel must have a vapor outlet stream connected and flow is set at 1E-06. Vessel composition is defined at initial state by specifying the charge or outlet stream composition.

Feed Stream

Set Stream 1 at the initial supply conditions T = 20 C, P = 4 bar a, F = 4000 kg/h

Control Valve

Size the control valve for 25000 kg/h with a pressure drop of 1 bar. Identify the connected controller

The valve is Fail Open (Signal to Close) requiring \( A_v = -0.0625 \) and \( B_v = 1.25 \). The control valve is after the inlet stream so mass flowrate transfer is not required.
Results

Excel plot comparing liquid level control using different Integral Action time (I) settings is shown. This has been prepared using the Chart → Data to Excel CSV File option.

A plot of mass flowrate of outlet Stream 5 shows the demand side mass flow schedule:

The following level plot has been obtained by using a P = 10% and I = 5 min. Try different settings to try and improve control. Study effect of changing the proportional band on performance.
Case D3.07 Control of Dead Time \(^{(1, p6)}\)

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.

The model considers a step change in flow from 5000 kg/h to 5500 kg/h in a process exhibiting a dead time of 1 minute. The controller is calibrated for 2500 to 7500 kg/h and the control valve is linear with a $C_v$ of 14.

For a 1 minute dead time the natural period is fixed at 2 minute 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.
Case D3.08 Control of Capacity – Tank Level (1, p18)

Capacity is exhibited where mass or energy can be stored such as in a tank with volume $V$. The rate of change of tank contents equals the difference between inflow and outflow.

$$\frac{dv}{dt} = F_i - F_o$$

$V/F$ is the retention time constant.

The non-self-regulating case, having a fixed outflow using a metering pump, will result in the tank overfilling or emptying for any change in inflow; an integrating process cannot balance itself. Replacing the pump with a valve will result in a self-regulating process.
Case D3.09 Two Capacity – Tank Displacer Level (7)

A common method used in the measurement of tank level is a displacer mounted in an external chamber with the displacer being linked to the transmission system by means of a torque tube.

This measuring chamber creates a two capacity process that introduces a lag with a time constant of chamber volume divided by the maximum flow rate at which liquid can enter.

This arrangement creates hydraulic resonance with a period that varies with the distance between the bounded surfaces. The natural period for this arrangement can be derived:

\[
\tau_n = 2\pi \sqrt{\frac{L_1 + L_2}{2g}}
\]

Where

- \(L_1\) Tank 1 liquid level
- \(L_2\) Displacer liquid level plus inter-connecting pipe length

The simulation connects the primary tank to the displacer chamber using two control valves to allow for the bi-directional balancing flow. The level controller is measuring the liquid level in the displacer chamber and manipulating the control valve on the outlet of the primary tank.

Throttling the chamber connecting valve will reduce the amplitude of this resonance but not the period. However this enables the use of a narrower proportional band and at the same time reducing the valve movement due to waves.
Case D3.14 Tank Level Controller Tuning

This model introduces the concept of using dynamic simulation as a training tool, in this case the selection of control modes and level controller tuning.

The graphs below show the effects of proportional only control and proportional plus integral action control.

Note the reduction in offset when the proportional band is reduced from 25 % to 5%.

When integral action is used the offset is completely eliminated.

If level control is critical such as in steam drum level on boilers or distillation column reboilers then integral action is essential. However if the tank is being used as a surge tank feeding a process unit where it is important to keep the flow as constant as possible the level is allowed to float between limits requiring proportional only control.
Section 4

Heat Exchangers

Contents

4.1 Simple Theory
4.2 Fouling
4.3 Design Optimisation
4.4 TEMA Heat Exchanger Layout Designation

<table>
<thead>
<tr>
<th>Case/File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>D4.01</td>
<td>Heat Exchanger Temperature Control</td>
</tr>
<tr>
<td>D4.02</td>
<td>Heat Exchanger 3 way Valve Control</td>
</tr>
<tr>
<td>D4.03</td>
<td>Shell and Plate Heat Exchanger</td>
</tr>
</tbody>
</table>

4.1 Simple Theory

Shell and tube heat exchangers are used extensively throughout the process industry and as such a basic understanding of their performance is important to both process and instrument engineers. This section provides a condensed review of the key terms and parameters involved in the design and operation of shell and tube heat exchangers.

The heat transfer performance of shell and tube heat exchanger involves many interacting parameters, which can be summarised as follows:

- Process fluid state on shell side and tube side
- Stream temperature specifications
- Shell side and tube side pressure drop
- Shell side and tube side
- Selection of heat transfer models and fouling coefficients for shell side and tube side
- Heat exchanger TEMA\(^{(4)}\) layout and number of passes.

The basic layout for a countercurrent shell and tube heat exchanger is shown:-

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

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

Where:
- \(Q\) is the heat transferred per unit time \((kJ/h, Btu/h)\)
- \(U\) is the overall heat transfer coefficient \((kJ/h-m^2\cdot°C, Btu/h-ft^2\cdotºF)\)
- \(A\) is the heat-transfer area \((m^2, ft^2)\)
- \(\Delta T_{\text{lm}}\) is the log mean temperature difference \(ºC, ºF\)
- \(C_{p(t)}\) is the liquid specific heat tube side \((kJ/kg\cdotºK, Btu/lb\cdotºF)\)
- \(C_{p(s)}\) is the liquid specific heat shell side \((kJ/kg\cdotºK, Btu/lb\cdotºF)\)
- \(w\) is tube side flow \(W\) shell side flow \((kg/h, lb/h)\)
Case D4.01 Heat Exchanger Temperature Control

A typical arrangement is shown for liquid-liquid temperature control which does not provide good control as the controlled variable is influenced by the capacity and thermal lags of the heat exchanger. This arrangement is acceptable if one side undergoes a phase change such as steam. Process water, varying with temperature, is cooled to a controlled temperature by manipulating the flow rate with 15°C cooling water.

