

The new batch reactor heat transfer  
and chemical properties calculator



Version 5 – Volume 1

# Delta T Reactor

**OPERATING & REFERENCE MANUAL**

**VOLUME 1**

**REACTOR VESSEL HEAT TRANSFER**

**PROCESS CALCULATOR**

Version 5

Issue: January 2003

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# The new batch reactor heat transfer and chemical properties calculator



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## 1 GENERAL FEATURES

### 1.1 Introduction

Delta T Reactor – Reactor Vessel Heat Transfer Process Calculator (referred to simply as Delta T in this manual) is a design and rating program providing detailed heat transfer analysis and calculation of agitation power for vertical cylindrical process vessels, reactors and fermenters fitted with external heat transfer jackets and/or internal coils. The user may dimension and configure the vessel freely. The user specifies the following items:

- vessel internal diameter
- vessel straight side
- bottom dish type
- vessel wall thickness
- vessel wall conductivity
- vessel lining thickness
- vessel lining conductivity
- agitator type
- agitator diameter/speed
- agitator geometry
- vessel baffling
- jacket type
- jacket geometry and options

The user chooses the vessel and jacket fluids from the database. Initial vessel and entry jacket temperatures are chosen. Fluid quantities in the vessel and jacket flowrates are specified. The user may specify exotherm as a function of time and also vessel and jacket fouling factors.

The single-point output gives a detailed presentation of heat transfer coefficients, heat flows and pressure drops. The time-base output allows the thermal history to develop over time. This feature allows the calculation of vessel heat-up and cool-down times and the behaviour of the vessel temperature under the effects of exotherm and agitator absorbed power.

Other features of Delta T include:

- units toggle feature
- loadable standard vessel data
- liquid properties
- separate liquid selection screen
- user-defined liquids
- job store, retrieve, clear and print-out

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## 1 GENERAL FEATURES (continued)

### 1.2 System Requirements

Delta T requires the following hardware and software configuration:

- MS Windows 95 or later
- Hard disk (5 MB required)
- VGA or better monitor
- MS Windows compatible printer recommended

Delta T is supplied on CD and may be updated by email.

### 1.3 Software Installation from CD or Email Download

Select or make a new folder (say "C:\DeltaT"). From Windows Explorer run the executable installation program from the supplied CD or download folder and install to the new folder.

### 1.4 General Operation

This section sets out some general notes on how to get around the program and to make heat transfer calculations.

#### Help Screens

In each module of Delta T, accessing the Help Menu gives assistance in understanding module functionality, data entry and option selection.

#### Local Menu

The Local Menu allows access to options such as Calculate, Graphical Display, and Steam on Coil or Jacket.

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## 1 GENERAL FEATURES (continued)

### Main Menu

The Main Menu enables movement between the various program main modules.

### Utilities Menu

The Utilities Menu gives access to utility features such as Program Status, User-Defined Liquids, Liquid Properties and Standard Vessel Data.

### Selection of Options

Screen options are selected from List Boxes (simple or drop-down).

### Data Entry

When a numerical entry is made, the entry is completed by pressing (enter) or by moving focus to another location.

### Screen Warnings

Entry of out-of-range data (e.g. temperature too high or too low) results in a warning message being printed to the message box and rejection of the entered data.

## 1.5 Heat Flow Sign Convention

The following sign convention is used throughout the program: any heat flow or transfer which tends to increase the vessel temperature is positive (e.g. heat transfer into the vessel, exotherm in the vessel). Any heat flow or transfer which tends to decrease the vessel temperature is negative (e.g. heat transfer out of the vessel, endotherm in the vessel).

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## 2 VESSEL INPUT

Details of the entry items are as follows:

### 2.1 Description

The user enters up to 20 characters giving a title or reference to the current job. Any combination of letters and numbers may be used.

### 2.2 Vessel Internal Diameter

This is entered in mm or inch. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch).

### 2.3 Vessel Straight Side

This is the tangent-to-tangent line distance along the straight side of the vessel. The value is entered in mm or inch. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch). The straight side dimension must lie in the range 0.05 to 20 times the vessel internal diameter.

### 2.4 Bottom Dish Type

The user selects from the following dish types:

- ASME 6% Torispherical Dish
- 2:1 Semi-Ellipsoidal Dish
- Hemispherical Dish
- 60 degree Conical End
- Flat End

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## 2 VESSEL INPUT (continued)

### 2.5 Wall Thickness

This is the thickness of the outer pressure-retaining wall of the vessel. The value must be entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

### 2.6 Wall Conductivity

The value is entered in mW/m.K or Btu/ft.hr.F. The entered value must lie in the range 1 to 100,000,000 W/m.K (0.00058 to 58,000 Btu/ft.hr.F). Table 2.15 gives representative values of conductivities of metals and glasses in units of W/m.K and Btu/ft.hr.F.

### 2.7 Lining Thickness

This is the thickness of the inner protective wall lining of the vessel. The value is entered in mm or inch. Zero lining thickness may be entered. If a non-zero value is entered, however, then the entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

### 2.8 Lining Conductivity

The value is entered in W/m.K or Btu/ft.hr.F and the entered value has the same limits as the wall conductivity. If zero lining thickness has been entered, this entry may be omitted.

### 2.9 Vessel Liquid

The vessel liquid is chosen by selecting the Select Liquids option from the Main Menu. See Section 5 for details on the operation of the Liquid Selection module.

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## 2 VESSEL INPUT (continued)

### 2.10 Temperature

The vessel temperature is entered in degrees F or C and must lie between the property limit temperatures for the selected vessel fluid. These property limit temperatures may be inspected in Liquid Properties Module.

### 2.11 Percent Full

The entered value must lie in the range 20 to 100%. Note that 100% full means full to the top tangent line of the vessel.

### 2.12 Vessel Fouling Factor

The thermal resistance of deposits on the vessel internal wall is entered here. Typical values may be obtained from Perry and other sources. The fouling factor is entered in sqft.hr.F/btu or sqm.K/W. The input value must lie in the range 0 to 10 sqm.K/W (0 to 57 sqft.hr.F/btu).

### 2.13 Ambient Temperature

The ambient temperature is entered in degrees F or C. The entered value must lie between -20 C and 50 C.

### 2.14 Vessel Nominal and Fluid Volumes

On entry of the basic vessel dimensions, the vessel nominal volume (to top tan line excluding top dish) is displayed. When vessel percent full is also entered, the vessel fluid volume is displayed.

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## 2 VESSEL INPUT (continued)

### 2.15 Table - Thermal Conductivities of Some Metals & Glasses

Material	Btu/ft.hr.F	W/m.K
Ceramic Glass	0.5 - 0.7	0.9 - 1.2
Hastelloy B	5 - 8	9 - 14
Inconel	8 - 9	14 - 16
SS 304/316	9 - 10	15 - 17
Monel	9 - 12	15 - 21
Titanium	10 - 11	17 - 19
Bronze (75% Cu, 25% Sn)	14 - 16	24 - 28
Mild Steel	25 - 27	43 - 48
Low Alloy Steel	25 - 35	43 - 61
Tantalum	31 - 33	53 - 57
Aluminum Bronze (5% Al)	46 - 50	80 - 87
Brass (70% Cu, 30% Zn)	56 - 66	97 - 114
Copper	180 - 220	310 - 380

Note: Values vary depending on material grade and purity. Values generally fall with rise in temperature.

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## 3 AGITATOR INPUT

### 3.1 General

The program offers the following selection of agitators:

Turbines/Paddles  
Propellers  
Anchors  
Helical Ribbons

The agitators may be selected to operate in baffled or unbaffled vessels, except in the case of anchors and helical ribbons which are assumed to operate in unbaffled vessels only. The number and size of the baffles are specified by the user. The user can select a range of technical options for each selected agitator type.

It is important to note that the user may separately specify details for each type of agitator in a single design session. Values and options selected for one agitator type do not affect values and options selected for another agitator type. The current agitator selection is defined by the last agitator option viewed.

For each agitator selection, the following common items are required in each case. Note however that the selected values are unique to each agitator type selection.

#### Agitator Type

Agitator type is selected from Turbines/Paddles, Propellers, Anchors and Helical Ribbons.

#### Agitator Diameter

Agitator diameter may be entered in inch or mm. A zero value of agitator diameter may be entered. If, however, a non-zero value is entered then the entered value must lie in the range 1 to 100,000 mm (0.04 to 4,000 inch).

#### Agitator Speed

Agitator speed is entered in RPM. A zero value may be entered. If, however, a non-zero value is entered then the entered value must lie in the range 1 to 10,000 RPM.

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## 3 AGITATOR INPUT (continued)

### Agitator Absorbed Power

The power transmitted to the vessel fluid by the action of the agitator may have a significant heating effect on the fluid. In the normal course of data entry the program calculates and displays the absorbed power. Section 10 gives details of the calculation routines used. For the program to compute the absorbed power, all of the Agitator Input and Vessel Temperature, Internal Diameter, Straight Side Percent Full must be specified.

### 3.2 Turbines/Paddles

#### Number of Turbines

The specified number must be between 0 and 4.

#### Number of Blades

The specified number must be between 2 and 12.

#### Blade Width

The entered value must lie between 1 and 100,000 mm (0.04 and 4000 inches). The entered value must be less than the vessel height. Blade width is equal to blade height only when the blade is vertical.

