PROCESS SIMULATION

DYNAMIC MODELLING & CONTROL

Design, Implementation and Operation

SAMPLER

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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.

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.

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

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

The iterative process can be based on 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 columns, recycle loops and controllers may converge faster in this mode. Pressure Nodes require this calculation mode.

The AutoCalc mode uses rigorous logic to determine the calculation sequence. This mode is not recommended on new models.
The chart below shows the basic steps involved in setting up a steady simulation.

1. Create the flowsheet incorporating dynamic unit operations - select components and thermodynamic method - enter feed stream and equipment specifications. These steps are identical to the ones performed for steady-state simulation.

2. Determine the initial state for a dynamic simulation. This may include calculating the flowsheet in steady state and adjusting several parameters by hand - sizing the equipment such as control valves, tank geometry and hydraulics of distillation columns.

3. Set dynamic run parameters such as simulation time, simulation step size, defining objects and parameters to be recorded.

4. 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.

5. Interpret the results and optimize the model.

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:
Section 2

Dynamic Simulation Basics

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2.1 Introduction

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</table>
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 ($P_i$) and outlet ($P_o$) pressures to be specified where $P_i$ is taken from the inlet stream. $P_o$ can be specified directly or overtaken indirectly by an assigned UnitOp in the model. A mass balance must be maintained around the control valve. 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 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)

![Optional mass flow rate transfer](image)

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 database 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.

![Flowsheet Diagram](image)

**Engineering Units**

Format Menu

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.

**Components and Define Thermodynamics**

1. Click button in the toolbar.

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. Open Thermodynamic Menu and define K and H values by clicking button in the toolbar.

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.
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:

<table>
<thead>
<tr>
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<th>Value</th>
<th>Units</th>
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<tbody>
<tr>
<td>Temperature</td>
<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.
Section 3

Process Measurement and Control

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3.3 Control Valves

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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](image)

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:
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.

\[ D_E = \text{Diesel in Methyl Ester Flow (m}^3\text{/h)} \quad E = \text{Methyl Ester Flow (m}^3\text{/h)} \quad D_S = \text{Diesel Flow from Ship (m}^3\text{/h)} \quad V_P = \text{Bio-diesel Product Volume Fraction} \]

We have:

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

Rearranging gives:

\[ D_E = \frac{E (1 - V_E)}{V_E} \quad \text{and substituting for } D_E \text{ leads to the following:} \]

\[ E = \frac{V_P D_S}{(1 - V_P/V_E)} \quad \text{and} \quad \frac{D_E + E}{D_S} = \frac{1}{(V_E/V_P - 1)} \]

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.
3.2 Orifice Plate Flowmeters

The differential pressure measured and unrecovered pressure loss across a square edge concentric orifice plate is dependent on the pressure tap location; as shown in the diagrams below. It can be seen that full flow taps (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:

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

For gases

\[ W = K \cdot d^2C \sqrt{\frac{h \cdot p_r \cdot M}{T_f}} \]
Sizing Methods


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

\[
S = \frac{W_m}{N D^2 F_a F_m \sqrt{G_f} \sqrt{h_m}}
\]

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:

\[K_r = \frac{1 - \beta^2}{C\beta^4}\]

\[C = \frac{C_d}{(1 - \beta^4)^{1/5}}\]

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:

\[
S = \frac{W_m}{N D^2 F_a F_m F_c \sqrt{G_f} \sqrt{h_m}}
\]

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.
3.3 Control Valves \(^{(2,3)}\)

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.

For a detailed review of valve sizing issues refer to Emerson Process Management, Fisher Control Valve Handbook, 4\(^{th}\) Edition\(^{(3)}\). Piping installation factors affect the valve performance which are reviewed here.

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 \(\frac{1}{2}D\). 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 \(^{(3)}\)

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 \(\Delta P < C_i^2(\Delta P_s)\)

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

Where:

- \(q\) liquid flow rate \((m^3 / h)\)
- \(C_f\) 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 \(\Delta P \geq C_i^2(\Delta P_s)\)

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

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

Where:

- \(P_1\) upstream pressure (bar)
- \(P_2\) downstream pressure (bar)
- \(P_x\) 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:

\[
C_v = 0.032 \left( \frac{\mu \cdot q}{\Delta P} \right)^{0.667}
\]
Control Valve Sizing Correction for Reducers

The valve sizing is adjusted by the Piping Geometry Factor, \( F_p \), which for a valve installed between identical reducers, is given by:

\[
F_p = \left( 1 + \frac{\sum K}{N_2} \left( \frac{C_v}{d^2} \right)^2 \right)^{-0.5}
\]

\( \sum K = K_1 + K_2 = 1.5 \left( 1 - \beta^2 \right) \)

Where:

- \( d \) nominal valve size (in or mm)
- \( \beta \) \( d/D \)
- \( N_2 \) 0.00214 (mm) and 890 (in) and \( C_v \) is valve sizing coefficient at 100% opening.

For liquid sizing we have a modified coefficient:

\[
C_v = \frac{q}{N_1 F_p \sqrt{G_f}} \sqrt{\frac{P_1 - P_2}{G_f}}
\]

Where:

- \( N_1 \) 0.0865 (m³/h, kPa), 0.865 (m³/h, bar), 1.00 (gpm, psia)
- \( G_f \) specific gravity referenced to water at 60°F

CHEMCAD allows for entry of \( F_p \) correction factor in the control valve sizing calculation procedure.

CHEMCAD calculates the equivalent length of fittings using the pipe friction factor and not the friction factor at fully turbulent conditions. This procedure is acceptable at fully turbulent conditions. However under laminar and transitional flow conditions results should be checked, using the relationships presented here, to ensure acceptable design conditions. If it is found that the pressure loss is significantly increased through the use of the prevailing friction factor the user can modify the equivalent length by adding an additional \( L/D \) correction.