Case D4.02 Heat Exchanger 3 way Valve Control

This arrangement provides superior control because the lags introduced by the heat exchanger no longer influence the control.
Section 5

Batch Distillation

Contents

5.1 Introduction
5.2 Operation and Control
5.3 Thermodynamics
5.4 Mass and Energy Balances
5.5 Process Simulation

<table>
<thead>
<tr>
<th>Case/File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>D5.01</td>
<td>Batch Distillation No Heat Transfer</td>
</tr>
<tr>
<td>D5.02</td>
<td>Batch Distillation with Dynamic Reactor and Column</td>
</tr>
<tr>
<td>D5.03</td>
<td>Batch Distillation with Control System</td>
</tr>
</tbody>
</table>

References

5.1 Introduction

Batch distillation techniques are used extensively in the Specialty, Fine Chemicals and Pharmaceutical Industries to achieve a variety of processing objectives, namely:

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

The simplest form of batch distillation involves a single flash separation which is used where a large difference in volatility exists between the components. Such a distillation does not need a fractionating column between the batch still, normally a stirred jacketed reactor, and the condenser. Simple batch distillation, also referred to as pot to pot, provides one theoretical plate of separation.

A typical batch distillation arrangement utilizing a stirred batch reactor, packed column, overhead condenser and a single accumulator (receiver) is shown, with the nomenclature used in this article.

![Batch Distillation Flow Diagram](image)

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. Overheads are continuously withdrawn in accordance with the reflux control strategy. Cuts(fractions) are taken by switching to different accumulators(receivers), following a time, temperature or overhead composition strategy.
Batch distillation with rectification can be operated as follows:

- **Constant reflux ratio**, giving varying overhead composition. Distillation is continued until the desired composition is achieved in the still or the distillate receiver.
- **Constant overhead composition**, by 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.
- **Repetitive 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 low-boiling trace component.
- **Minimum time by 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. 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 including operational temperature difference, jacket heating media and heat transfer considerations (4, 5).

### 5.2 Operation and Control

The operation and control of a batch distillation is determined by the mass and energy balances, with the primary objective being to minimise distillation time. If conditions are fixed at the still then conditions at the top of the column can be varied and vice-versa.

The best strategy is to control the heat input at the still to maximise the distillate draw rate and sustain the desired reflux ratio. The still bottoms temperature will increase as the distillation proceeds reducing the temperature driving force. If the heating medium is steam the heat input can be controlled by the flowrate or pressure and if heat transfer fluid the heat input can be maintained by increasing the temperature. Alternatively if the heating medium conditions are fixed, the distillation pressure can be reduced to increase the temperature driving force, if necessary, in incremental steps as the distillation temperature increases throughout the distillation.

At constant pressure, the top and bottom temperatures are an indication of composition. If the product is the still residues the distillation is continued until the bottom temperature reaches a target limit. If the product is the distillate the column top temperature is controlled by increasing the reflux ratio as the distillation proceeds to maintain the target temperature. There will come a point when the still heat input will not be able to sustain the increasing reflux ratio at which point the column top temperature will start to increase and the distillation is stopped.

The operating instructions can determine the distillation by specifying temperature cut off values or time steps can be given with an established distillation. If repetitive batch distillations are to be carried out it may be desirable to shorten the distillation time by the use of intermediate fractions between the component fractions.

The basic instrumentation required will include still bottoms and column top temperatures, still pressure and possibly control, reflux and distillate flow control and level measurements as determined by the plant configuration. Still heat input control will be determined by the heating medium used and the jacket services configuration.(5)

To start the distillation, apply heat to the still and continue until stable conditions at total reflux have been achieved. Now start distillate draw at fixed reflux ratio for bottoms composition or variable reflux for top composition. If there are distillate cuts involved separate receivers will be required.

It is not desirable to store hot liquids e.g. hydrocarbons, nor to cool the reflux as this causes internal reflux which leads to additional still heat input, so rundown coolers should be installed appropriately.
5.3 Thermodynamics

To calculate the vapour pressure and concentrations at temperatures other than a solvent’s atmospheric boiling point the following can be used:

Antoine Equation (base 10)
\[
\log_{10} p = A - \frac{B}{(C + t)}
\]

Antoine Equation (natural)
\[
\ln p = A_e - \frac{B_e}{(C_e + T)}
\]

Where:
\[
\ln p = 2.303 \log_{10} p
\]

\[p\] vapor pressure of component mm Hg
\[t\] temperature °C
\[T\] temperature °K
\[A, B, C\] Antoine coefficients (base 10) for each pure solvent
\[A_e, B_e, C_e\] Antoine coefficients (natural) for each pure solvent

The coefficients can be converted using:
\[
A = \frac{A_e}{2.303}, \quad B = \frac{B_e}{2.303}, \quad C = C_e - 273
\]

The Cox equation is an approximation based on Antoine coefficient \(C\) being in the range 210 – 250. This allows \(A\) and \(B\) to be calculated from two known points on the vapour pressure/temperature relationship and the estimation of the relative volatility of an ideal binary mixture throughout the operating temperature range.

\[
\log_{10} p = \frac{A}{t + 230}
\]

We can derive:
\[
\alpha = \frac{p_1}{p_2}, \quad \log_{10} \alpha = \log_{10} p_1 - \log_{10} p_2 = \frac{(A_1 - A_2) - (B_1 - B_2)}{t + 230}
\]

Where:
\(\alpha\) relative volatility based on Raoults law

Subscripts
1, 2 component 1 or 2 parameter, where 1 represents the more volatile component (mvc)

Note:
\(\alpha\) will increase as the temperature is reduced, achievable by operating at a reduced pressure.

For ternary mixtures in a simple distillation, a plot of liquid compositions on triangular axes is known as a Residue Curve. The residue curve is defined as being the locus of the liquid composition remaining behind in the still bottoms during a simple equilibrium distillation process. The residue curve depends on the starting liquid composition from which a family of curves can be generated to create a Residue Curve Map (RCM) which is used to determine the viability of a distillation and provides a great amount of insight into the separation of a mixture.

All residue curves originate at low-boiling pure components or azeotropic compositions (low-boiling nodes) and end at high boiling compositions (high-boiling nodes). An RCM with more than one origin for residue curves has more than one distillation region.

Intermediate boiling pure components or azeotropes that are not nodes are called saddles. In a distillation region (three sided) with one saddle, all residue curves track back toward the solitary saddle. However in a region with two non-adjacent saddles (four sided) some residue curves track toward one saddle whilst others track towards the other saddle.