#### Blade Angle

The value entered must lie between 0 degrees (horizontal) and 90 degrees (vertical).

#### Baffle Width

The value may be entered in mm or inch. The entered value must lie between 1 and 100,000 mm (0.04 and 4000 inches). The entered value must be less than the vessel radius.

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## 3 AGITATOR INPUT (continued)

### Number of Baffles

The specified number must be between 0 and 8.

### 3.3 Propellers

#### Number of Propellers

The entered number must lie between 0 and 4.

#### Pitch/Diameter Ratio

The entered value must lie in the range 0.1 thru 2.0

#### Bottom Clearance

The entered value must lie in the range 1 thru 100,000 mm (0.04 thru 4000 inches). In addition, the entered value should lie between 10% and 90% of the vessel liquid height. For multiple propellers, enter the average value of bottom clearance.

#### Baffle Width

The value may be entered in mm or inch. The entered value must lie between 1 and 100,000 mm (0.04 and 4000 inches). The entered value must be less than the vessel radius.

#### Number of Baffles

The specified number must be between 0 and 8.

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## 3 AGITATOR INPUT (continued)

### 3.4 Anchors

#### Blade Width

The entered value may be in mm or inch and must lie between 1 and 100,000 mm (0.04 thru 4000 inches). The entered value must be less than the radius of the vessel.

#### Agitator Height

The value may be entered in mm or inch. The entered value must lie between 1 and 100,000 mm (0.04 and 4000 inches). The entered value must be less than the vessel height.

### 3.5 Helical Ribbons

#### Blade Width

The entered value may be in mm or inch and must lie between 1 and 100,000 mm (0.04 thru 4000 inches). The entered value must be less than the radius of the vessel.

#### Ribbon Height

The value may be entered in mm or inch. The entered value must lie between 1 and 100,000 mm (0.04 and 4000 inches). The entered value must be less than the vessel height.

#### Pitch/Diameter Ratio

The user may select a value in the range of 0.1 to 2.0.

#### Number of Ribbons

The entered value must lie in the range 0 thru 3.

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## 4 JACKET AND COIL INPUT

In the Jacket and Coil Input Screens, the details of the selected jacket and coil are entered. The user may choose to have one jacket and/or one coil.

### 4.1 General

#### Jacket Type

This is the most important entry in Jacket Input. There are six jacket options to select from as follows:

- Half-Pipe Coils
- Conventional Jackets
- Conventional Jackets with Spiral Baffles
- Conventional Jackets with Agitation Nozzles
- User-Defined Jackets
- Dimple Jackets

#### Jacket Options

The user will note that as different jacket options are selected, in certain cases, the type of information required by the program changes. There are however types of information required by the program which remain the same over all jacket options. These common options are described in this section. The following sections describe those options that vary with type of jacket.

There is one important point to note about the common options. Although the type of information required does not vary with jacket type, an entry or choice made for one jacket selection will not apply to another jacket selection. The user may choose a different jacket fluid and flowrate for each selection of jacket type. This facility allows up to six completely different jacket designs to be developed in parallel for a single selection of vessel characteristics.

#### Jacket Liquid

The user selects the jacket liquid from the liquids database. Section 11 lists the fluids available in the database. The user may toggle steam on the jacket using the local menu.

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## 4 JACKET AND COIL INPUT (continued)

### Total Flowrate

This is the total flowrate of jacket fluid through all parallel passes. The value is entered in LPM or USGPM. The value must lie in the range 0 to 600,000 LPM (0 to 160,000 USGPM). If a value of 0 is selected for the flowrate, during computations, a small minimum flowrate based on a mean jacket velocity of 0.005 m/s (0.016 ft/s) is substituted for the input zero value.

### Entry Temperature

This is the temperature of the cooling or heating fluid entering the jacket in degrees C or F. The entered value must lie between the lower and higher property limit temperatures for the jacket fluid selected. These property limit temperatures may be inspected using the Liquid Properties facility.

### Jacket Fouling Factor

The fouling factor for the selected jacket is entered in sqft.hr.F/Btu or in sqm.K/W. The value must lie in the range 0 to 10 sqm.K/W (0 to 57 sqft.hr.F/btu).

### Note on Jacket Extent

The extent of the jacket is defined by specifying the percentage of the straight side area covered by the jacket and by specifying whether the bottom dish is covered by jacket. It should be noted that if the bottom dish is not to be covered by jacket, then the minimum coverage of the straight side permitted is 20%.

### Note on Steam Flowrate

If steam is toggled on the jacket, the user is not permitted to input the flowrate as in the case of a liquid. The program computes the correct flowrate in accordance with the provisions of Section 10 and displays the calculated flowrate in the Single-Point Output.

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## 4 JACKET AND COIL INPUT (continued)

### 4.2 Half-Pipe Coils

#### Half-Pipe Size

The user can select from 1, 1.5, 2, 2.5, 3, 4, 6 and 8 inch half-pipe coils.

#### At Centres

The user selects the centre-to-centre distance of adjacent coils. This distance is entered in mm or inch. The entered value must lie in the range 0.1 mm to 10,000 mm (0.004 to 400 inch). If the entered value is not at least as great as the half-pipe outside diameter an error will be detected.

#### Development

Half-pipe coils are fabricated normally either in 120 or 180 degree cross-section development.

#### Number of Parallel Passes

To limit velocity or pressure drop, especially on large vessels, it is common to split the flow into a number of parallel passes. The program allows up to eight parallel passes. In the case of half-pipe coils, Delta T does not differentiate between zoned and interleaved passes.

#### Percent Straight Side

This is the percentage of the straight side covered by the jacket. In the case of half-pipe coils, this parameter interprets the spaces between adjacent coils as being part of the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

#### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

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## 4 JACKET AND COIL INPUT (continued)

### Half Pipe Schedule

The program offers the user the option of selecting Schedule 10, 40 or 80 as required.

### 4.3 Conventional Jackets

#### Jacket Gap

This is the gap between the outer surface of the vessel and the inner surface of the jacket. The entry is made in mm or inch. The entered value must lie between 0.1 and 10,000 mm (0.004 to 400 inch).

#### Percent Straight Side

This is the percentage of the straight side covered by the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

#### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

#### Jacket Wall Thickness

The value is entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

#### Jacket Entry

This option selects whether the jacket fluid enters at the bottom or the top of the jacket. At low flowrates in conventional jackets, this factor determines whether natural convection 'aids' or 'opposes' the effects of forced convection.

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## 4 JACKET AND COIL INPUT (continued)

### 4.4 Conventional Jackets with Spiral Baffles

#### Jacket Gap

This is the gap between the outer surface of the vessel and the inner surface of the jacket. The value must lie between 0.1 and 10,000 mm (0.004 to 400 inch).

#### Passage Width

This is the centre-to-centre distance between adjacent baffles. The entered value must lie between 0.1 and 10,000 mm (0.004 to 400 inch).

#### Number of Parallel Passes

To limit velocity or pressure drop, it is common to split the flow into a number of parallel passes. The program allows up to eight parallel passes. Delta T does not differentiate between zoned and interleaved passes.

#### Percent Straight Side

This is the percentage of the straight side covered by the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

#### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

#### Jacket Wall Thickness

The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

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## 4 JACKET AND COIL INPUT (continued)

### 4.5 Conventional Jackets with Agitation Nozzles

#### Percent Baffle Leakage

In this form of jacket construction, a percentage of the jacket fluid leaks past the baffles. The value must lie in the range 0 to 75% (a typical value might be 25 to 30%). Liquid that leaks past the baffle shares in the temperature rise or fall in the jacket but does not contribute to the fluid velocity which promotes convective heat transfer.

#### Jacket Gap

This is the gap between the outer surface of the vessel and the inner surface of the jacket. The entry is made in mm or inch. The entered value must lie between 0.1 and 10,000 mm (0.004 to 400 inch).

#### Number of Inlets with Nozzles

The conventional jackets of reactors are often fitted with agitation nozzles to impart a swirl flow to the jacket fluid to aid heat transfer. The program allows up to 8 entry nozzles to be specified. When the user loads vessel dimensional data from the Standard Vessel Data option in the Utilities Menu, the standard DIN recommendation is loaded and displayed.

#### Number of Inlets without Nozzles

Reactor manufacturers often recommend that one inlet nozzle without an agitation nozzle is installed on the vessel jacket. Flow through this nozzle joins the general flow in the jacket but does not assist in generating jacket fluid swirl. Up to 8 nozzles may be specified. When the user loads vessel dimensional data from the Standard Vessel Data option in the Utilities Menu, the standard DIN recommendation is loaded and displayed.

#### Nozzle Throat Size

This value in inch or mm specifies the minimum internal nozzle throat diameter. This value is important for the calculation of the additional momentum imparted to the jacket fluid to promote fluid swirl. If the user loads nozzle data from the Standard Vessel Data option on the Utilities Menu for standard Pfaudler or De Dietrich nozzles, this data is supplied and displayed automatically.

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## 4 JACKET AND COIL INPUT (continued)

### Nozzle K Value

This value allows the program to compute nozzle pressure drop, an important parameter which determines the pumping duty required to supply the jacket. The value is defined as:

$$K = 1 \times 10^7 \Delta P / \rho q^2$$

Where  $\Delta P$  is in Pa,  $\rho$  is in  $\text{kg/m}^3$  and  $q$  is in  $\text{m}^3/\text{sec}$ . This value can be entered by the user or is supplied automatically when the user loads nozzle data from the Standard Vessel Data option on the Utilities Menu for standard Pfaudler or De Dietrich nozzles.