To overcome these problems the Darby 3K Method can be used which is valid over a wide range of \( Re \) and fitting size. Where we have:

\[
K_f = \frac{K_m}{Re} + K_i \left( 1 + \frac{K_d}{D_{in,nom}^{0.3}} \right)
\]

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

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

<table>
<thead>
<tr>
<th>Nomenclature for General Equations (Note: units in fps, some equations are unit specific)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f )</td>
</tr>
<tr>
<td>( Re )</td>
</tr>
<tr>
<td>( \rho )</td>
</tr>
<tr>
<td>( D )</td>
</tr>
<tr>
<td>( d )</td>
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<tr>
<td>( a )</td>
</tr>
<tr>
<td>( v )</td>
</tr>
<tr>
<td>( p )</td>
</tr>
<tr>
<td>( H )</td>
</tr>
</tbody>
</table>
Control Valve and Actuator Construction

Control Valve Body Types

- Reverse Double-Ported Globe
- Angle
- Three-Way with Balanced Plug

Eccentric Disc Control Valve with Rotary Shaft Actuator

Sliding Stem Diaphragm Actuator

Direct Acting  Reverse Acting
Control Valve CHEMCAD Calibration

For Reverse control action specify Controller Parameter \( \text{Error} = X_{\text{set}} - X \)
Increasing Measurement with Decreasing Controller Output gives Cooling for Fail Open Valve.
Decreasing Measurement with Increasing Controller Output gives Heating for Fail Closed Valve.

For Direct control action specify Controller Parameter \( \text{Error} = X - X_{\text{set}} \)
Increasing Measurement with Increasing Controller Output opens Fail Closed Valve e.g. Level control on tank outlet or Pressure control on tank outlet.
Decreasing Measurement with Decreasing Controller Output opens Fail Open Valve e.g. Level control on tank inlet or Pressure control on tank inlet.

### SINGLE CONTROL VALVE OPERATIONS

<table>
<thead>
<tr>
<th>ACTION</th>
<th>CONTROL OUTPUT</th>
<th>POSITION</th>
<th>STATE</th>
<th>LOGIC EQUATION</th>
<th>COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mA</td>
<td>%</td>
<td></td>
<td></td>
<td>A_v</td>
</tr>
<tr>
<td>FAIL CLOSED</td>
<td>4</td>
<td>0</td>
<td>Closed</td>
<td>0</td>
<td>(0 = 4A_v + B_v)</td>
</tr>
<tr>
<td>FAIL OPEN</td>
<td>4</td>
<td>100</td>
<td>Open</td>
<td>1</td>
<td>(1 = 4A_v + B_v)</td>
</tr>
<tr>
<td>OPEN</td>
<td>20</td>
<td>0</td>
<td>Closed</td>
<td>0</td>
<td>(0 = 20A_v + B_v)</td>
</tr>
</tbody>
</table>

### DUAL CONTROL VALVE OPERATIONS IN SPLIT RANGE

<table>
<thead>
<tr>
<th>ACTION</th>
<th>CONTROL OUTPUT</th>
<th>POSITION</th>
<th>STATE</th>
<th>LOGIC EQUATION</th>
<th>COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mA</td>
<td>%</td>
<td></td>
<td></td>
<td>A_v</td>
</tr>
<tr>
<td>FAIL CLOSED</td>
<td>12</td>
<td>50</td>
<td>Closed</td>
<td>0</td>
<td>(0 = 12A_v + B_v)</td>
</tr>
<tr>
<td>FAIL OPEN</td>
<td>4</td>
<td>0</td>
<td>Open</td>
<td>1</td>
<td>(1 = 4A_v + B_v)</td>
</tr>
<tr>
<td>OPEN</td>
<td>12</td>
<td>50</td>
<td>Closed</td>
<td>0</td>
<td>(0 = 12A_v + B_v)</td>
</tr>
</tbody>
</table>

### 3 Way Valve

<table>
<thead>
<tr>
<th>ACTION</th>
<th>CONTROL OUTPUT</th>
<th>POSITION</th>
<th>STATE</th>
<th>LOGIC EQUATION</th>
<th>COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>mA</td>
<td>%</td>
<td></td>
<td></td>
<td>A_v</td>
</tr>
<tr>
<td>Fail Open Signal to Close</td>
<td>4</td>
<td>12</td>
<td>Open</td>
<td>0</td>
<td>(0 = 4A_v + B_v)</td>
</tr>
<tr>
<td>Fail Closed Signal to Open</td>
<td>4</td>
<td>20</td>
<td>Closed</td>
<td>0</td>
<td>(0 = 20A_v + B_v)</td>
</tr>
</tbody>
</table>
**Section 4**

**Heat Exchangers**

**Contents**

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

<table>
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<tr>
<th>Fluid Flow and Control Valves</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:

![Shell and Tube Heat Exchanger Diagram](image)

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

\[ Q = U \cdot A \cdot \Delta T_{lm} = w \cdot \left( C_{p(t)} \cdot (t_2 - t_1) \right) = W \cdot \left( C_{p(s)} \cdot (T_1 - T_2) \right) \]

Where:

- \( Q \) = heat transferred per unit time (kJ/h, Btu/h)
- \( U \) = the overall heat transfer coefficient (kJ/h-m² · °C, Btu/h-ft² · °F)
- \( A \) = heat-transfer area (m², ft²)
- \( \Delta T_{lm} \) = log mean temperature difference (°C, °F)
- \( C_{p(t)} \) = liquid specific heat tube side, (kJ/kg·°K, Btu/lb·°F)
- \( C_{p(s)} \) = liquid specific heat shell side, (kJ/kg·°K, Btu/lb·°F)
- \( w \) = tube side flow, \( W \) = shell side flow (kg/h, lb/h)
The log mean temperature difference (LMTD) $\Delta T_{lm}$ for countercurrent flow is given by:

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

Where:

- $T_1$ inlet shell side fluid temperature
- $T_2$ outlet shell side fluid temperature
- $t_1$ inlet tube side temperature
- $t_2$ outlet tube side temperature

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

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

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

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


It should be noted that the heat exchanger configuration correction factor should be >0.75.

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

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

The combined fouling coefficient $h_f$ can be defined as follows:

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

The individual heat transfer coefficients depend on the nature of the heat transfer process, the stream properties and the heat transfer surface arrangements. The heat exchanger layout depends on the heat transfer area (HTA) so an initial estimate is required based on a trial value of the OHTC. Typical values for the OHTC are shown in General Data Section 10.

The heat curves for sensible heat and condensing applications are shown:
4.2 Fouling Considerations

The fouling factors chosen can have a significant effect on the design and again typical values are shown in General Data Section 10.

It can be shown that the design margin achieved by applying the combined fouling film coefficient is given by:

$$\frac{A_f}{A_C} = 1 + \frac{U_C}{h_f}$$

Where: \(A_C\) is the clean HTA, \(A_f\) is the dirty or design HTA and \(U_C\) is the clean OHTC.