The RCM and mass balance identifies feasible operations as the distillate and bottoms will lie on the same residue curve, which must be in the same distillation region. For heterogeneous azeotropes, overlaying the RCM with the liquid/liquid phase equilibrium (binodal) diagram indicates valid operational conditions.
Case D5.02 Batch Distillation with Dynamic Reactor and Column

Components and thermophysical options are the same as in Case D5.01. The CHEMCAD flowsheet is shown:

For dynamic column use any SCDS for UnitOp 2. In this case SCDS 3 format has been selected, which has no reboiler or condenser. Batch Reactor will serve as reboiler.

Steady state Heat Exchanger HTXR UnitOp 3 will condense top vapor totally. Dynamic Vessel DVSL UnitOp 4 acts as reflux drum, steady state Divider UnitOp 5 provides reflux/distillate split and Dynamic Vessel DVSL UnitOp 6 acts as the receiver.

Process Specifications

Stream 1, dry Saturated Steam at 12 bar (vf = 1.0) with Stream 2 Condensate Return at 4 bar

The stream calculator shows that heat change ΔH across the jacket is 2.18 MJ/kg. Heat duty 436 MJ/h achieved with 200 kg/h steam.
Section 6

Continuous Distillation

Contents

6.1 Introduction
6.2 Fundamentals
6.3 Operation and Control
6.4 Simulation Considerations
6.5 Simulations

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References

6.1 Introduction

This section reviews the continuous distillation process by considering the basic chemical engineering relationships for vapour liquid equilibrium, mass and energy balances and their impact on control system design and operation.

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

- Separation and purification of hydrocarbon mixtures
- Purification of organic solvents
- Water removal and drying.
- 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 affect performance.
- Control loops are interactive rendering stable control difficult if incorrect selection.

6.2 Fundamentals

**Mass Balance**

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, 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 \( \frac{D}{F} \) determines the relative composition of each product such that if feed composition \( z \) changes then \( \frac{D}{F} \) must be manipulated to maintain constant \( x \) and \( y \).
6.3 Operation and Control

The operation and control of a continuous distillation is constrained by the mass and energy balances. If conditions are fixed at the reboiler then conditions at the top of the column can be varied and vice-versa.

The distillation operation is determined by the top and bottom specifications and is driven by the component purification requirements. At constant pressure the temperature profile in a column is used to determine the composition profile.

The temperature in the upper section of the column, above the feed point, can be controlled by adjusting the reflux ratio. The temperature in the lower section of the column, below the feed point, can be controlled by adjusting the heat input to the reboiler. However the reboiler heat input must be sufficient to maintain a constant liquid level in the column bottoms and to heat the feed and reflux to the respective bubble points.

If the heating medium is steam the heat input can be controlled by the flowrate or pressure and if heat transfer fluid the heat input can be maintained by increasing the temperature. Alternatively if the heating medium conditions are fixed, the distillation pressure can be reduced to increase the temperature driving force.

Consider the control loop configurations shown with the reflux drum and column bottoms on level control. Level control is essentially mass balance control so with this configuration the mass balance cannot be manipulated directly. Reflux on flow control results in variations in the boil up rate and reflux rate affect the distillate flow and we know the D/F ratio has a great effect on product quality.

It can be concluded that component quality specifications cannot be set independently for the distillate and bottoms.

The boil up rate has an immediate effect on the bottoms flow which if excessive could result in no bottoms flow or if too low to sustain the reflux an increase in light ends in the bottoms. When bottoms flow is under level control, as shown, the heat input can be fixed at any desired value. A stable arrangement is to control the reboiler heat input based on the column differential pressure which will set the vapour flow constant.

Variations in feed condition can have a significant impact on the column operation. A reduction in temperature increases the internal reflux at the feed point and an increase in temperature or if flashing occurs the vapour flow will increase above the feed point. It is desirable for the feed condition be held constant for stable column operation.
The reflux flow determines the column composition profile so smooth delivery is important for stable column operation. When distillate flow is manipulated for composition control it can be seen that reflux is a dependent variable and the reflux drum level mass balance, that is level, must be satisfied by manipulating the reflux flow. Changing the distillate flow will have no effect on top tray composition if the reflux or vapour flow is not changed accordingly which is the reflux ratio.

The conventional control system is to use a cascade system in which the reflux drum level controller output sets the reflux controller set point. This method results in the composition control response lagging as a result of the delay injected by the reflux drum.

The diagram shows a control system that injects a lead action if the distillate flow increases and a lag on decrease. The level controller output is passed via a computing unit where it is trimmed with a modified signal from the composition controller output.

Reflux flow is set according to \[ L = m - KD \]

The graphs, from Case D6.06, show the effect of constant K on the reflux flow response curves which sets the lead-lag ratio while the lag time varies with the reflux drum time constant and the level controller tuning parameters. This scheme eliminates the time lag associated with the reflux drum and introduces a reflux flow lead lag action following distillate flow changes which improves composition control.
Case D6.06 Distillation Column Overhead Control

A distillation column overhead control system which improves the composition control response characteristics by introducing lead lag features to reflux flow control has been discussed.

The simulation process flow diagram is shown.

\[ L = m - KD \]

The coefficient \( K \) sets the lead lag ratio while the lag time varies with the retention time of the reflux drum and the level controller tuning parameters as shown in the curves below:

A special feature of the simulation is the dynamic vessel outlet flow being dependent on two control valves. The control valve calculated flows are summed and fed forward to the dynamic vessel output stream using controller 9.
Case D6.07 Distillation Column Feedforward Control

The material balance based on the more volatile component 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 \( y \).

This simulation sets the steam flow in a preset ratio to the feed stream and the distillate flow based on the above relationship. The column bottoms mass balance is maintained by reboiler level control.

The distillation is based on ethanol and water which exhibits an azeotrope at 78°C with a 0.96 weight fraction as shown in the xy plot.

The SCDS column has 30 stages with the feed on stage 15. Column top pressure is 1.5 bar and differential pressure is 0.1 bar with a total condenser. The cut streams are reboiler recirculation rate which is set in dynamic vessel 7 and the reflux flow which is the overhead vapor flow minus the distillate flow which is determined from the mass balance relationship.