### Percent Straight Side

This is the percentage of the straight side covered by the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

### Jacket Wall Thickness

The value is entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

## 4.6 User-Defined Jackets

### Equivalent Diameter

This is 4 times the flow area divided by the flow perimeter. The value is entered in mm or inch. The value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch).

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## 4 JACKET AND COIL INPUT (continued)

### Flow Area per Pass

The value is entered in sq mm or sq inch. The entered value must lie in the range 0.1 to 1.0x10<sup>8</sup> sq mm (0.00015 to 155,000 sq.inch).

### Number of Parallel Passes

To limit velocity or pressure drop, especially on large vessels, it is common to split the flow into a number of parallel passes. The program allows up to 40 parallel passes.

### Percent Straight Side

This is the percentage of the straight side covered by the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

### Jacket Wall Thickness

The value is entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

## 4.7 Dimple Jackets

### Jacket Gap

This is the maximum clearance between the outside of the vessel and the inside of the jacket. The value may be entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

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## 4 JACKET AND COIL INPUT (continued)

### Dimples on Centres

This is the centre to centre distance between dimples which are assumed to be in a square array. The entered value must lie in the range 1 thru 100,000 mm (0.04 thru 4000 inches). See  $d_c$  on diagram on page 25.

### Dimple Diameter (1)

This is the diameter of the dimple where it meets the outside of the vessel as measured inside the jacket. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch). The entered value must be less than 90% of the Dimples on Centres. See  $d_1$  on diagram on page 25.

### Dimple Diameter (2)

This is the diameter of the dimple where it meets the outer jacket. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inches). The entered value must be less than the Dimples on Centres. See  $d_2$  on diagram on page 25.

### Percent Straight Side

This the percentage of the straight side covered by the jacket. The entered value must lie in the range 0 to 100 percent (20 to 100% if no jacket is specified on the bottom dish).

### Jacket on Dish

The options are to have the jacket covering the bottom dish or to have no jacket on the bottom dish.

### Jacket Wall Thickness

The value is entered in mm or inch. The entered value must lie in the range 0.1 to 10,000 mm (0.004 to 400 inch).

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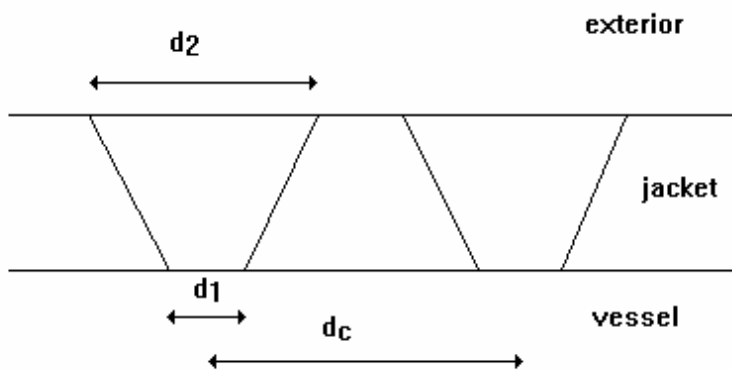
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## 4 JACKET AND COIL INPUT (continued)

### Number of Baffles

To increase jacket velocity in dimple jackets, flow-dividing baffles may be built into the jacket. Zero baffle leakage is assumed. The number must lie in range 0 thru 8.

### Definition Sketch for Input Dimensions



# The new batch reactor heat transfer and chemical properties calculator



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## 4 JACKET AND COIL INPUT (continued)

### 4.8 Internal Helical Coils

#### Tube Internal Diameter

This value is entered in mm or inch. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch).

#### Tube External Diameter

This value is entered in mm or inch. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4000 inch).

#### Number of Parallel Passes

To limit velocity or pressure drop, especially on large coils, it is common to split the flow into a number of parallel passes. The program allows up to eight parallel passes.

#### Coil Diameter

The value is entered in mm or inch. The entered value must lie in the range 1 to 100,000 mm (0.04 to 4,000 inch).

#### Number of Coil Turns per Pass

This is the number of turns of helical coil per parallel pass. The value must lie between 1 and 1000.

#### Percent Immersion

This parameter is the percent of the available heat transfer area which is immersed in the vessel liquid. The entered value must lie between 20 and 100.

## The new batch reactor heat transfer and chemical properties calculator



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### 4 JACKET AND COIL INPUT (continued)

#### Total Flowrate

This is the total flowrate of coil fluid through all parallel passes. The value is entered in LPM or USGPM. The value must lie in the range 0 to 600,000 LPM (0 to 160,000 USGPM). If a value of 0 is selected for the flowrate, during computations, a small minimum flowrate based on a mean coil velocity of 0.005 m/s (0.016 ft/s) is substituted for the input zero value.

#### Entry Temperature

This is the temperature of the cooling or heating fluid entering the coil in degrees C or F. The entered value must lie between the lower and higher property limit temperatures for the coil fluid selected. These property limit temperatures may be inspected using the Liquid Properties facility.

#### Coil Fouling Factor

The fouling factor for the coil is entered in sqft.hr.F/Btu or in sqm.K/W. The value must lie in the range 0 to 10 sqm.K/W (0 to 57 sqft.hr.F/btu).

#### Note on Steam Flowrate

If steam is toggled on the coil, the user is not permitted to input the flowrate as in the case of a liquid. The program computes the correct flowrate in accordance with the provisions of Section 10 and displays the calculated flowrate in the Single-Point Output.

# The new batch reactor heat transfer and chemical properties calculator



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## 5 LIQUID SELECTION

### Category List

The available categories of compounds are displayed in the top list box. These categories are:

- Alkanes
- Alkenes/Alkynes
- Halogenated Organics
- Ethers
- Ketones/Aldehydes
- Acids/Anhydrides
- Alcohols/Phenols
- Esters
- Benzene Derivatives
- Heterocycles/Polycycles
- Organic Nitrogen Compounds
- Organic Sulfur Compounds
- Inorganic Compounds
- Aqueous Solutions/Heat Transfer Liquids
- User-Defined Liquids
- User-Defined Mixtures

The current category will be shown highlighted on the screen. Clicking on a required category selects that category. When a category name is selected the compound list is automatically loaded and partially displayed.

### Compound List

At the bottom is a list box giving the list of compound formulas and names belonging to the currently selected category. Clicking on a compound name causes that compound to be selected.

# The new batch reactor heat transfer and chemical properties calculator



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## 5 LIQUID SELECTION (continued)

### Synonyms and Structural Formula

Directly beneath the partial list of compounds are given synonyms and the structural formula for the currently selected compound. This feature is available for the Enhanced Database version of the program.

### Searching for Compounds

As explained above, the compounds are displayed in category groups. Within each category, the compounds are stored in formula order. If the user knows which category the compound of interest belongs to and how many carbon atoms in the chemical formula, then it is easy to locate the compound quickly.

If, on the other hand, only the name or a fragment of the name is known, it will be more convenient to use the Search facility available. The user simply enters the name fragment in the Search text box and clicks on the Search command button. The search facility will locate in turn every compound in the database in which the string is found either in the compound's primary name or in its synonyms. The String Search facility is easy to use and prompts and warnings are displayed on the screen.

### Assignment of Selected Liquids

When a liquid is selected by clicking on its name in the Compounds List Box, that liquid is assigned to the currently selected assignment: Vessel, Jacket (6 options), Internal Coil or Database.

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT

### 6.1 Single-Point Output

When all items on the input screens have been entered and any detected errors corrected (see Section 6.3), the computation is carried out by transferring control to the Single Point Output Screen via the Main Menu and pressing the Calculate button. When this has been done, the Single-Point Output screen is calculated and displayed. For Jackets, the following coefficients are displayed:

- Jacket Film Coefficient
- Jacket Fouling Coefficient
- Vessel Wall Coefficient
- Vessel Lining Coefficient
- Vessel Fouling Coefficient
- Vessel Film Coefficient
- Overall Coefficient

The quoted coefficients are all referred to the vessel internal surface.

For Internal Helical Coils the following coefficients are displayed:

- Internal Tube Film Coefficient
- Internal Tube Fouling Coefficient
- Tube Wall Coefficient
- External Tube Fouling Coefficient
- External Tube Film Coefficient
- Overall Coefficient

The quoted coefficients are all referred to the tube outer surface.

The following additional information is displayed:

- Vessel Temperature
- Jacket Inlet Temperature
- Jacket Outlet Temperature
- Actual Heat Transfer Area
- Heat Transfer Rate
- Jacket Pressure Drop

For Internal Helical Coils, coil temperatures and pressure drop are quoted. For Conventional Jackets with Agitation Nozzles, nozzle pressure drop is also quoted.

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT (continued)

### 6.2 Time-Base Output

Control is transferred to the Time-Base Output Module via the Main Menu after completion of data input.

The user inputs a value of time in hours, specifies values of exotherm (if any), and presses the Calculate button. The program calculates the vessel temperature and other quantities at 0%, 20%, 40%, 60%, 80%, and 100% of the input time. The starting point for the calculation is specified in the Input Screens. The calculation automatically takes into account any input value of exotherm and absorbed agitator power.