<table>
<thead>
<tr>
<th>Fouling Resistances</th>
<th>Fouling Coefficients</th>
<th>Clean OHTC</th>
<th>Design Margin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inside</td>
<td>Outside</td>
<td>Inside</td>
<td>Outside</td>
</tr>
<tr>
<td>0.002</td>
<td>0.001</td>
<td>500</td>
<td>1000</td>
</tr>
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</tr>
<tr>
<td>0.001</td>
<td>0.001</td>
<td>1000</td>
<td>1000</td>
</tr>
</tbody>
</table>

Corrosion Fouling

Heavy corrosion can dramatically reduce the thermal performance of the heat exchanger. Corrosion fouling is dependent on the material of construction selection and it should be possible to eliminate altogether with the right choice. However if economics determine that some corrosion is acceptable and no data is available from past experience an allowance of \(\frac{1}{16}\) in (1.59 mm) is commonly applied.

Pressure Drop

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

<table>
<thead>
<tr>
<th>Process Description</th>
<th>Pressure Drop (psi)</th>
<th>Pressure (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid streams with no phase change</td>
<td>10</td>
<td>70</td>
</tr>
<tr>
<td>Vapour streams with no phase change</td>
<td>2</td>
<td>14</td>
</tr>
<tr>
<td>Condensing streams</td>
<td>2</td>
<td>14</td>
</tr>
<tr>
<td>Boiling streams</td>
<td>1</td>
<td>7</td>
</tr>
</tbody>
</table>

4.3 Design Optimisation

CCTHERM always searches from a small size to a large size which ensures the minimum possible excess area consistent with satisfying the user specified shell side and tube side pressure drop and velocity design constraints.

If the design is pressure drop or velocity limited leading to an oversized area the user can relax the pressure drop and/or the velocity design constraint and possibly adjust tube pitch or diameter to make the design a heat transfer area limited design.

CCTHERM issues a message at the end of its search advising if the design is pressure drop, velocity or area limited to assist in the optimization process.

The heat exchanger design can be forced by setting design limits to constrain certain parameters. For example restricting tube length to meet an installation constraint will result in an increase in the number of tubes and hence shell diameter. Standard shell sizes are used so an increase in diameter from 8" to 10" could lead to an oversize of 56% derived from the increase in shell area ratio.

To achieve final design optimisation the user should switch to the rating mode and adjust tube length until the desired area safety margin has been achieved.
### 4.4 TEMA Heat Exchanger Layout Designation

<table>
<thead>
<tr>
<th>Front End</th>
<th>Shell Types</th>
<th>Rear End</th>
<th>Head Types</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Channel and Removable Cover</td>
<td>One Pass Shell</td>
<td>Fixed Tubesheet Stationary Head</td>
</tr>
<tr>
<td>B</td>
<td>Bonnet (Integral Cover)</td>
<td>Two Pass Shell with Longitudinal Baffle</td>
<td>Fixed Tubesheet Stationary Head</td>
</tr>
<tr>
<td>C</td>
<td>Channel Integral with Tubesheet and Removable Cover</td>
<td>Split Flow</td>
<td>Fixed Tubesheet Stationary Head</td>
</tr>
<tr>
<td>D</td>
<td>Special High Pressure Closure</td>
<td>Double Split Flow</td>
<td>Outside Packed Floating Head</td>
</tr>
<tr>
<td>E</td>
<td></td>
<td>Divided Flow</td>
<td>Floating Head with Backing Device</td>
</tr>
<tr>
<td>F</td>
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<td>G</td>
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<tr>
<td>Z</td>
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</tbody>
</table>

**TEMA CLASS** | **APPLICATION**
---|---
R | Severe requirements of petroleum and related process applications
C | Moderate requirements of commercial and general process applications
B | Chemical process service
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. A variable temperature process water 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 Thermodynamics
5.3 Mass and Energy Balances

<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.

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. However reduced pressure operation is sometimes required to achieve the desired separation, to reduce operating temperature for economic reasons, or when processing temperature sensitive materials.

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

The boil up rate achievable with stirred jacketed reactors is dependent upon many factors including operational temperature difference, jacket heating media and heat transfer considerations\(^4, 5\).

**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 flow rate 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.
6.1 Introduction

It is recommended that the SCDS UnitOp is used for building fully integrated models because it has a greater number of connection points.

SCDS 1 and SCDS 21-24 icons are the most developed having built in dynamic vessels and control loops. However for our initial exercise we will use SCDS Column 1 icon.

For refinery operations the Tower UnitOp is more suitable as it includes pump around and stripping facilities.
6.2 Column Specification

The stage numbering convention in CHEMCAD is from top to bottom, 1 to N. A stage is considered the space above a plate. If a condenser is present it is stage 1; if a reboiler is present it is stage N. To model a column which has ten stages plus condenser and reboiler 12 stages (10+condenser+reboiler = 12) must be specified.

If a condenser is present, the feed must not enter stage 1, as that is the reboiler. Top stage feeds should enter stage 2, the top stage (plate), if a condenser is present. Likewise, if a reboiler is present a bottom plate feed is connected to stage (N-1), not stage N.

6.3 Convergence

Typically the user has a product specification, mass fraction of a key component in either the bottoms or tops, for a column design or to achieve with an existing column.

Converging a column model in simulation is similar to converging a column in the real world; it is difficult to go directly to high purity separation. It is best to start with an easy target, such as reflux ratio and bottoms flowrate. Once the column is converged to this simple specification, we ‘tightly’ the specifications toward the target specification. Use the following procedure:

1. Set up the column: number of stages, condenser, reboiler, operating pressure.
2. Generate TPxy and RCM plots to verify that the target is thermodynamically feasible with the selected VLE K model.
3. On the SPECIFICATIONS page, set ‘loose’ specifications such as ‘Reflux Ratio’ and ‘Bottoms Flowrate’ or Reboiler Heat Input.
4. Run the column and converge. Change the specifications if necessary.
5. Go to the CONVERGENCE page of the column dialog. Set the initial flag to 0 Reload Column Profile. This setting instructs CHEMCAD to use the current converged profile as it’s starting point (initial conditions) in iterative calculations.
6. On the SPECIFICATIONS page change to more tight specifications. Run the column.

If the column converges, tighten the specifications and run again. If the column fails to converge, do not save the profile of the failed attempt. Relax the specifications and run the column again. Repeat from step 5 until you reach the target.