The reboiler heat transfer area is 200 m\(^2\) with a heat transfer coefficient of 400 kcal / h-m\(^2\)-°C and a dynamic vessel 1.5 m diameter by 3 m tan-tan height.
Section 7

Batch Reactors

7.1 Introduction
7.2 Thermal Design Fundamentals
7.3 Process Design Considerations
7.4 Reactor Parameters
7.5 Performance Characteristics
7.6 Jacket / Coil Services Configurations

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<td>Reactor Indirect Heating – Direct Cooling</td>
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<td>D7.02</td>
<td>Reactor Indirect Heating – Indirect Cooling</td>
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<tr>
<td>D7.03</td>
<td>Reactor Jacket Circulation Hydraulics</td>
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<td>Cryogenic Batch Reactor System</td>
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<tr>
<td>D7.05</td>
<td>Batch Reactor Kinetics</td>
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References

7.1 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.
7.2 Thermal Design Fundamentals (6, 7)

Heat Transfer

A typical batch reactor system is shown which defines the key variables for determining the basic thermal ratings.

The fundamental equation for heat transfer across a surface area \( A \) is given by:

\[
Q = U \cdot A \cdot \Delta T_m = V_j \cdot C_p \cdot (t_2 - t_1)
\]

The mean temperature difference \( \Delta T_m \) for a batch reactor with contents temperature \( T \) and services inlet and outlet temperatures \( t_1 \) and \( t_2 \) is approximated by:

\[
\Delta T_m = T - \frac{(t_1 + t_2)}{2}
\]

The overall heat transfer coefficient \( U \) is the sum of the individual resistances as follows:

\[
\frac{1}{U} = \frac{1}{h_i} + \frac{1}{h_{fi}} + \frac{1}{k_w / x} + \frac{1}{h_o} + \frac{1}{h_{fo}}
\]

When considering glass lined equipment the reactor wall thermal conductivity \( k_w \) includes the glass thickness \( x_g \) and metal wall thickness \( x_m \) with the thermal conductivities for glass \( k_g \) and metal \( k_m \) to give the following:

\[
k_w = \frac{x_m + x_g}{x_g / k_g + x_m / k_m}
\]

The inside fouling coefficient \( h_{fi} \) and outside fouling coefficient \( h_{fo} \) are determined by practical experience and there is extensive literature available on this subject. The combined fouling coefficient \( h_f \) is given by:

\[
h_f = \frac{h_{fi} \cdot h_{fo}}{h_{fi} + h_{fo}}
\]
7.6 Jacket / Coil Services Configurations

Jacket services system configurations in common use are presented. The dynamic simulation plots presented are all based on a 6300L Glass Line Reactor fitted with an impeller agitator rotating at 90 rpm. The reactor contents at the start of the simulation are 4000 kg of Toluene.

Direct Jacket Heat / Direct Cool

These systems involve the connection of the appropriate supply and return services directly to the reactor jacket/coils. There are many arrangements in use from total manual to fully automatic control involving forced circulation with steam/water mixing facilities.

Temperature ranges from $-20^\circ C$ to $180^\circ C$ with water, steam or ethylene glycol/water can be used but ethylene glycol/water should not be used above its boiling point.

This arrangement provides good thermal response due to there being no heat transfer lags associated with heat exchangers. However, to provide combined heating/cooling facilities requires automatic valve sequencing and jacket/coil blowdown routines when changing services. This results in discontinuous control, with the exception of steam water mixing systems, which can lead to operational problems if handling exothermic reactions.

![Diagram of direct heating and cooling system]

The scheme above shows the basic system with automatic control of the steam and cooling water services. The changeover between heating and cooling modes can be done manually or automatically involving a timed sequence of valve switching operations. The changeover is not seamless as with a single fluid system and requires careful consideration if used on exothermic reactions.

A study of the heat up and cool down curves demonstrates the fast response of these systems. However the rate of change of jacket wall temperature can lead to thermal shock problems with glass lined equipment and possibly product problems with the high wall temperatures that can be experienced.

The heat-up curves for a direct system, shown below, have been modelled using 4 barg steam pressure.

Operational problems associated with this system and the mixing system, shown following, include cross contamination of services, jacket fouling and corrosion and the need for sequenced control routines when changing services from heat to cool.

These systems are not always cheaper than other alternatives.
Ciba Geigy and Wiegand developed a steam jet water mixing heater which provides a wide range of heating duties using water as a single phase in the operating range 5°C to 180°C.

This arrangement requires careful design in relation to air removal, thermal expansion and pressurisation facilities, if operating above the boiling point. The service returns from high operating temperatures require special automatic blowdown facilities.

The heat up curves for the mix system have been modelled using 9 barg steam pressure, an initial inlet temperature of 150°C and 20000 kg/h water circulation rate. It can be seen that the heat up time is increased by 50% due to the rate of jacket temperature increase being significantly slower. This type of system allows for better control of jacket temperature conditions but with the loss of heat input capability.
Case D7.01 Reactor Indirect Heating – Direct Cooling

Reactor jacket temperature control systems require a constant recirculation flow rate at all times. This requires that the simulation maintains a mass balance in the incompressible fluid circulation loop by removing the same flow from the loop as is admitted. This is achieved by setting the Divider 7 Stream 11 output equal to Control Valve 3 calculated flow rate. This valve controls the -40ºC Syltherm XLT coolant flow to the jacket.

Jacket mixing nozzle pressure drop is not calculated rigorously. The DataMap facility is used to calculate the pressure drop and set the jacket outlet pressure. See Case D7.02 for the correlations and further details.