The entered value of time must lie between 0.01 and 1000 hours. Values of exotherm at each time point are entered on this screen. The magnitude of the exotherm (or endotherm) cannot exceed 5000 kW (17.5 million btu/hr).

The program main output gives values of the following:

- Vessel Temperature
- Overall Heat Transfer Rate
- Cumulative Heat Transfer

Detailed output for both jacket and coil may be accessed from the Local Menu. This detailed output gives Exit Temperatures, Heat Transfer Coefficients and Heat Transfer Rates for both jacket and coil as function of time.

When the output is complete, the user may toggle the output data between US and Metric units.

Other values of time can be entered and the time-base calculation repeated as required.

There are a number of important other features in the Time-Base module:

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT (continued)

### Jacket Temperature Regime

This is selected from the Regime menu. The user can select between the following:

- Constant Inlet Temperature Regime
- Regime where temperature tracks the Vessel Temperature by a specified amount (to be entered by the user). For example the user can specify 20 C. In this case the maximum absolute difference between the jacket and vessel temperatures will not exceed 20 C.
- Heat Transfer Rate Limited Regime: In this case the temperature differential between the jacket and vessel is adjusted automatically so that the rate of heat transfer is limited to an amount specified by the user.

### Search for Time for specified Temperature

In the normal calculation, the user specifies the time and the temperature development over that period is computed. Once this basic calculation has been executed, the user can enter a temperature value and search for the time required to reach the specified temperature.

### Enter Vessel, Jacket or Coil Temperatures

The user can specify vessel initial temperature, current jacket inlet temperature or coil inlet temperature on this screen without having to go back to the Vessel Input, Jacket Input or Coil Input screens.

## 6.3 Program Status

The Program Status screen (which may be accessed from the Utilities Menu) provides the user at any time with status reports, error messages and additional technical information. The displayed messages depend on the stage of data entry and calculation. When calculation is initiated, the Program Status screen will be presented if incomplete or incorrect data is detected.

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT (continued)

### During Data Entry

If the Calculate option is selected during the data entry phase before all entries are complete, Program Status screen will respond with the message "Data Entry not Complete".

### When Data Entry is Complete

When the Calculate option is selected after completion of data entry, a check is carried out on the entered data and errors found are reported on. A complete list of possible errors is given in the next section. To proceed further, the user must return to the data entry screens and correct the reported errors.

### After Calculation

If the calculation detects a jacket or vessel temperature outside the permitted range for the jacket or vessel fluid, this will be reported at this stage. Note that this occurrence does not cause interruption of the calculation. When a calculated temperature is out-of-range, the properties are calculated at the nearest fluid property limit temperature and the calculation is allowed to proceed.

### Additional Process Information

As well as reporting run-time errors at this time, additional technical information is given as follows: Jacket Reynolds Number, Jacket Prandtl Number, Jacket Velocity, Vessel Reynolds Number, Vessel Prandtl Number.

This screen also reports un-insulated vessel heat losses to or heat gains from the environment which is assumed to be still air at the ambient temperature entered in the Vessel Input module. This is a special information-only feature. Elsewhere in Delta T a completely insulated vessel is assumed.

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT (continued)

### 6.4 Program Status Error Messages

The following is a complete listing of possible errors that may be detected in the input data after completion of data entry.

**Straight Side Out of Range:** This error occurs if the vessel straight side is more than 20 times or less than 0.05 times the vessel internal diameter.

Wall Thickness > 0.25 Vessel Diameter

Lining Thickness > 0.25 Vessel Diameter

Agitator Diameter > Vessel Diameter

Half Pipe Centres < Half Pipe Diameter

**Half-Pipe Centres too large:** This error occurs when the entered Half-Pipe centre-to-centre distance is greater than the height of the jacket.

**Baffle Spacing too large:** This error occurs when the baffle spacing is greater than the jacket height divided by the number of parallel passes.

Tube ID > Tube OD

Tube OD > 0.25 Vessel Diameter

**Too Many Coil Turns:** This error occurs when the number of coil turns per pass multiplied by the tube diameter is greater than the vessel straight side.

Jacket Equivalent Diameter > Vessel Straight Side

Coil Diameter > Vessel Diameter

**Flow Area too small:** This error occurs when the flow area specified for a user-defined jacket is less than the area of a circle with the specified equivalent diameter as diameter.

**Jacket Specification Error:** This error occurs when no jacket is specified on the bottom dish and less than 20% of the straight side is specified to be covered by jacket.

# The new batch reactor heat transfer and chemical properties calculator



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## 6 OUTPUT (continued)

Jacket Flow Area/Nozzle Area < 1: The jacket flow area for an agitated conventional jacket must exceed the combined nozzle throat areas.

Vessel Temperature out of range: This occurs if the vessel temperature is outside the permitted range for the chosen liquid.

Jacket Temperature out of range

Vessel Coefficient equal to zero: This occurs when the agitator speed is zero and the vessel and jacket temperatures are equal. It will also happen if agitator speed is zero and a user-defined liquid is specified in the vessel with constant specific volume (and thus with zero coefficient of expansion).

Dimple Diameter (1) > 90% Dimple Centres: The dimple diameter (1) is the diameter of the dimple in a dimple jacket at the point where the jacket meets the outside of the vessel shell. This provision in the program stops the user from specifying a dimple jacket with zero flow area.

Dimple Diameter (2) > Dimple Centres: The dimple diameter (2) is the diameter of the dimple at the outside of the jacket. The dimple circles cannot intersect.

Blade Width > Vessel Radius

Blade Width > Vessel Height

Agitator Bottom Clearance > Vessel Height

Agitator Height > Vessel Height

Propeller is less than 10% of the liquid height off the bottom.

Propeller is less than 10% of the liquid height from the liquid surface.

Coil Temperature out of range for Coil Liquid

Coil Steam Temperature <= Vessel Temperature

Vessel to Coil Coefficient equal to zero

# The new batch reactor heat transfer and chemical properties calculator



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## 7 LIQUID PROPERTIES

The Liquid Properties module is a stand-alone feature that enables the user to select any fluid from the database (including user-defined liquids), and to calculate the physical properties at any temperature within the available temperature range for that liquid.

The liquid may be selected by the user by choosing the Select Liquids option from the local menu.

The output properties are as follows:

- Viscosity
- Specific Volume
- Specific Heat
- Thermal Conductivity
- Expansivity
- Low-Limit Temperature
- High-Limit Temperature

The properties displayed may be toggled between US and Metric units via the local menu.

The liquids available in the database are set out in Section 11.

# The new batch reactor heat transfer and chemical properties calculator



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## 8 USER-DEFINED LIQUIDS

This module allows the user to define up to 50 new liquids and to add them permanently to the database. Each liquid is defined by the following quantities.

Viscosity  
Conductivity  
Specific Heat  
Specific Volume  
Low-Limit Temperature  
High-Limit Temperature

The user defines these quantities over the temperature range by specifying two reference temperatures and values of Viscosity, Conductivity, Specific Heat and Specific Volume at these temperatures.

### Reference Temperatures

The reference temperatures are the temperatures for which the property values are entered. These must be less than 1300 K and must not be closer to each other than 1 K.

### Viscosity

The program fits a log viscosity versus inverse temperature function to the entered data. The values entered at the two reference temperatures may be the same, but if this is so then no variation in viscosity will be calculated over the temperature range. This is normally a significant matter for viscosity. The entered values must lie between 0.001 cp and  $1.0 \times 10^9$  cp.

### Conductivity

The program fits a straight line function to the entered data to represent the conductivity over the temperature range. If identical values are entered for conductivity at the two reference temperatures, conductivity will be constant over the temperature range. The entered values must lie in the range 0.6E-03 and 0.6E+6 Btu/ft.hr.F (1.0E-03 to 1.0E+06 W/mK).

# The new batch reactor heat transfer and chemical properties calculator



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## 8 USER-DEFINED LIQUIDS (continued)

### Specific Volume

The program fits a straight line density function to the entered data to represent the specific volume over the temperature range. If identical values are entered, specific volume will be constant over the temperature range. This may not be of significance for specific volume but the derived values of the expansion coefficient will be identically zero and thus all calculated natural convection coefficients will also be zero. This is clearly a serious matter if natural convection is likely to be a significant mechanism of heat transfer. Entered values must lie between 16 and 0.00016 cuft/lb (1 and 0.00001 cum/kg).

### Specific Heat

The program fits a straight line function to the entered data to represent the specific heat over the temperature range. If identical values are entered, specific heat will be constant over the temperature range. Entered values must lie between 0.0024 and 24 Btu/lb.F (10 and 100,000 J/kg.K).

### Low and High Limit Temperatures

These define the range of applicability of the calculated properties. The same limitations that apply to the reference temperatures apply here too. In addition, the entered high-limit temperature must be greater than the entered low-limit temperature.

### Liquid Name

Having entered the physical property data, the user must specify the user-defined liquid name. The use of (left) and (right) at the top screen location will scroll through the current user-defined liquid names. The user enters the liquid name in the usual way while the cursor is located at the top screen location.