Often, it is difficult to obtain the first convergence on a column. If the column is run with no condenser or reboiler, one does not have the option of ‘loose’ specifications. If the column has a condenser or reboiler, relaxing specifications does not always help.

1. On the convergence page of the column dialog, specify estimates if you can make reasonable estimates. Note that a bad guess will make the column more difficult to converge than no estimate.
2. Remove non key components from the feed(s) to obtain the first convergence. Now set the initial flag to 0 Reload Column Profile, return the other components, and run the unit again.
3. Specify a larger number of iterations on the convergence page of the column dialog. The default is 50, but possibly 52 iterations will find the answer.
4. Try an alternate column model. If you are currently using the SCDS try the same separation with a TOWER or vice versa. The two models use different mathematical models; often one will find an answer in 10 iterations while the other is difficult to converge. It is not possible to obtain different answers with the columns; the models are numerical methods to find a stable composition profile.
5. Consider a partial condenser. If you have a condenser present but have a significant amount of light ends, you may have difficulty converging the column. The default condenser type, total, requires that no vapor leaves stage 1. If light ends are present, this may not be possible without cryogenic temperatures. Changing condenser mode to partial allows the light ends gases to slip past the condenser.
Section 7

Batch Reactors

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

<table>
<thead>
<tr>
<th>Case/File Name</th>
<th>Description</th>
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<tbody>
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<td>Reactor Indirect Heating – Direct Cooling</td>
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<tr>
<td>D7.02</td>
<td>Reactor Indirect Heating – Indirect Cooling</td>
</tr>
<tr>
<td>D7.03</td>
<td>Reactor Jacket Circulation Hydraulics</td>
</tr>
<tr>
<td>D7.04</td>
<td>Cryogenic Batch reactor System</td>
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<td>D7.05</td>
<td>Storage Tank Heating</td>
</tr>
<tr>
<td>D7.06</td>
<td>Batch Reactor Kinetics</td>
</tr>
</tbody>
</table>

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

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:

\[
Q = U \Delta T_m = V f C_p j (t_2 - t_1)
\]

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:

\[
h_f = \frac{h_{fi} h_{fo}}{h_{fi} + h_{fo}}
\]
The stirred batch reactor inside film coefficient $h_i$ is predicted using the Sieder-Tate equation defined as follows:

$$Nu = C \cdot Re^{0.667} \cdot Pr^p \left( \frac{\mu_h}{\mu_w} \right)^q$$

- $Nu$ Nusselt number
- $Re$ Reynolds number
- $Pr$ Prandtl number
- $\mu_b$ process side bulk viscosity
- $\mu_w$ process side viscosity at the wall
- $C, p, q$ empirical constants available from manufacturer

$$Nu = \frac{h_i D}{k_i}$$

- $D$ reactor inside diameter
- $k_i$ process fluid thermal conductivity

$$Re = \frac{\rho n d^2}{\mu_b}$$

- $n$ impeller rotation rate
- $d$ impeller diameter
- $\rho$ process fluid density

$$Pr = \frac{C_p \mu}{k}$$

$C_p$ process fluid specific heat

In low viscosity applications $\frac{\mu_b}{\mu_w}$ approaches unity and is ignored.

<table>
<thead>
<tr>
<th>AGITATOR TYPE</th>
<th>C</th>
<th>p</th>
<th>q</th>
<th>RANGE</th>
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</thead>
<tbody>
<tr>
<td>IMPELLER (3 BLADES)</td>
<td>0.33</td>
<td>0.33</td>
<td>0.14</td>
<td>$2 \times 10^4 &lt; Re &lt; 2 \times 10^6$</td>
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<tr>
<td>ANCHOR</td>
<td>0.55</td>
<td>0.25</td>
<td>0.14</td>
<td>$5 \times 10^3 &lt; Re &lt; 4 \times 10^4$</td>
</tr>
<tr>
<td>TURBINE (6 BLADES)</td>
<td>0.44</td>
<td>0.33</td>
<td>0.24</td>
<td>$200 &lt; Re &lt; 1 \times 10^3$</td>
</tr>
</tbody>
</table>

The outside film coefficient $h_o$ depends on the type of heat transfer surface, namely external jacket(s) with or without mixing nozzles, external half coil(s) or internal coil(s). For coils and half coils (refer Appendix II) the outside film coefficient $h_o$ is determined using the following:

$$Nu = \frac{h \cdot d_{equ}}{k_o} = 0.027 \left( Re \right)^{0.8} \left( Pr \right)^{0.33}$$

$$d_{equ} = \frac{4 \cdot X \cdot Flow \cdot Cross \cdot Sectional \cdot Area}{Wetted \cdot Perimeter \cdot for \cdot Heat \cdot Transfer}$$

$Re$ is calculated using $d_{equ}$ with $h_o$ being evaluated under actual process conditions.

The outside film coefficient $h_o$ for baffled jackets without mixing nozzles are calculated using the above relationships. For mixing nozzle applications, manufacturers’ proprietary methods are used to calculate $Re$, raised to a modified coefficient, depending on whether turbulent or laminar flow conditions.
To establish the thermal rating of the reactor a heat balance is made to establish the heat up and cool down rates based on agreed design parameters using the following:

\[ Q = 3600 \ U \ A \left( T - t_i \right) = \frac{dT}{d\theta} \left( W \ C_{pr} + M \ C_p + m \ C_{pr} \right) 60 \]

where \( Q \) is reactor heat duty in kJ/h and \( \frac{dT}{d\theta} \) is the temperature change in °C/m.