The typical control system uses a reactor contents temperature on reactor jacket temperature cascade control loop with the heating and cooling valves operating in split range. The heating heat exchanger has a constant steam supply pressure of 10 bar to ensure that condensate return is maintained under all load conditions. Temperature control uses a 3 way bypass valve to eliminate the thermal lags associated with this type of system see Case D4.02

Common simulation problems are summarised below:

For vapour to be removed from the reactor mixed phase must be selected and product draw schedule set to maintain constant pressure

Jacket Origin Stream 2 and Jacket Connection Stream 1

Jacket is full of liquid so liquid fraction is always 1. This feature can be used on steam heated systems to test for condensate build up

Make sure the connected streams are specified on General Information

To model full jacket/coil arrangement Thermal mode 5 is always selected. If special reactors are being used Isothermal mode will establish heat duty requirements which can then be checked independently
Section 8

Emergency Relief

Contents

8.1 Introduction
8.2 Relief System and Piping Headers

Emergency Relief Simulations

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<td>Dynamic Relief Two Vessels</td>
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<tr>
<td>D8.02</td>
<td>Dynamic Relief Three Vessels</td>
</tr>
<tr>
<td>D8.03</td>
<td>Fire Induced Runaway Reaction</td>
</tr>
</tbody>
</table>

8.1 Introduction

This section does not discuss relief device sizing methods and procedures; for further information refer to Chemical Engineering in Practice or other appropriate publications. This section reviews the behavior of emergency relief systems in the dynamic state. Dynamic simulation of the total relief system can establish the adequacy of the relief device and blowdown system under real conditions of venting flow including the onset of two phase flow.

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 Layer of Protection Analysis (LOPA) and 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.

A pressure relief device is either a relief valve or a bursting (rupture) disc or a combination of both. On chemical reactors the bursting 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 reseat, unless used in conjunction with a safety valve.

In mitigation 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, ±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 relief systems 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.

8.2 Relief System Piping and Headers

Refer to Section 10 for details of configuration and simulation of pipe networks.

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
D8.01 Dynamic Relief Two Vessels

This simulation investigates the dynamic relieving behaviour of two identical vessels, containing the single component ethylene, when subjected to a coincident external fire. This model tests for the suitability of the vent header under coincident relieving conditions. It can also be used to check for the impact of two phase flow and for variable back pressure conditions.

Dynamic Vessel (DVSL) requires the inlet, liquid outlet, vapour outlet and relief streams to be connected as shown. The initial condition can be specified by level, in which case the vessel contents composition and state (P, T) are taken from the outlet stream specification. Alternatively the composition and level can be specified in the DVSL dialogue screen. The Flash with Heat Duty Thermal Mode is selected where the actual heat duty comes from the Relief Device fire model selected, which in this case is API520/521.

Pressure nodes are used to drive the pipe network to a balanced state; their detailed application and use are discussed in Chemical Engineering in Practice.

The header inlet nodes are set for variable pressure with the inlet flow coming from the current stream rate, determined by the relief valves, and the outlet flow being determined by the downstream piping. The outlet node is set for fixed pressure at 14.696 psia; this node can be used to check for the effects of variable back pressure. The initial node pressures are all set at 14.696 psia with no pressure limits required.

The main parameters are shown in the simulation flowsheet.

Thermodynamics selected: K Model – Peng Robinson and H Model – Peng Robinson
Relief conditions selected: Vessel Model – HEM and Vent Model – HEM
Dynamic simulation settings: Run Time 5m with a step size of 0.1m

The relief valve stream has automatically been assigned to Stream 4. If more streams are connected to DVSL check that the automatic assignment agrees with the flowsheet.

Pressure Data
- Set pressure: 250 psia
- Back pressure: 14.696 psia
- Max pressure: 14.696 psia
- Stream ID: 4
Section 9

Risk Assessment

Contents

9.1 Assessment Techniques
9.2 Hazard and Operability HAZOP
9.3 As Low As Reasonably Practical ALARP
9.4 Layer of Protection Analysis LOPA
9.5 Consequence Analysis – Dynamic Simulation

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<td>D9.01</td>
<td>Wash Water Heat Recovery System</td>
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<td>Ammonia Scrubbing System</td>
</tr>
<tr>
<td>D9.03</td>
<td>Storage Tank Heating System</td>
</tr>
</tbody>
</table>

References

3. HSE, “Lines of Defence/Layers of Protection Analysis in the COMAH Context”
   www.digitalrefining.com/article/1000487
9.1 Assessment Techniques

Hazard and Risk assessment in the Process Industry is based on established techniques. Risk assessment analyses the risk either qualitatively, rating risk from low to high, or quantitatively by assigning numerical factors based on field data or published databases.

Risk assessment has to demonstrate that the measures for prevention and mitigation result in a level of risk that is As Low as Reasonably Practical (ALARP).

A Hazard Identification (HAZID) study provides a methodology to identify specific hazards.

A Hazard and Operability (HAZOP) study identifies qualitatively specific hazards associated with the process plant and its operation, providing a basis for challenging the design and assessing the risks.

Layer of Protection Analysis (LOPA) is a semi-quantitative method applied to prevent or mitigate the risk by applying Independent Protection Layers (IPLs). LOPA is used to reduce the risks to ALARP.

The overall approach to risk analysis and reduction is summarised in the flow chart below, showing the application of IPLs to achieve an acceptable risk and challenging the requirement for a Safety Instrument System (SIS).

<table>
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<th>Level</th>
<th>Interpretation</th>
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<tbody>
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<td>&gt; $10^{-4}$/yr</td>
<td>Unacceptable</td>
<td>Risk cannot be justified except in extraordinary circumstances</td>
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<td>ALARP or tolerable</td>
<td>Undesirable, tolerable risk only if further risk reduction is impractical or the cost is not proportionate to the benefit gained.</td>
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<td>Class III</td>
<td>&lt; $10^{-6}$/yr</td>
<td>Acceptable</td>
<td>Negligible risk.</td>
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</table>
9.5 Consequence Analysis – Dynamic Simulation

The hazard analysis and risk assessment techniques discussed are subjected to detailed studies by teams of specialists with the appropriate experience. These processes result in a series of actions to evaluate and mitigate the risk identified. In the initial design phase and even on existing plant it can be difficult to predict the outcomes from some “What If” the scenarios presented.

Dynamic simulation of a process plant based on the proposed or existing mass and energy balances and incorporating actual equipment sizing specifications allows the consequences of process deviations and equipment failure to be predicted with some confidence.

The dynamic simulation is controlled by an action matrix in Excel which can drive process abnormalities and deviations and force equipment failure conditions such as control valve or pump maloperation. The ability to stress test combinations of equipment and control system failures provides the opportunity to analyse outcomes which may not have been identified in risk assessment studies.