## The new batch reactor heat transfer and chemical properties calculator



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### 8 USER-DEFINED LIQUIDS (continued)

#### Calculate/Save

Once all the data has been entered, selection of this option from the local menu calculates the liquid parameters and stores these for future recall and calculation. In addition the actual data entered by the user to define the liquid is also stored for future reference.

Before final acceptance by the program of the input data, a check is carried out to see if any of the properties go outside the permitted range of values over the temperature range: if this occurs, a warning will be printed in the message box and the user will have to correct the input values before the fluid is accepted.

#### Load Liquid Data

This option allows the user to recall data entered previously for a user-defined liquid. This data may be amended and the liquid properties redefined as required for calculation and storage to the same or a different location.

# The new batch reactor heat transfer and chemical properties calculator



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## 9 UTILITIES

### 9.1 Storing Current Job

This facility allows the user to store a job at any stage for future retrieval. The facility requests a filename to be entered which must meet the usual requirements for a DOS filename. If an input/output error occurs during the storing process, a warning will be printed in the message box. The user can correct the problem and retry the storing process.

### 9.2 Retrieving Existing Job

This allows the user to retrieve a job that was stored at an earlier time. The filename of the job must be entered. If an input/output error occurs during the job retrieval process, a warning message will be printed to the message box. Retrieving a job automatically overwrites any current job in memory.

In storing and retrieving jobs only the variables associated with the input screens are stored and retrieved. Any output must be recalculated after retrieval.

### 9.3 Printing Current Job

This facility produces a professional quality formatted printout of the contents of the input and output screens including the additional technical parameters presented in the Program Status screen.

### 9.4 Clearing Current Job

This feature clears all variables associated with the input and output screens and resets the standard defaults.

## The new batch reactor heat transfer and chemical properties calculator



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### **9 UTILITIES (continued)**

#### **9.5 Standard Vessel Data**

This utility allows the user to load pre-defined dimensional and other data for DIN-standard vessels. All of the critical dimensions are loaded and the values are carefully adjusted to give best-fit to the required program values – in particular heat transfer area and jacket gap. The user may also load proprietary Pfaudler and De Dietrich data on agitation nozzles.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE

### 10.1 Introduction

The following heat transfer regimes are modelled in Delta T and are described in this Technical Reference.

#### Heat Transfer in Closed, Curved Channels

This covers flows in Half-Pipe Coils, Conventional Jackets fitted with Spiral Baffles, Internal Helical Coils and in User-Defined Jackets. Turbulent, laminar and transitional flow regimes are covered. The effects of entrance flow regimes and natural convection are taken into account.

#### Heat Transfer in Flow in Annular Channels

This analysis covers flows in conventional jackets and conventional jackets fitted with agitation nozzles. Curvature, entrance effects and natural convection are taken into account.

#### Heat Transfer on Vessel Internal Surface

The correlations used in Delta T cover a range of agitator selections and the turbulent and laminar regimes. Natural convection correlations are included for non-agitated vessels.

#### Heat Transfer on the outside of Helical Coils

The correlations employed cover turbulent and laminar forced convection. Natural convection correlations are included for non-agitated vessels.

#### Heat Transfer in Dimple Jackets

New correlations for pressure drop and heat transfer have been developed by Madison Technical Software.

#### Condensation Heat Transfer in Jackets

Correlations are presented for condensation on vertical surfaces and in horizontal ducts.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

This technical reference also sets out extensive information on:

- Absorbed Agitator Power
- Pressure Drop Calculations
- Vessel Temperature vs Time functions

Section 10.14 lists the technical literature used as reference in the formulation of the equation and correlation basis for Delta T.

### 10.2 Notation

A	Area
c	Specific Heat
C	Coefficient, Clearance
d	Diameter
$d_v$	Vessel Internal Diameter
e	Absolute Roughness, Efficiency
f	Friction Factor, Heat exchange factor
g	Acceleration due to Gravity
H	Vertical Dimension
$H_{ab}$	Height of Agitator off tank bottom
$H_{liq}$	Height of Liquid in tank
h	Heat Transfer Coefficient
L	Flow Length, Length
k	Thermal Conductivity, Rate Constant
n	Number
N	Agitator Speed (revolutions/unit time)
M	Mass
P	Power, Perimeter
p	Pressure
q	Volume Flowrate
R	Heat exchange factor
T	Absolute Temperature
t	Time, Thickness
U	Overall Heat Transfer Coefficient
V	Velocity
w	Mass Flowrate
W	Width
$X_a$	Vertical Agitator Blade Height

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Greek Symbols

$\beta$	Expansion Coefficient
$\Delta P$	Pressure Difference
$\Delta T$	Temperature Difference
$\theta$	Angle
$\lambda$	Pitch of propeller or helical ribbon
$\mu$	Viscosity
$\rho$	Density

### Subscripts

a	Agitator, Area
an	Anchor
b	Bulk
baff	Baffle
bl	Blade
c	Curved Flow, Coil, Center-to-Center
e	Equivalent
fc	Forced Convection
f	Fouling
fb	Fully Baffled
g	Lining
i	Inside
j	Jacket
L	Longitudinal, Laminar
m	Metal
n	Nozzle
nc	Natural Convection
o	Outside
pb	Partially Baffled
ribb	Ribbon
t	Tangential, Turbulent
ub	Unbaffled
v	Vessel
w	Flowrate, Wall

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Dimensionless Numbers

Ge	Entrance Correction
Gr	Grashof Number $g.\beta.H^3.\rho^2.\Delta T/\mu^2$
Gz	Graetz Number $(\pi/4).Re.Pr.Rt$
Nu	Nusselt Number $h.d/k$
Pr	Prandtl Number $c_p\mu/k$
Re	Reynolds Number = $d\rho V/\mu$ (general) = $d_a^2\rho N/\mu$ (agitated vessels)
Vi	Viscosity Ratio $\mu_b/\mu_w$
Rt	Dimensional Ratio $d/L$
Po	Power Number $P/\rho N^3.d_a^5$
Cu	Curvature Correction

### 10.3 General

The convection formulas presented here are presented in the form of dimensionless numbers defined in Section 10.2. The following general points apply:

#### Equivalent Diameter

Unless otherwise stated, the diameter dimension is the equivalent diameter equal to 4 times the flow area divided by the flow perimeter. This definition is applied to all closed ducts, circular and non-circular.

#### Reynolds Number

For flow in an agitated vessel, the Reynolds Number is expressed in terms of agitator diameter and agitator speed. Agitator speed is expressed in revolutions per unit time.

#### Units

In the interpretation of the equations, any consistent set of units may be used. Delta T uses SI units for internal calculation.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Accuracy of the Package

The equations used in Delta T are a compendium of published correlations with interpolations developed by Madison Technical Software. The accuracy of the basic equations is of the order of 10% in the laminar and turbulent regions. ESDU gives excellent data on formula accuracy. Little or no reliable published data is available for heat transfer in the transitional region: Delta T employs logarithmic interpolation between the upper laminar limit and the lower turbulent limit. Accuracy in this region is of the order of 25%.

### Liquid Properties

The package comes with a built-in database of the transport properties of a range of liquids. These are listed in Section 11. The representation of these properties as functions of temperature is by cubic interpolation on a uniform tabulation of values. Accuracy is generally better than 1-2%.

### Overall Heat Transfer Coefficient

For heat transfer through a vessel wall, the overall heat transfer coefficient is defined as:

$$1/U = 1/h_j + 1/h_{jf} + 1/h_m + 1/h_g + 1/h_{vf} + 1/h_v$$

with,

- $h_j$  = Jacket Film Coefficient referred to vessel id
- $h_{jf}$  = Jacket Fouling Coefficient referred to vessel id
- $h_m$  = Vessel Metal Wall Coefficient referred to vessel id
- $h_g$  = Vessel Lining Coefficient referred to vessel id
- $h_{vf}$  = Vessel Fouling Coefficient
- $h_v$  = Vessel Film Coefficient

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

The calculated U-value refers to the vessel internal surface. For heat transfer through the wall of an internal helical coil,

$$1/U = 1/h_i + 1/h_{if} + 1/h_m + 1/h_{of} + 1/h_o$$

with,

$h_i$  = Internal Tube Film Coefficient referred to tube od

$h_{if}$  = Internal Tube Fouling Coefficient referred to tube od

$h_m$  = Tube Wall Coefficient referred to tube od

$h_{of}$  = Tube Outside Fouling Coefficient

$h_o$  = Tube Outside Film Coefficient

The calculated U-value refers to the tube outside surface.

### Factors of Safety

No arbitrary factors of safety have been employed in Delta T on the computed coefficients or other quantities. The output results from the program are mid-range estimates from the specified correlations. It is normal practice to use factors of safety in heat transfer work: this, however, has been left to the discretion of the user.

## 10.4 Application of Formulas

### Half-Pipe Coils

The correlations set out in section 10.5 are applicable to heat transfer in half-pipe coils.