The reactor duty, kJ/h, is calculated from:

\[ Q = 3600 \ U \ A \left( T - t_i \right) \]

The rate of temperature, °C/m, change is calculated from:

\[ \frac{dT}{d\theta} = \frac{Q}{\left( W \ C_{pr} + M \ C_p + m \ C_{pr} \right) 60} \]

The time \( \theta \) (min) for temperature change from \( T_1 \) to \( T_2 \) can be calculated \((8, Eq 18.7)\) using mean values for the specific heat and \( U \) in the temperature range under consideration:

\[ \theta = \frac{\left( W \ C_{pr} + M \ C_p + m \ C_{pr} \right)}{U \ A} \ln \left( \frac{T_1 - t_i}{T_2 - t_i} \right) \]

The boil up rate \( V \) (kg/h) without reflux is calculated from:

\[ V = \frac{Q}{L} \]

For total reflux the heat input is given by:

\[ Q = V \ C_p \left( T_{bp} - T_c \right) \]

The total heat input\((5, 12)\) to reduce the reactor contents from \( N_0 \) to \( N_1 \) mols at different operating conditions are given by:

For variable top composition (constant reflux ratio)

\[ Q_T = L \left( R + 1 \right) \int_{N_1}^{N_i} dN \]

For constant top composition (variable reflux ratio)

\[ Q_T = L \int_{N_i}^{N_1} dN \int_{R_o}^{R_1} \left( R \right) dR \]

Both relationships indicate that the reflux ratio must be kept to a minimum, subject to satisfying the desired separation specification, to optimise the heat input.
Section 8

Emergency Relief

Contents

8.1 Introduction
8.2 Relief System and Piping Headers

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<td>D8.01</td>
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<tr>
<td>D8.02</td>
<td>Dynamic Relief Three Vessels</td>
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<tr>
<td>D8.03</td>
<td>Fire Induced Runaway Reaction</td>
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8.1 Introduction

To achieve safe operation of chemical processes, particularly when involving exothermic reactions, requires a combination of preventative and protective measures. Preventative measures minimise the occurrence of an event and include:-

- Automatic control systems including the use of independent hardwired alarm and trip systems based on 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.

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.

A pressure relief device is either a relief valve, 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.

To mitigate against the loss of containment, due to operation of a bursting disc sized for the worst case scenario, the installation of a smaller bursting disc/relief valve combination in parallel set at a lower relief pressure can be considered. This smaller system operates in the event of nuisance pressure build ups, due to maloperation, without total loss of containment. This technique has the disadvantage, due to the poor set pressure tolerance of bursting discs typically, ±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.

### Relief System Pressures

- Design Pressure + 10%
- Design Pressure
- Set Pressure + 10%
- Set Pressure
- Pressure rise due to runaway reaction
- Safety valve starts to open
- Valley discharges full capacity, and pressure continues to rise but at reduced rate
- Peak pressure occurs at design pressure +10%

### 8.2 Relief System Piping and Headers

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

- Branch pipe from reactor to the header to be not less than the outlet diameter of relief device.
- Branch pipe to enter main header as a 45 degree T, flow through branch.
- All 90° bends to have maximum R/D consistent with layout constraints.
- Main header to slope towards the blowdown drum and enter tangentially.
- Consideration to be given to nitrogen inerting to prevent explosive mixtures.
- Provision of adequate inspection and test facilities to ensure headers are clear.
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, as described in Section 5. 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.
The vessel pressures and relief valve back pressures are shown in the plots. The back pressure conditions will be acceptable in this coincident relief situation provided the relief valves' capacity and operation are not affected by the superimposed back pressure. In this case balanced valves should be given consideration.

Case D8.02 Dynamic Relief Three Vessels

The previous case is now extended to study the behaviour of three identical vessels subjected to a coincident external fire relieving into a common header system. The main parameters are shown in the simulation flowsheet.

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


Section 9

Engineering Fundamentals

Contents

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9.2 Fluid Flow Synopsis
9.3 Mass and Energy Balance Fundamentals
9.4 Process Measurement Technology Synopsis

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</tr>
<tr>
<td>D9.01</td>
</tr>
<tr>
<td>D9.02</td>
</tr>
</tbody>
</table>

References

Maths and Units

Fluid Flow

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

The following can be proved using the above procedure:

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

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

\[
\text{a}^{\frac{1}{3}} = \sqrt[3]{a^2} \text{ is the cubed root of a}^2
\]

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>Note 1</th>
<th>Prefix</th>
<th>Symbol</th>
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</tr>
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</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>
</tr>
</thead>
<tbody>
<tr>
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<td>0.2931E-03</td>
<td>10E-06</td>
</tr>
<tr>
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<td>kWh</td>
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<tr>
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<td>105.5E06</td>
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</tbody>
</table>

1000 Btu = \( 10^3 \) Btu = 1E03 Btu = 1.055E06 joule = 0.2931 kWh = 10E-03 therm
9.2 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:

\[
q = a_1 v_1 = a_2 v_2 \quad \Rightarrow \quad D_1^2 v_1 = D_2^2 v_2 \quad \Rightarrow \quad \frac{D_2^2}{D_1^2} = \frac{v_2}{v_1} = \beta
\]

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 predict 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:

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

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 \( L \):

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

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:

\[
\left( \frac{dP}{dL} \right)_f = f \frac{\rho v^2}{2g \ D}
\]
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:

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

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

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
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.

\[ x_i = \frac{m_i \cdot M W_S}{1000} \]

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:

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

The weight fraction $w_i$ of a component in an aqueous solution is calculated from:

\[ w_i = \frac{M_i \cdot M W_i}{\rho_S \cdot \ln 1000} \]

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/m³) is given by:

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

The gas inlet concentration of component $A$ can be converted from mole fraction to mg/m³ using:

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

Weight fraction is converted to mole fraction as follows:

\[ \frac{w_i / M W_i}{w_i / M W_i + (1-w_i)/18} \]
ppm (w), ppm (v), mg/m³, mole fraction and weight fraction

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

Pollutants in gases
Consider at 20°C
\[
\text{ppm}_v = \frac{\text{mg}}{\text{m}^3} = \frac{\text{mg}}{\text{m}^3} \times \frac{22.415}{\text{MW}} = \frac{\text{mg}}{\text{m}^3} \times \frac{24.055}{\text{MW}}
\]

Pollutants in liquids
Consider for water, where L is a litre and \( \rho \) is liquid density:

\[
\text{ppm}_w = \frac{\text{mg}}{\text{L} \times \rho} = \frac{\text{mg}}{\text{L}} = \frac{\text{ppm}_w \times 10^6}{\text{MW}}
\]

For example, trichloroethylene (MW 131.4 g/mol) has a consent limit for drinking water, using preferred units, of 0.005 mg/L = 0.005 ppm(w). Therefore the consent limit as a weight fraction is 0.005x10^{-6} and as a mole fraction is 0.000684x10^{-6}.