CHEMCAD simulations can be linked to Excel using the Tools → DataMap facility. Conditions such as stream and unit operation properties or equipment operating status are scheduled in the table at the desired time in the simulation.

In the spreadsheet below the current dynamic run time is sent to cell A2. The VLOOKUP function transfers data matching the current run time from the action matrix to the active Row 2. The formula for cell B2 “VLOOKUP(A2,A8:I135,2,TRUE)” transfers the value in column B from the row in the schedule that matches the current simulation step time in cell A2.

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</tr>
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<tr>
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<td>Output pressure</td>
<td>&lt;None&gt;</td>
<td>1</td>
<td>1.00000</td>
</tr>
</tbody>
</table>

The foregoing DataMap and Excel action matrix are applied in Case 9.00 Simulation Scheduler.
Case D9.00 Simulation Scheduler

The previous action matrix is linked to the CHEMCAD simulation as shown below:

The convergence page to achieve the required interaction between CHEMCAD and Excel is set up on the Run → Convergence screen as shown:

The action matrix allows for the manipulation of inlet flow, pump pressure, controller set points, controller auto/manual select and control valve position in manual mode. The combination of events and equipment failures to be tested will have been determined from the hazard studies.

The control valve operating mode is set by entering 0 for Normal and 4 for Manual setting of the valve position in the matrix cell. Other conditions that can be set are Power Failure (1), Manually Close (2) and Manually Open (3).

The run time step size value should be appropriate for the process under consideration which in this case is 5 seconds which must be entered in minutes as 0.0833 with a total run time of 60 minutes.


**Section 10**

**Pipe Networks**

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10.1 Fluid Flow Synopsis
10.2 Piping Design
10.3 Centrifugal Pumps
10.4 Pipe Networks

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<tr>
<th>Case/File Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>D10.01</td>
<td>Cooling Water Distribution Balancing</td>
</tr>
<tr>
<td>D10.02</td>
<td>Biodiesel Blender</td>
</tr>
</tbody>
</table>

Fluid Flow

10.1 Fluid Flow Synopsis

Process and manufacturing facilities require extensive piping systems to distribute services and process fluids at acceptable flows and pressures for satisfactory equipment operation.

Fluid flow through a pipe, valve, fitting or nozzle will result in a pressure drop in the direction of the flow. Fluid mechanics enables the calculation of the pressure drop through a pipe, valve or nozzle as a function of the flowrate. Process equipment such as compressors or pumps, use experimentally determined performance curves to predict the flow pressure drop relationships.

The fundamental relationship for incompressible fluid flow in a circular pipe is known as the continuity equation and is given by:

\[ q = a_1 v_1 = a_2 v_2 \]

\[ D_1^2 v_1 = D_2^2 v_2 \]

\[ \frac{D_2^2}{D_1^2} = \frac{v_2}{v_1} = \beta \]

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

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

Where in consistent units:

- \( q \): volumetric flowrate
- \( a \): pipe cross sectional area
- \( v \): fluid velocity
- \( D \): pipe internal diameter
- \( \beta \): pipe diameter ratio
- \( p \): fluid pressure
- \( w \): fluid density
- \( g \): gravitational constant
- \( z \): elevation
- \( h_L \): head loss due to friction

Subscript 1 refers to conditions at inlet and is treated as the smaller diameter
Subscript 2 refers to conditions at outlet and is treated as the larger diameter

A dimensionless number called the Reynolds Number (\( Re \)) is used to prediction the fluid flowing state (laminar, transitional or turbulent) which is then used in the selection of the appropriate pressure drop correlation. Using the fps system of units, for a fluid of density \( \rho \) (lb/ft\(^3\)) and viscosity \( \mu \) (lb/ft-s) flowing in a circular pipe of inside diameter \( d \) (ft) with a velocity \( v \) (ft/s) we have:

\[ Re = \frac{v \cdot d \cdot \rho}{\mu} \]

The units equation ft/s x ft x lb/ft\(^3\) x ft-s/lb shows that \( Re \) is dimensionless.

The friction factor \( f \) is introduced which is dependent on the Reynolds Number and pipe wall roughness \( \varepsilon \). The Darcy-Weisbach equation is used to calculate, in consistent units, the friction head loss \( h_L \) of fluid flowing in a pipe of length \( L \):

\[ h_L = f \cdot \frac{L \cdot v^2}{D \cdot 2g} \]

In terms of the Darcy-Weisbach or Moody friction factor the pressure loss due to friction for a fluid with density \( \rho \) is given by:

\[ \left( \frac{dP}{dL} \right)_f = \frac{f \cdot \rho v^2}{2g \cdot D} \]
In using reference data care should be taken to ensure the correct friction factor data is being used.

The Fanning friction factor $f_F$ is commonly used in Chemical Engineering and is related to the Darcy friction factor $f$ as follows:

$$f = 4f_F$$

The form of the Darcy equation using the Fanning friction factor becomes:

$$h_L = \frac{2f_F L}{D} \frac{v^2}{g} \quad \text{or in the more common form} \quad h_L = \frac{4f_F L}{D} \frac{v^2}{2g}$$

For laminar flow conditions (Reynolds Number $Re < 2300$).

The Darcy friction factor is given by $f = \frac{64}{Re}$ and the Fanning is given by $f_F = \frac{16}{Re}$.

For an independent check of the friction factor the Moody diagram is used. Knowing the pipe flow $Re$ and the pipe roughness coefficient $\varepsilon$ (units of m or ft), giving the relative roughness $\varepsilon/D$ (consistent units), the friction factor can be determined.

Unfortunately friction factors are sometimes quoted without definition and incorrect use can lead to significant errors. CHEMCAD Pipe UnitOp uses the Darcy form throughout.

The laminar flow line formula will allow verification of the diagram friction factor being used. Check friction factor at $Re=1000$; if Darcy $f = 0.064$ and if Fanning $f_F = 0.016$.

**Moody Diagram – Darcy Friction Factor**

Example:
Friction factor for cast iron pipe $D = 500$mm, $\varepsilon = 0.5$ mm ($\varepsilon/D = 0.001$) with Re of 300000 is 0.026
Case 10.01 Cooling Water Distribution Balancing

A problem frequently experienced on process plant is the balancing of utility systems. This case considers a typical cooling water system where it is required to supply three heat exchangers.