Not all of the outside surface of the vessel that is nominally covered by half-pipe coil will in fact be in contact with the circulating liquid. In order to be able to fabricate the half-pipe, it is necessary to allow a spacing between adjacent coils, typically about 1". This spacing does however contribute significantly to the total heat transfer area. The following method is employed in Delta T to estimate the total effective heat transfer area provided by a half-pipe coil.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

Define

$$1/h = 1/h_v + 1/h_{vf}$$

$h_v$  = Vessel Film Coefficient

$h_{vf}$  = Vessel Fouling Coefficient

$t$  = Total wall thickness =  $t_m + t_g$

$k$  = Mean Wall Conductivity

$$= (t_m + t_g) / (t_m/k_m + t_g/k_g)$$

$b$  = half-spacing between adjacent half-pipe coils

Then,

$$\eta = \text{fin efficiency} = (\text{Exp}(2mb) - 1) / (mb(\text{Exp}(2mb) + 1))$$

where,

$$m = (h/(k.t))^{0.5}$$

$$A_{\text{eff}} = A_{\text{hp}} + \eta \cdot A_{\text{sp}}$$

where,

$A_{\text{eff}}$  = Effective Heat Transfer Area

$A_{\text{hp}}$  = Area actually covered by Half-Pipes

$A_{\text{sp}}$  = Area between Half-Pipes

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Conventional Jackets

In a conventional jacket, the flow is partly in a tangential direction and partly in a vertical direction. Section 10.6 gives correlations for heat transfer coefficients in tangential flows in an annular channel. The heat transfer coefficient in a conventional jacket is calculated from these correlations using a mean effective curvature diameter for the overall flow through the jacket of

$$d_c = d_v / \cos(\theta) \text{ where } \tan(\theta) = 2H_j / \pi d_v$$

Vertical flow in a conventional jacket in the laminar regime may be 'opposing' or 'aiding' in that the effects of natural convection can counteract or assist the effects of forced convection. For example, a coolant entering at the bottom of the jacket will give rise to aiding flow with resulting higher heat transfer coefficients than in the case where coolant enters at the top of the jacket.

### Conventional Jackets with Spiral-Wound Baffles

The correlations in section 10.5 can be applied to conventional jackets fitted with spiral-wound baffles.

To increase the velocity of the circulating fluid in the jacket, baffles are often fitted in conventional jackets. The baffles are usually welded to the vessel outer surface and the outer jacket is placed around the baffles, sometimes being tack-welded or plug-welded into place. A portion of the circulating liquid may leak past the baffles and thus not assist in promoting the heat transfer. The proportion of liquid that does leak will depend on the details of construction and the tolerances observed during fabrication. A typical figure is 10 to 30% leakage.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Conventional Jackets with Agitation Nozzles

To increase the rate of heat transfer in conventional jackets, the circulating liquid can be injected tangentially into the jacket so as to cause a swirl flow around the jacket. A basic momentum balance analysis is given by Bollinger (Chem Eng, September 1982). Taking this as a starting point the following expression for the mean swirl flowrate can be developed:

$$w_s = w_n \cdot \{((B+K)^2 - (B+K) + B \cdot A_j/A_n)^{0.5} - B\}$$

$w_n$  = mass flowrate into jacket from nozzles

$$B = d_e/(2fL)$$

$K$  = constant between 0 and 1 dependent on the relative positions of entry and exit nozzles in the jacket. Set equal to 0.5

$A_j$  = Jacket Flow Area

$A_n$  = Sum of Nozzle Throat Flow Areas

$d_e$  = Equivalent Diameter of Jacket

$f$  = Darcy Friction Factor for the Swirl Flow (see 10.11)

$L$  = Flow Length of Jacket (approx  $\pi \cdot d_v$ )

When the swirl flow,  $w_s$ , has been computed, the heat transfer coefficient is calculated from the correlations set out in section 10.5.

Pressure drop through an agitation nozzle is computed from the following

$$K = 1 \times 10^7 \Delta P / \rho q^2$$

Where

$\Delta P$  = pressure differential across nozzle (Pa)

$\rho$  = fluid density (kg/m<sup>3</sup>)

$q$  = flowrate through nozzle (m<sup>3</sup>/sec)

For a range of proprietary nozzles (Pfaudler and De Dietrich), the Standard Vessel Data utility gives values of  $K$ .

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Internal Helical Coils

The correlations set out in section 10.5 are applicable to internal flows in helical coils. For heat transfer from the outer surface of helical coils the correlations presented in section 10.8 are used.

### User-Defined Jackets

For jackets not covered by the specific options provided by Delta T, the user can employ the User-Defined Jacket facility.

The jacket geometry is expressed at input stage in terms of equivalent diameter, flow area and number of parallel passes. The correlations set out in section 10.5 are applicable.

### Dimple Jackets

See Section 10.11.3 for details of heat transfer in dimple jackets.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### 10.5 Heat Transfer in Closed, Curved Channels

#### General

This section covers heat transfer by forced and natural convection in closed, curved channels. The results of this section are directly applicable to Half-Pipe Coils, flow inside Helical Coils, Conventional Jackets with Spiral Baffles and User-Defined Jackets. Flow in Conventional Jackets or Conventional Jackets with Agitation Nozzles are treated separately.

The limits of the transitional zone are functions of curvature, Prandtl Number and Reynolds Number. In the Delta T routines the following limits are used.

Lower Limit of the Transitional Zone:

$$Re_1 = 15000 \text{ for } d_e/d_c > 0.30706$$

$$Re_1 = 2000 \cdot (1 + 13.2 \cdot (d_e/d_c)^{0.6}) \text{ for } d_e/d_c < 0.30706$$

Upper Limit of the Transitional Zone:

$$Re_2 = 15000$$

In the above relations,

$d_e$  = equivalent channel diameter

$d_c$  = coil diameter

Specific references for this section are,

ESDU items 78031, 68006, 67016 and 68007  
Oliver, Chem Eng Sc, Vol 17, p335, 1962

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Laminar Flow with High Curvature

For  $B = Re^{0.5} \cdot (d_e \cdot Pr / d_c)^{0.25} > 3.2$

then the high curvature formula applies:

$$Nu_{fc} = 0.984B(1 - 1.48/B + 23.2/B^2 - 120/B^3 + 212/B^4) \cdot \nu_i^{0.14}$$

In the high curvature region, natural convection effects are suppressed by the flow curvature. All properties are evaluated at the bulk temperature.

### Laminar Flow with Low Curvature

For  $B = Re^{0.5} \cdot (d_e \cdot Pr / d_c)^{0.25} < 3.94$

the calculation is the same as for straight tubes with no curvature effects but with entrance and natural convection effects.

The forced convection component is,

$$Nu_{fc} = 3.66 + 0.1082 \text{ Gz} / (1 + 0.06634 \text{ Gz}^{0.67}) \cdot \nu_i^{0.14}$$

with all properties evaluated at the bulk temperature. This formula was derived by interpolation between formulas given by ESDU and Perry.

The natural convection component in horizontal flow is,

$$Nu_{nc} = 0.3543 (\text{Gr} \cdot \text{Pr})^{0.25} \cdot \nu_i^{0.14}$$

$$\text{Gr} = \beta \cdot g \cdot d^3 \cdot \rho^2 \cdot \Delta T / \mu^2$$

$\Delta T$  = mean value of  $T_w - T_b$

This formula is derived from the ESDU correlation. All properties are evaluated at the wall temperature.

Combining forced and natural convection components,

$$Nu^3 = Nu_{fc}^3 + Nu_{nc}^3$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### Turbulent Flow

For  $Re > Re_2$

$$Nu = 0.0225 Re^{0.795} Pr^{0.495} \exp(-0.0225 \ln^2(Pr)) Cu Ge Vi^m$$

with,

$$Cu = (1 + 0.059(Re.(d_e/d_c)^2)^{0.34}$$

$$Ge = 1 + 4.9167 Rt(1 - \exp(-0.30/Rt)) \text{ for } Re.(d_e/d_c)^2 < 4.72$$

$$Ge = 1 \text{ for } Re.(d_e/d_c)^2 > 4.72$$

This entrance correction factor is the average of ESDU correlations for right angle edge entry and 90 degree mitre bend entry.

and,

$$m = 0.30 \text{ for } T_w < T_b$$

$$m = 0.18 \text{ for } T_w > T_b$$

## 10.6 Heat Transfer in Flow in Annular Channels

### Laminar Flow with High Curvature

$$\text{For } B = Re^{0.5} (d_e Pr / d_c)^{0.25} > 4.9$$

$$Nu = 0.984 B (1 - 1.48/B + 23.2/B^2 - 120/B^3 + 212/B^4) Vi^{0.14}$$

This presentation is derived from ESDU Item 78031. Note that the secondary currents induced by the flow curvature suppress natural convection and entrance effects. All properties are evaluated at the bulk temperature.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### Laminar Flow with Low Curvature

For  $B = Re^{0.5} \cdot (d_e \cdot Pr / d_c)^{0.25} < 3.94$

the forced convection component is,

$$Nu_{fc} = 4.86 + 0.09525 \{Gz / (1 + 0.0525 Gz^{0.67})\} \cdot Vi^{0.14}$$

with all properties evaluated at the bulk temperature. The formula for  $Ge$  is a generalization by Madison Technical Software of the Norris & Streid formula for  $Gz > 55$  and the standard  $Gz = 0$  result.