We have defined: 1 g-mole of any gas occupies 22.415 litre(dm³) at 0°C and 1 atmosphere. Therefore we can say that the same g-mole of any gas will occupy the same volume giving:

\[
\text{Mole} \% = \text{Volume} \%
\]

For a Total Flow of \( W \) (kg/h) and a mixture density of \( \rho_{G0} = \frac{M}{2241.5} \) (kg/m³) we have:

\[
\text{Volumetric Flow} = \frac{W}{\rho_{G0}} = \frac{2241.5W}{\sum P_i M_i} \text{ (Nm}^3/\text{h)}
\]

Where average MW
\[
\overline{M} = \frac{\sum P_i M_i}{100} \text{ (kg/kmol)}
\]

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

\[
\rho_c = \frac{M_w}{22.415} \times \frac{P_i}{Z_i} \times \frac{273}{T_i} \text{ kg/m}^3
\]

where 22.415 is in units of litre(dm³)/g-mole or m³/kg-mole of any gas at NTP(0°C,1atm), \( M_w \) is molecular weight g/mol or kg/kmol.

<table>
<thead>
<tr>
<th>Component</th>
<th>MW (kg/kmol)</th>
<th>% v/v</th>
<th>Volume in 1 m³</th>
<th>Mass in 1 m³</th>
<th>% w/w</th>
<th>Mass Flow</th>
<th>Molar Flow</th>
<th>% mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>M_A</td>
<td>P_A</td>
<td>V_A = \frac{P_A}{100}</td>
<td>P_A M_A 2241.5</td>
<td>\frac{100 P_A M_A}{\sum P_i M_i}</td>
<td>\frac{W P_A M_A}{\sum P_i M_i}</td>
<td>\frac{W P_A}{\sum P_i M_i}</td>
<td>P_A</td>
</tr>
<tr>
<td>B</td>
<td>M_B</td>
<td>P_B</td>
<td>V_B = \frac{P_B}{100}</td>
<td>P_B M_B 2241.5</td>
<td>\frac{100 P_B M_B}{\sum P_i M_i}</td>
<td>\frac{W P_B M_B}{\sum P_i M_i}</td>
<td>\frac{W P_B}{\sum P_i M_i}</td>
<td>P_B</td>
</tr>
<tr>
<td>C</td>
<td>M_C</td>
<td>P_C</td>
<td>V_C = \frac{P_C}{100}</td>
<td>P_C M_C 2241.5</td>
<td>\frac{100 P_C M_C}{\sum P_i M_i}</td>
<td>\frac{W P_C M_C}{\sum P_i M_i}</td>
<td>\frac{W P_C}{\sum P_i M_i}</td>
<td>P_C</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>\sum P_i M_i 2241.5</td>
<td>100 W 2241.5</td>
<td>100</td>
<td>W</td>
<td>\frac{100 W}{\sum P_i M_i}</td>
<td>100</td>
</tr>
</tbody>
</table>

Molar and Mass Relationships for Mixture with “i” Species
9.4 Process Measurement Technology Synopsis

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.
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.
Magnetic Flowmeter

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

The following guidelines should be considered when selecting flow meter sizes.

<table>
<thead>
<tr>
<th>Service Conditions</th>
<th>Fluid</th>
<th>Reasonable Velocities</th>
<th>Pressure Drop</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>m/s</td>
<td>ft/s</td>
<td>kPa / m</td>
</tr>
<tr>
<td>General Service and Process Piping</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquids, non-viscous</td>
<td>0.9 to 4.6</td>
<td>3.0 to 15</td>
<td>Line size meter</td>
</tr>
<tr>
<td>Erosive slurries</td>
<td>0.9 to 4.6</td>
<td>3 to 6</td>
<td>Same ∆P as pipe</td>
</tr>
<tr>
<td>Coating forming liquids</td>
<td>1.8 to 4.6</td>
<td>6 to 16</td>
<td></td>
</tr>
</tbody>
</table>

Vortex Shedding Flowmeter

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

The following guidelines should be considered when selecting flow meter sizes.

On gas or steam the flow velocities are in the range

\[
\sqrt{\frac{74}{\rho}} \text{ to } 79 \text{ m/s} \quad \rho \text{ density } \frac{\text{kg}}{\text{m}^3} \quad \sqrt{\frac{50}{\rho}} \text{ to } 260 \text{ ft/s} \quad \rho \text{ density } \frac{\text{lb}}{\text{ft}^3}
\]

Process fluid viscosity requires the Reynolds Number to be greater than 20000
Linear performance is achieved for Reynolds Number in the range 20000 to 7.0 E06
Coriolis Flowmeter

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

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

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

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

Thermal Dispersion Flowmeter

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

Ultrasonic Flowmeter

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

Costings

The following sequence gives an indication of comparative costs with the lowest cost first:
Turbine → Magnetic → Vortex → Thermal → Ultrasonic → Positive Displacement → Coriolis.
The chart shows typical flow meter selection criteria and applications:

- **VAPOUR PHASE**
  - **GAS**
    - **SELECT**
    - **VORTEX**
      - 1. Invasive > wetted
    - **THERMAL MASS**
      - 2. Non-invasive > wetted
    - **CORIOLIS**
      - 3. Non-contact
    - **AXIAL TURBINE**
      - (Clean Gas)
  - **STEAM**
    - **VORTEX**
      - 1. Invasive > wetted
    - **TARGET**
      - (Saturated)
    - **CORIOLIS**
      - 2. Non-invasive > wetted
    - **ULTRASONIC**
      - (Clean Gas)

- **SLURRY PHASE**
  - **LIQUID**
    - **HIGH VISCOSITY**
      - **MAGNETIC**
        - 1. Invasive > wetted
      - **CORIOLIS**
        - 2. Non-invasive > wetted
    - **LOW VISCOSITY**
      - **MAGNETIC**
        - 1. Invasive > wetted
      - **CORIOLIS**
        - 2. Non-invasive > wetted

1. Invasive > wetted
2. Non-invasive > wetted
3. Non-contact
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($\varepsilon_R$) 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 $\varepsilon_R$ 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 $\delta\varepsilon_R$ of the liquid and the vapour space or between the two liquids are higher. Special designs, involving coated and twin probes, are used when $\delta\varepsilon_R < 1.0$, 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 $\varepsilon_R$, 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.