Process

Cooling water is supplied to the header at a temperature of 15°C, pressure of 5 bar at 35000 kg/h. The cooling tower is designed for an optimum return temperature of 25°C. A restriction orifice is installed in the return line and is sized based on a differential pressure of 0.5 bar.

Control valve positions are adjusted to achieve the desired heat exchanger duties whilst satisfying the temperature return specification.

The heat exchanger duties are UnitOp7 → 60 kW, UnitOp13 → 80 kW and UnitOp17 → 125 kW.

The control valves are adjusted manually in operating mode Fix valve position, adjust flow rate.

This model could be readily adapted for other utility systems such as heat transfer fluids and steam. The simulation can be extended for studying process dynamics.
Section 11

Process Measurement

11.1 Introduction

Reliable and accurate measurement sensor 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.

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® (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®, PROFIBUS PA and FOUNDATION™ being the most common. Modbus® 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™ 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. An understanding of the fundamentals of process control is essential before beginning work on dynamic simulation. Process Control Systems by Shinskey[1] 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 provide an introduction to dynamic simulation and simple control loop applications.
11.2 Flow

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 being 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 the highest specification for same value. Accuracy is important for stock and custody monitoring, with reproducibility, the ability of the sensor to reproduce its reading, being important for control.

Positive Displacement Flowmeter

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 ±0.05% rate for μ = 0.2 - 5 cps and ±0.25% rate for μ > 5cps over 10:1 turndown. Advancements in accuracy from ±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.

Turbine Flowmeter

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 ±0.5% rate for μ = 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.
11.3 Level

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 ±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 ± 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. The reflectivity requires the liquid dielectric constant(ε) to be ≥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 ε and turbulent conditions. Method is suitable for custody transfer with accuracy ±0.5mm 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 δε of the liquid and the vapour space or between the two liquids are higher. Special designs, involving coated and twin probes, are used when δε < 1.0, conductivities > 100 μmho, coating effects or vessel material is non-conducting. Typical accuracies claimed are ±0.25% span and is dependent on fluid properties, so is not suitable for changing conditions. Maximum conditions 200°C at 100 bar and 400 °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 ε, conductivity, density or humidity. Maximum conditions 150°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 °C at 100 bar.

The conductivity point level method requires a liquid conductivity > 0.1 μmho and is frequently used on utility and effluent pump control systems.
Section 12

Engineering Fundamentals and Data

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12.2 Process Engineering Units
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   Typical Overall Heat Transfer Coefficients
   Typical Fouling Resistance Coefficients
   Reactor Heat Transfer Data
12.4 General Engineering Data
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   Pipe and Tube
      Modelling Pipe Fittings
      Commercial Steel Pipe Dimensions
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      Modelling Control Valves
      Control Valve Flow Coefficient Units
      Control Valve Sizing Coefficients
      Worcester Ball Valve Coefficients
      Atomac Valve Coefficients
      Flowserve Inline Strainers

References

12.1 Basic Arithmetic

A basic understanding of practical mathematics is frequently sufficient for an engineer working in a general design or operating process plant environment. Note, we are not considering academic study, specialist areas or research and development.

Fractions and Indices (Powers)

Two numbers, such that their product is unity, are called reciprocal numbers; for example \( \frac{4}{4} \) and \( \frac{1}{4} \). A powerful concept is to use letters in place of numbers to represent a specific parameter or variable. So we can state that \( \frac{a}{b} \) is the reciprocal of \( \frac{b}{a} \) which in our example gives \( a=4 \) and \( b=1 \).

If \( m \) is a positive whole number and \( a \) is any number, where \( m \) is the index (power) of \( a \), the short and convenient way of writing \( \underbrace{a \times a \times a \ldots} \) where there are \( m \) number of \( a \)'s is \( a^m \).

The following rule \( a^m \times a^n = a^{m+n} \) always applies and it can be shown that:

For \( m = 0 \), we have \( a^0 \times a^m = a^{0+n} = a^n \) making \( a^0 = 1 \), note this means \( 10^0 = 1 \)
For \( m = 1 \) and \( n = -1 \), we have \( a^1 \times a^{-1} = a^{0} = 1 \) making \( a^{-1} = \frac{1}{a} \), note this means \( 10^{-1} = \frac{1}{10} \)

The following can be proved using the above procedure:

\[
\begin{align*}
\text{if } m &= 2, \quad a^2 = \frac{1}{a^2}, \\
\text{if } m &= \frac{1}{2}, \quad a^{\frac{1}{2}} = \sqrt{a}, \text{ the square root of } a
\end{align*}
\]

Note that \( (a^m)^n = a^{mn} \) always applies and it can be shown that \( x^{p/q} = \sqrt[q]{x^p} \)

\( a^{\frac{2}{3}} = \sqrt[3]{a^2} \) is the cubed root of \( a^2 \)

Number Convention SI Units – Prefixes

From the above we can deduce that fractions such as \( 1/10 = 10^{-1} \), \( 1/100 = 10^{-2} \) and so on. Numbers in the form \( 10^7 \) cannot be conveniently represented in computer programs, so the scientific notation is used where the \( 10^7 \) is now \( E07 \). Note E is not related to the mathematical constant e or the exponential function. The following conventions avoid errors in allocating the correct number of 0’s.

<table>
<thead>
<tr>
<th>Factors</th>
<th>Prefix</th>
<th>Symbol</th>
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</thead>
<tbody>
<tr>
<td>( 10^{-12} )</td>
<td>E-12</td>
<td>pico</td>
</tr>
<tr>
<td>( 10^{-9} )</td>
<td>E-09</td>
<td>nano</td>
</tr>
<tr>
<td>( 10^{-6} )</td>
<td>E-06</td>
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</tr>
<tr>
<td>( 10^{9} )</td>
<td>E09</td>
<td>giga</td>
</tr>
<tr>
<td>( 10^{12} )</td>
<td>E12</td>
<td>tera</td>
</tr>
</tbody>
</table>

Note 1 Tip for setting power, make equal to number 0’s so 0.00001 = \( 10^{-5} \) and 100000 = \( 10^5 \)

Note 2 Refinery industry sometimes uses MM to signify \( 10^6 \)

Unit converters are now available from many sources so are not shown here. A typical example for energy is shown. The unit to be converted from is multiplied by the factor shown in column with the desired unit.