The natural convection component is,

$$Nu_{nc} = \pm 0.7287 (Gr \cdot Pr \cdot Rt)^m \phi^{0.33}$$

$$Gr = \beta \cdot g \cdot d^3 \cdot \rho^2 \cdot \Delta T / \mu^2$$

$$\Delta T = T_w - T_b \text{ at the inlet and } \phi = \text{Exp}(-0.4875 (\pi \cdot Nu / Gz)^{0.888})$$

In aiding flow, the + sign is used and  $m = 0.28$ . In opposing flow, the - sign is used and  $m = 0.25$ . All properties are evaluated at the wall temperature. Combining forced and natural convection components for aiding flow in all cases and for opposing flow when  $Nu_{fc} > Nu_{nc}$

$$Nu^3 = Nu_{fc}^3 + Nu_{nc}^3$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### Turbulent Flow

For  $Re > Re_2$

$$Nu = 0.0192 Re^{0.795} Pr^{0.495} \text{Exp}(-0.0225 \ln^2(Pr)) Cu Ge Vi^m$$

The leading coefficient 0.0192 is obtained as the product of the straight tube coefficient of 0.0225 and the correction for parallel plates (0.853)

$$Cu = 1 + 0.059(Re.(d_e/d_c)^2)^{0.34}$$

In the high curvature region, defined by  $Re.(d_e/d_c) > 4.72$  then  $Ge = 1$ ,  $m = 0.30$  for  $T_w < T_b$  and  $m = 0.18$  for  $T_w > T_b$

In the low curvature region, defined by  $Re.(d_e/d_c) < 4.72$  then

$$Ge = 1 + 5.7143 Rt.(1 - \text{Exp}(-0.07/Rt)) \text{ and } m = 0.176$$

This correlation for  $Ge$  is the same as the ESDU Item 81045 correlation

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.7 Heat Transfer on Vessel Internal Surface

#### Non-Agitated Vessels

The correlations used here are taken from Rohsenow et al

$$C_{lam} = 0.6707 / (1 + (0.492 / Pr)^{0.5625})^{0.4444}$$

$$Nu_{lam} = 2.8 / \ln(1 + 2.8 / (C_{lam} \cdot (Gr \cdot Pr)^{0.25}))$$

$$C_{turb} = 0.13 Pr^{0.22} / (1 + 0.61 Pr^{0.81})^{0.42}$$

$$Nu_{turb} = C_{turb} \cdot (Gr \cdot Pr)^{0.333}$$

Combining laminar and turbulent components of natural convection

$$Nu^6 = Nu_{lam}^6 + Nu_{turb}^6$$

$$Gr = g \cdot \beta \cdot H^3 \cdot \rho^2 \cdot \Delta T / \mu^2$$

$$\Delta T = \text{mean value of } T_w - T_b$$

All properties are evaluated at the film temperature,  $T_f = (T_w + T_b) / 2$

#### Agitated Vessels - General

The correlations used in this section have been extensively revamped for Delta T version 5. For heat transfer on vessel internal surface, the following references have been used:

- |                       |                       |
|-----------------------|-----------------------|
| o W R Penney          | o Bondy & Lipka       |
| o Uhl                 | o Ackley              |
| o Nagata              | o Holland and Chapman |
| o Chapman and Holland | o Skelland et al      |
| o Chapman et al       | o Brooks and Su       |

The primary dimensionless numbers used here are:

$$Nu = h d_v / k \text{ for vessel-wall coefficients}$$

$$= h d_t / k \text{ for coil coefficients}$$

$$Re = \rho N d_a / \mu$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### Turbines and Paddles

The analyses of Penney, Brooks & Su and Holland & Chapman are used.

#### Fully Baffled Vessels

$$\begin{aligned} \text{Nu}_{fb} &= h d_v/k \\ &= K \text{Re}^{0.67} \text{Pr}^{0.33} v_i^{0.14} G_1 G_2 G_3 \end{aligned}$$

$$G_1 = (5 x_a/d_a)^{0.2}$$

$$G_2 = (n_b/6)^{0.2}$$

$$G_3 = (\text{Sin}(\theta))^{0.5}$$

$x_a$  = vertical blade height =  $W_a \text{Sin}(\theta)$

$W_a$  = blade width

$\theta$  = blade angle from horizontal (flat vertical blade  $\theta = 90$  degrees)

$n_b$  = number of blades

$K = 0.54$  for  $\text{Re} < 400$

$= 0.74$  for  $\text{Re} > 10000$

$= 0.1679 + 0.0621 \ln(\text{Re})$  for  $400 < \text{Re} < 10000$

#### Unbaffled Vessels

The formula for baffled vessels is used with  $K = 0.54$  for all  $\text{Re}$ .

#### Partially Baffled Vessels

Delta T interpolates between the fully baffled and the unbaffled cases using the Baffling Parameter of Nagata (see Section 10.9):

$$\text{Nu}_{pb} = \text{Nu}_{fb} - N_a(\text{Nu}_{fb} - \text{Nu}_{ub})$$

#### Note on Retreating-Blade Turbines

Active consideration was given to separate treatment for retreating-blade turbines. The available correlations (Cummings & West and Ackley) are not consistent with each other nor with the correlations for flat-blade turbines. We feel that the presented correlations for flat turbines will give reasonable and consistent values for retreating-blade turbines.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Propellers

We use the relations presented by Penney which were developed from the results of Ackley, Nagata and Strek.

#### Fully Baffled Vessels

$$\begin{aligned} \text{Nu} &= h d_v/k \\ &= 0.50 \text{Re}^{0.67} \text{Pr}^{0.33} v_i^{0.14} G_1 \end{aligned}$$

$$\begin{aligned} G_1 &= 1.29 (\lambda/d_a)/(0.29 + (\lambda/d_a)) \\ \lambda &= \text{propeller pitch} \end{aligned}$$

#### Unbaffled Vessels

$$\begin{aligned} \text{Nu} &= h d_v/k \\ &= 0.37 \text{Re}^{0.67} \text{Pr}^{0.33} v_i^{0.14} G_1 G_2 G_3 \end{aligned}$$

$$G_1 = 1.29 (\lambda/d_a)/(0.29 + (\lambda/d_v))$$

$$G_2 = (d_v/(3 d_a))^{0.25}$$

$$G_3 = (H_a/H_{liq})^{0.15}$$

#### Partially Baffled Vessels

The Nusselt number is estimated by interpolation between the fully baffled case and the unbaffled case using the Nagata Baffle Parameter (see 10.7.3).

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 10 TECHNICAL REFERENCE (continued)

### Anchors and Helical Ribbons

Only the case of mixing in an unbaffled vessel is considered. We have combined, extended and extrapolated the results of Penney

The basic formula is

$$\text{Nu} = h d_v/k$$
$$= \phi_1(\text{Re}) \phi_2(C_a/d_v) \phi_3(\lambda/d_v) \text{Pr}^{0.33} \nu^{0.14}$$

$$C_a = (d_v - d_a)/2$$

$\lambda$  = ribbon pitch

The terms of this equation are detailed as follows:

(1) Base Function  $\phi_1(\text{Re})$

For helical ribbons (based on the case of  $C_a/d_v = 0.02$  and  $\lambda/d_v = 0.25$ ),

$$\phi_1(\text{Re}) = K \text{Re}^n, \text{ with}$$

$$K = 0.98 \quad n = 0.33 \quad \text{for } \text{Re} < 9$$
$$K = 0.68 \quad n = 0.50 \quad \text{for } 9 < \text{Re} < 135$$
$$K = 0.30 \quad n = 0.67 \quad \text{for } 135 < \text{Re}$$

For anchors based on the case of  $C_a/d_v = 0.02$

$$\phi_1(\text{Re}) = K \text{Re}^n, \text{ with}$$

$$K = 1.05 \quad n = 0.33 \quad \text{for } \text{Re} < 12$$
$$K = 0.69 \quad n = 0.50 \quad \text{for } 12 < \text{Re} < 100$$
$$K = 0.32 \quad n = 0.67 \quad \text{for } 100 < \text{Re}$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### (2) Effect of Agitator Clearance $\phi_2(C_a/d_v)$

Penney gives a graphical presentation of the effect of agitator clearance on heat transfer coefficient. This data has been curve-fitted by Madison Technical Software as follows

$$h(x)/h(0.02) = 1.455(1 - x^{0.116 - 0.046 \ln(x)}) = \phi_2(x) \text{ for } x > 0$$

$$h(0)/h(0.02) = 1.455$$

where  $x = C_a/d_v$

### (3) Effect of Ribbon Pitch $\phi_3(\lambda/d_v)$

For anchors,  $\phi_3 = 1$

For helical ribbons, Penney gives data for  $\lambda/d_v = 0.25$  and  $0.5$ . From this data

$$\begin{aligned} h(x)/h(0.25) = \phi_3(x) &= 0.920/x^{0.06} && \text{for } Re < 11 \\ &= 0.801/x^{0.16} && \text{for } 11 < Re < 170 \\ &= 0.697/x^{0.26} && \text{for } 170 < Re \end{aligned}$$

### (4) Limits of Applicability

$$0.10 < \lambda/d_v < 2.0 \qquad 0.0 < C_a/d_v < 0.20$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.8 Heat Transfer on Tube Outer Surface

#### Non-Agitated Conditions

The ESDU correlation for natural convection on the outer surface of tubes is (ESDU Item 69004).

$$\text{Nu} = \text{Exp}(0.0545 + 0.0922 \ln(\text{Pr}) - 0.0147 \ln^2(\text{Pr}) + 0.118 \ln(\text{Gr.Pr}) + 0.00485 \ln^2(\text{Gr.Pr})) \cdot \text{Vi}^{0.137}$$

All properties are evaluated at the bulk temperature.

$$\text{Gr} = \beta \cdot g \cdot d_e^3 \cdot \rho^2 \cdot \Delta T / \mu^2$$

$d_e$  = tube outside diameter

$\Delta T$  = mean value of  $T_w - T_b$

#### Turbines

We use Penney and Nagata as references in this section. The results apply to all turbines and paddles.