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

Conductivity → Capacitance → Tuning fork → Hydrostatic→ Displacer → Ultrasonic → Load cell → Radar→Nucleonic.
The charts show level instrumentation selection criteria and applications:

CONTINUOUS TYPE

ELECTRONIC TYPE

MECHANICAL TYPE

MECHANICAL

ELECTRONIC

RADAR 2
(Interface)

DISPLACER 1
(Interface)

FLOAT 1

RADAR 2

NUCLEONIC 3
(Interface)

SERVO FLOAT 1

MAGNETIC FLOAT 1

NUCLEONIC 3

CAPACITANCE 1
(Interface)

TUNING FORK 1

CAPACITANCE 1

ULTRASONIC 2

ULTRASONIC 2

HYDRAULIC 1

HYDRAULIC 1

1 Invasive > wetted
2 Non-invasive > wetted
3 Non-contact

POINT TYPE

PROCESSED APPLICATION

STORAGE

MIXED PROPS

FLUID

CLEAN

TANK FARM

DUTY

DAY/SURGE

RADAR 3, 2
GUIDED
400°C, 399 barg

RADAR 3, 2
400°C, 399 barg

RADAR 1

RADAR 3

NUCLEONIC 1
(Noisy, flash)
2% span

NUCLEONIC 1
(Noisy, flash)
2% span

SERVO FLOAT 1

SERVO FLOAT 1

RF CAPACITANCE 1

RF CAPACITANCE 1

150°C, 2 barg

HYDROSTATIC 1
(Atmospheric)

HYDROSTATIC 1
(Atmospheric)

1 Invasive > wetted
2 None invasive > wetted
3 None contact

Mixed Props:
Flashy, boiling, foaming
Surface fouling, precipitates
Varying density, viscosity

LOAD CELLS 3

LOAD CELLS 3

55
Pressure

Pressure Terminology and Units

Process pressure is defined as the force applied to a surface area with typical units as follows:

<table>
<thead>
<tr>
<th>from</th>
<th>to</th>
<th>psi</th>
<th>kg/cm²</th>
<th>bar</th>
<th>mm Hg</th>
<th>atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>psi</td>
<td>psi</td>
<td>1</td>
<td>0.07031</td>
<td>0.06895</td>
<td>51.715</td>
<td></td>
</tr>
<tr>
<td>kg/cm²</td>
<td>psi</td>
<td>14.223</td>
<td>1</td>
<td>0.9807</td>
<td>735.6</td>
<td></td>
</tr>
<tr>
<td>bar</td>
<td>kg/cm²</td>
<td>14.504</td>
<td>1.0197</td>
<td>1</td>
<td>750.06</td>
<td></td>
</tr>
<tr>
<td>mm Hg</td>
<td>bar</td>
<td>0.01934</td>
<td>0.00136</td>
<td>0.00133</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>atm</td>
<td>mm Hg</td>
<td>14.696</td>
<td>1.0332</td>
<td>1.01325</td>
<td>760</td>
<td></td>
</tr>
</tbody>
</table>

Pressure is measured in terms of absolute, gauge or vacuum pressure. The relationship between these definitions is shown in the diagram below.

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:

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

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

So we have the following absolute pressure relationships:

1 atm = 14.696 psi = 1.01325 bar which is equivalent to 0 psig and 0 barg
30 psig = 44.696 psia = 3.082 bara

It is recommended that absolute pressures are stated as “psia” and “bara” to prevent confusion. Many literature sources quote absolute and gauge pressures interchangeably leading to confusion.

In level measurement a liquid of density \( \rho \) and level \( H \) gives a static head pressure of \( \rho H \) and for a tank at atmospheric pressure \( p_a \) the level transmitter HP connection pressure will be \((\rho H + p_a)\). If the pressure transmitter LP side is connected to the tank vapour space the transmitted signal is proportional to \( \rho H \).

If the HP and LP connections are continually immersed in the liquid level the transmitted signal can be used to determine the liquid density.
Section 10

General Engineering Data

Contents

Dished End Dimensions
Commercial Steel Pipe Dimensions
Stainless Steel Pipe Dimensions
Typical Overall Heat Transfer Coefficients
Typical Fouling Resistance Coefficients
Reactor Heat Transfer Data

Reference

Storage Tank Ends

Depth Ratio = 0.249 to 0.317

<table>
<thead>
<tr>
<th>Di/Do mm</th>
<th>ri mm</th>
<th>r Approx mm</th>
<th>hi mm</th>
<th>Volume litre</th>
</tr>
</thead>
<tbody>
<tr>
<td>900</td>
<td>1372</td>
<td>50</td>
<td>112</td>
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</tr>
<tr>
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<tr>
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Based on ANSI B36.10:1970 and BS 1600 Part 2: 1970

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Based on ANSI B36.19:1965 and BS 1600 Part 2: 1970

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<td>211</td>
</tr>
<tr>
<td>Steam</td>
<td>Heavy organics</td>
<td>106</td>
<td>159</td>
</tr>
</tbody>
</table>
## Fouling Resistance Coefficients

### Cooling Water Fouling Resistances/Coefficients

<table>
<thead>
<tr>
<th>Hot Fluid Temperature</th>
<th>Up to 240 °F</th>
<th>240 to 400 °F</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Water</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Unit Select</td>
<td>Resistance ft² h°F / Btu</td>
<td>Resistance ft² h°F / Btu</td>
</tr>
<tr>
<td>Boiler Blowdown</td>
<td>2.00E-03</td>
<td>2.00E-03</td>
</tr>
<tr>
<td>Boiler Feed (Treated)</td>
<td>1.00E-03</td>
<td>5.00E-04</td>
</tr>
<tr>
<td>Brackish Water</td>
<td>2.00E-03</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>City Water</td>
<td>1.00E-03</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>Condensate</td>
<td>5.00E-04</td>
<td>5.00E-04</td>
</tr>
<tr>
<td>Cooling Tower</td>
<td>1.00E-03</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>Distilled Water</td>
<td>5.00E-04</td>
<td>5.00E-04</td>
</tr>
<tr>
<td>Engine Jacket (Closed System)</td>
<td>1.00E-03</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>Hard Water (Over 15 Grains/Gal)</td>
<td>3.00E-03</td>
<td>3.00E-03</td>
</tr>
<tr>
<td>Muddy Or Silty Water</td>
<td>3.00E-03</td>
<td>2.00E-03</td>
</tr>
<tr>
<td>River Water</td>
<td>2.00E-03</td>
<td>1.00E-03</td>
</tr>
<tr>
<td>Sea Water</td>
<td>5.00E-04</td>
<td>5.00E-04</td>
</tr>
<tr>
<td>Spray Pond</td>
<td>1.00E-03</td>
<td>1.00E-03</td>
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</tbody>
</table>