<table>
<thead>
<tr>
<th>to</th>
<th>Btu</th>
<th>joule</th>
<th>kWh</th>
<th>therm</th>
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<td></td>
<td></td>
<td></td>
<td></td>
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<td>0.2931E-03</td>
<td>1E-06</td>
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<tr>
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<td>3.6E06</td>
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<td>100E03</td>
<td>105.5E06</td>
<td>29.31</td>
<td>1</td>
</tr>
</tbody>
</table>

1000 Btu = \( 10^3 \) Btu = \( 1E03 \) Btu = \( 1.055E06 \) joule = \( 0.2931 \) kWh = \( 1E-03 \) therm
Formulae

The concept of using letters in place of numbers provides a powerful technique to define specific relationships and to perform units conversion. This approach allows the development, in many fields, of formulae to provide a statement in general terms of a whole series of particular facts or physical relationships.

Velocity, acceleration and distance

Let \( t \) represent time in seconds (s)

The reciprocal of time is called frequency \( f \) so \( f = 1/t \)

with units of 1/s or in the index form s\(^{-1}\).

If a stirrer in a vessel rotates once in half a second it will rotate 2 times per second or 2/s or 2s\(^{-1}\).

\( t/60 \) represents time in minutes obtained from units equation (s x m/60s), note the s cancels out.

\( t/3600 \) represents time in hours obtained from units equation (s x h/3600s)

\[ (v-u)/t \] represents the change in speed over \( t \) seconds the acceleration \( a \) (ft/s \times 1/s) giving units ft/s\(^2\).

This leads to the formula

\[ a = (v-u)/t \] ft/s\(^2\) or ft-s\(^{-2}\).

The distance travelled in time \( t \) is given by

\[ s = ut + t(v-u)/2 \] ft, number group unit is ft

Substituting for \( (v-u) = at \) gives

\[ s = ut + \frac{1}{2}at^2 \] ft, number group unit is ft

Temperature Conversion

To convert from °F to °C we have:

\[ °F = 9/5 °C + 32 \]

A temperature of -10°C is equivalent to

\[ °F = 9/5 \times -10 + 32 = 14 \]

Pressure Conversion

Absolute pressure \( p_a \) is the pressure above a total vacuum and gauge pressure \( p_g \) is the pressure above or below atmospheric pressure \( p_{atm} \) giving:

\[ p_a = p_g + p_{atm} \text{ for } p_g > p_{atm} \quad p_a = p_g - p_{atm} \text{ for } p_g < p_{atm} \]

At atmospheric pressure \( p_{atm}(kg/m^2) \), the absolute pressure \( p_a(kg/m^2) \) at the bottom of a column of liquid with a density \( p(kg/m^3) \) and height \( H(m) \) is:

\[ p_a = Hp + p_{atm} \text{, check units RHS = kg/m}^3 \times m = kg/m^2 = \text{LHS} \]

To convert \( p_a \) from kg/m\(^2\) to bar.

We know 1 kg/cm\(^2\) = 0.98065 bar and 1 cm\(^2\) = 0.0001 m\(^2\) so 1/10\(^{-4}\) = 10\(^4\) kg/m\(^2\) = 0.98065 bar

1.0197 x 10\(^4\) kg/m\(^2\) = 1 bar leading to \( p = Hp / (1.0197 \times 10^4) \) bar.

\( p_{atm} = 1.01325 \) bar, so a \( p_g \) of 5 barg is equivalent to \( p_a \) of 6.01325 bar and a vacuum \( p_g \) of 0.5 barg is equivalent to \( p_a \) of 0.51325 bar.

Power to pump liquids

The following example demonstrates the rigorous application of unit conversions and the use of a formula to calculate the power to pump a liquid. The theoretical power to pump \( Q \) (litres/min) of liquid, with density \( p(kg/m^3) \), against a differential head \( h(m) \) or \( \Delta p(bar) \) is given by:

\[ P = Qhp/(6116x10^3) = Q\Delta p/600 \text{ kW} \]

Density of water \( \rho_{H2O} = 1 \) gm/cm\(^3\),

We need to convert to kg/m\(^3\) we know 1000 gm = 1 kg and 1 cm\(^3\) = 10\(^{-6}\) m\(^3\)

\( \rho_{H2O} = 1 \times 1/1000 \times 1/10^{-6} =1000 \) kg/m\(^3\), check units RHS =gm/cm\(^3\) x kg/gm x cm\(^3\)/m\(^3\) = kg/m\(^3\) = LHS

Power to pump 1000 litres/min of water 50 metres equals 1000x50x1000/(6116x10\(^3\)) = 8.167 kW

The overall efficiency \( \eta_o \), a fraction in range 0 – 1, is derived from the drive efficiency \( \eta_d \) the transmission efficiency \( \eta_t \) and the pumping efficiency \( \eta_p \) from \( \eta_o = \eta_d \times \eta_t \times \eta_p \).

The volumetric efficiency \( \eta_v = \frac{\text{actual pump flow } Q_{act}}{\text{theoretical pump flow } Q_t} \).
12.2 Process Engineering Units \(^{(3,4)}\)

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 also reviewed.

**Molality, Molarity, Mole Fraction and Mole Ratio**

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/m3) 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:

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

The weight fraction \(w_i\) of a component in an aqueous solution is calculated from:

\[
w_i = \frac{M_i MW_i}{\rho_{SO} \ln 1000}
\]

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

\[
M_{AB} = \frac{W_A / M_A + W_B / M_B}{W_A / M_A + W_B / M_B}
\]

For a system pressure \(P=1.01325\) bar and temperature \(T\) °K the inlet gas density (g/litre or kg/m\(^3\)) is given by:

\[
\rho_I = \frac{M_{AB}}{22.4} \left(\frac{273}{273 + T}\right)
\]

The gas inlet concentration of component \(A\) can be converted from mole fraction to mg/m\(^3\) using:

\[
y_A \times 10^6 \left[\frac{M_A}{22.4} \left(\frac{273}{273 \times T}\right)\right]
\]

Weight fraction is converted to mole fraction as follows:

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