### Chemical Processing Fouling Resistances/Coefficients

<table>
<thead>
<tr>
<th>Chemical Processing Fouling Coefficient Units</th>
<th>Resistance ft² h°F / Btu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gases &amp; Vapors</td>
<td>Acid Gases 2.50E-03</td>
</tr>
<tr>
<td></td>
<td>Stable Overhead Products 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Solvent Vapors 1.00E-03</td>
</tr>
<tr>
<td>Liquid</td>
<td>Caustic Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>DEG And TEG Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>MEA And DEA Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Stable Side Draw and Bottom Product 1.50E-03</td>
</tr>
<tr>
<td></td>
<td>Vegetable Oils 3.00E-03</td>
</tr>
</tbody>
</table>

### Industrial Fluids Fouling Resistances/Coefficients

<table>
<thead>
<tr>
<th>Industrial Fluids Fouling Coefficient Units</th>
<th>Resistance ft² h°F / Btu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gases &amp; Vapors</td>
<td>Ammonia Vapor 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Chlorine Vapor 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>CO2 Vapor 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Coal Flue Gas 1.00E-02</td>
</tr>
<tr>
<td></td>
<td>Compressed Air 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Engine Exhaust Gas 1.00E-02</td>
</tr>
<tr>
<td></td>
<td>Manufactured Gas 1.00E-02</td>
</tr>
<tr>
<td></td>
<td>Natural Gas Flue Gas 5.00E-03</td>
</tr>
<tr>
<td></td>
<td>Refrigerant Vapors (Oil Bearing) 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Steam (Exhaust, Oil Bearing) 1.80E-03</td>
</tr>
<tr>
<td></td>
<td>Steam (Non-Oil Bearing) 5.00E-04</td>
</tr>
<tr>
<td>liquids</td>
<td>Ammonia Liquid 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Ammonia Liquid (Oil Bearing) 3.00E-03</td>
</tr>
<tr>
<td></td>
<td>Calcium Chloride Solutions 3.00E-03</td>
</tr>
<tr>
<td></td>
<td>Chlorine Liquid 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>CO2 Liquid 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Ethanol Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Ethylene Glycol Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Hydraulic Fluid 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Organic Heat Transfer Media 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Methanol Solutions 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Molten Heat Transfer Salts 5.00E-04</td>
</tr>
<tr>
<td></td>
<td>Refrigerant Liquids 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Sodium Chloride Solutions 3.00E-03</td>
</tr>
<tr>
<td>Oils</td>
<td>Engine Lube Oil 1.00E-03</td>
</tr>
<tr>
<td></td>
<td>Fuel Oil #2 2.00E-03</td>
</tr>
<tr>
<td></td>
<td>Fuel Oil #6 5.00E-03</td>
</tr>
<tr>
<td></td>
<td>Quench Oil 4.00E-03</td>
</tr>
<tr>
<td></td>
<td>Transformer Oil 1.00E-03</td>
</tr>
</tbody>
</table>
Reactor Heat Transfer Data

This information was provided with the permission of Pfaudler Reactor Systems.

Thermal conductivity of glass $k_g = 6.9$ Btu/ft$^2$°F/in

Glass thickness can vary between 1 mm and 2 mm. Use 1.5mm(0.06in) thick as a good average.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density $\text{kg/m}^3$</th>
<th>Specific Heat $\text{kJ/kg °K}$</th>
<th>Thermal Conductivity $\text{W/m °K}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon Steel</td>
<td>8000</td>
<td>0.4</td>
<td>52</td>
</tr>
<tr>
<td>Stainless Steel</td>
<td>8000</td>
<td>0.5</td>
<td>16.2</td>
</tr>
<tr>
<td>Hastelloy C</td>
<td>8690</td>
<td>0.423</td>
<td>11.1</td>
</tr>
</tbody>
</table>

Outside film coefficient

For steam on the jacket side take an outside film coefficient of $8517$ W/m$^2$°K (1500 Btu/ft$^2$°F)

For water or other fluid on the jacket side, use the Pfaudler equations or consult the circulating nozzle leaflets.

Fouling coefficients

- Fouling on inner vessel: typical value $5678$ W/m$^2$°K (1000 Btu/ft$^2$°F)
- Fouling on jacket side: typical value $5678$ W/m$^2$°K (1000 Btu/ft$^2$°F)

<table>
<thead>
<tr>
<th>Product</th>
<th>XL 3410 (L)</th>
<th>RA60 1360 (L)</th>
<th>RA60 2270 (L)</th>
<th>RA84 9090 (L)</th>
<th>RA96 13640 (L)</th>
<th>hi</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>70</td>
<td>68</td>
<td>68</td>
<td>68</td>
<td>67</td>
<td>659</td>
</tr>
<tr>
<td>Toluene</td>
<td>59</td>
<td>55</td>
<td>55</td>
<td>55</td>
<td>56</td>
<td>232</td>
</tr>
<tr>
<td>Chloroform</td>
<td>60</td>
<td>57</td>
<td>57</td>
<td>57</td>
<td>57</td>
<td>259</td>
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<tr>
<td>Ethyl alcohol</td>
<td>57</td>
<td>54</td>
<td>54</td>
<td>53</td>
<td>54</td>
<td>213</td>
</tr>
<tr>
<td>Methyl alcohol</td>
<td>62</td>
<td>58</td>
<td>58</td>
<td>59</td>
<td>59</td>
<td>302</td>
</tr>
<tr>
<td>Acetone</td>
<td>62</td>
<td>59</td>
<td>59</td>
<td>58</td>
<td>58</td>
<td>284</td>
</tr>
</tbody>
</table>

Assumptions:
- glass thickness: 1.5 mm
- fouling steam side: 3333 Btu/h ft$^2$°F
- fouling process water: 1000 Btu/h ft$^2$°F
- fouling organic solvents: 1000 Btu/h ft$^2$°F
- Impellor speed: 90 rpm

Jacket side film coefficient

- steam: 1500 Btu/h ft$^2$°F
- water: 500 Btu/h ft$^2$°F
- Heat transfer fluid: 250 Btu/h ft$^2$°F
- Glycol/water mix: 30 Btu/h ft$^2$°F

Heat transfer fluid overall heat transfer coefficient $U_o$ can be estimated from $U_s$ as follows, where 1500 is the jacket film coefficient for steam and 250 is the jacket film coefficient for oil.

$$\frac{1}{U_o} = \frac{1}{U_s} + \frac{1}{1500} + \frac{1}{250}$$