#### Fully Baffled Vessels

$$\begin{aligned} \text{Nu} &= h d_t / k \\ &= 0.03 \text{Re}^{0.67} \text{Pr}^{0.33} \text{Vi}^{0.14} G_1 G_2 G_3 \end{aligned}$$

$$G_1 = (5 x_a / d_a)^{0.20} \text{ and } G_2 = (25 d_t / d)^{0.5}$$

$$G_3 = (d_v / H_{liq})^{0.15}$$

#### Unbaffled Vessels

$$\text{Nu} = h d_t / k = 0.08 \text{Re}^{0.56} \text{Pr}^{0.33} \text{Vi}^{0.14} G_1 G_2$$

$$G_1 = (5 x_a / d_a)^{0.15} \text{ and } G_2 = (15.6 d_t / d_v)^{0.50}$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Partially Baffled Vessels

The Nusselt number is estimated by interpolation between the fully baffled case and the unbaffled case using the Nagata baffle parameter (see 10.7.3).

### Propellers

We use the relations presented by Penney developed from the results of Ackley, Nagata, Oldshue and Skelland et al.

### Fully Baffled Vessels

$$Nu = h d_t/k = 0.016 Re^{0.67} Pr^{0.37} \nu_i^{0.14} G_1 G_2$$

$$G_1 = (3 d_a/d_v)^{0.10}$$

$$G_2 = (25 d_t/d_v)^{0.50}$$

### Unbaffled Vessels

$$Nu = h d_t/k = 0.05 Re^{0.62} Pr^{0.33} \nu_i^{0.14} G_1 G_2$$

$$G_1 = (33.3 d_t/d_v)^{0.50}$$

$$G_2 = (0.333 d_v/d_a)^{0.20}$$

### Partially Baffled Vessels

The Nusselt number is estimated by interpolation between the fully baffled case and the unbaffled case using the Nagata Baffle Parameter (see 10.7.3).

### Helical Ribbons and Anchors

To our knowledge, there are no published correlations for the heat transfer on the outside of coils in vessels agitated with helical ribbons or anchors. In order to provide a rough and ready working design for these situations, Delta T models the helical ribbon as a propeller and models the anchor as a paddle/turbine.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.9 Agitator Absorbed Power

#### General

The following references have been used:

- Penney & Bell
- Tatterson
- Uhl & Voznick
- Sawinsky et al
- Rushton et al
- Holland & Chapman
- Bates et al
- Nagata

#### Turbines

The generalised formulas of Nagata are adapted and presented here. These formulas apply to all types of turbines and paddles.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Unbaffled Vessels

Define the effective agitator blade width

$$W_{ae} = n_b W_a / 2$$

$$A = 14 + (W_{ae}/d_v)(670(d_a/d_v - 0.6)^2 + 185)$$

$$\log_{10}(B) = 1.3 - 4(W_{ae}/d_v - 0.5)^2 - 1.14(d_a/d_v)$$

$$n = 1.1 + 4W_{ae}/d_v - 2.5(d_a/d_v - 0.5)^2 - 7(W_{ae}/d_v)^4$$

$$z = (1000 + 1.2 \text{Re}^{0.66}) / (1000 + 3.2 \text{Re}^{0.66})$$

Then,

$$P_{Oub} = P / (\rho N^3 d_a^5) = A/Re + Bz^n G_1 G_2$$

$$G_1 = (H_{liq}/d_v)^m$$

$$m = 0.35 + W_{ae}/d_v$$

$$G_2 = (\sin(\theta))^{1.2}$$

$\theta$  = blade angle

The experimental data ranges for these relations are

$$0.3 < d_a/d_v < 0.80$$

$$0.05 < W_{ae}/d_v < 0.5$$

### Fully Baffled Vessels

For a baffled vessel, full baffling occurs when,

$$(W_{baff}/d_v)^{1.2} n_{baff} = 0.35$$

with  $W_{baff}$  = baffle width and  $n_{baff}$  = number of baffles

$$P_o = P_{ofb} = P_{Oub} \text{ at } Re = Re_c$$

$$Re_c = 25(d_a/d_v - 0.4)^2 / (W_{ae}/d_v) + (W_{ae}/d_v) / (0.11(W_{ae}/d_v) - 0.0048)$$

$$\text{If } \theta < 90 \text{ degrees then, } Re_c(\theta) = 104(1 - \sin(\theta)) Re_c$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Partially Baffled Vessels

$$Po = Po_{fb} - Na(Po_{fb} - Po_{ub})$$

$$Na = \text{Nagata Baffling Parameter} \\ = (1 - 2.9(W_{baff}/d_v)^{1.2} n_{baff})^2$$

When  $(W_{baff}/d_v)^{1.2} n_{baff} > 0.35$  then  $Na = 0.20$ .  $Po_{ub}$  is the power number with no baffling.

### Multiple Impellers

As an approximation, the following gives reasonable results,

$$Po(n_a = n_a) = n_a Po(n_a = 1)$$

### Propellers

We base our equations on the data of Bates at al given in Uhl "Mixing".

### Fully Baffled Vessels

$$Po_{fb} = 47/Re + 0.16(\lambda/d_a)^{1.6}(d_v/d_a)^{0.65}$$

### Unbaffled Vessels

$$Po_{ub} = 42/Re + 0.634(\lambda/d_a)/Re^{0.08}$$

### Partially Baffled Vessels

The Nusselt number is estimated by interpolation between the fully baffled case and the unbaffled case using the Nagata Baffling Parameter (see 10.7.3).

### Multiple Impellers

As an approximation, the following gives reasonable results,

$$Po(n_a = n_a) = n_a Po(n_a = 1)$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Anchors

We derive our equations from Sawinsky at al

#### Low Re Region (Re < 30)

$$Po = a(L/d_a)(d_v/C)^n/Re$$

$$a = 17$$

$$n = 0.45$$

$$L = (2 H_a + d_a)$$

$H_a$  = height of anchor

$$C = (d_v - d_a)/2$$

#### Moderate Re Region (30 < Re < 10000)

$$Po = (L/d_a) f(Re)$$

$$f(Re) = (0.567(d_v/C)^{0.45} - 0.121) g(Re) + 0.121$$

$$g(Re) = K Re^n$$

$$n = -0.889 \quad K = 20.57 \quad 30 < Re < 50$$

$$n = -0.827 \quad K = 16.14 \quad 50 < Re < 100$$

$$n = -0.721 \quad K = 9.906 \quad 100 < Re < 10000$$

#### High Re Region (Re > 10000)

$$Po = (L/d_a) f(Re)$$

$$f(Re) = (0.09668(d_v/C)^{0.45} + 1.5741)/Re^{0.28}$$

#### Limits on C/d<sub>v</sub>

The evidence is presented in the literature for  $C/d_v > 0.01$ . We allow use of the relations down to  $C/d_v = 0.005$ . For smaller values of  $C/d_v$ , the program uses the value calculated at  $C/d_v = 0.005$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Helical Ribbons

The low-Re formula is from Sawinsky et al. The higher-Re formula is derived by consideration of the low-Re formulas for ribbons and anchors and the higher-Re formulas for anchors.

#### Low Re Region (Re < 100)

$$Po = a(L/d_a)(d_v/C)^n/Re$$

with

$$a = 19$$

$$n = 0.45$$

$$L = n_{ribb}H_a(1 + (\pi.d_a/\lambda)^2)^{0.50}$$

$H_a$  = overall height of agitator

$\lambda$  = ribbon pitch

$$C = (d_v - d_a)/2$$

#### Higher Re Region (100 < Re)

For equal  $(L/d_a)$  and  $(d_v/C)$ , the low-Re values for ribbons are 19/17 times the low-Re values for anchors. The anchor curve however deviates from a straight line in the region above  $Re = 30$  while the relation for helical ribbons is linear up to  $Re = 100$ . The net effect at  $Re = 100$  is

$$P_{oribb}/P_{oanch} = 1/(1.0679 + 0.4088/(C/d_v)^{0.45})$$

This factor is applied for  $Re > 100$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.10 Condensation Heat Transfer in Jackets

#### General

The following basic assumptions are made in this analysis:

- Entry conditions are dry, saturated ( $X = 1$ )
- All entering vapour condenses
- Exit conditions are saturated liquid ( $X = 0$ )

The following condensing surface configurations and flow regimes are considered:

- Gravity controlled flow in vertical ducts
- Stratified flow in horizontal ducts

The correlations presented for vertical ducts are applicable to condensation in conventional jackets and dimple jackets. The correlations developed for horizontal ducts are applicable to half-pipe coils, baffled conventional jackets, user-defined jackets and internal coils.

Note that the correlations used assume gravity-control of the condensate film thickness. No allowance has been made for vapour-shear control of the condensate film which may occur in the initial portion of the jacket at very high condensing rates; heat transfer coefficients in a vapour-shear control regime may be several times greater than in a gravity-control regime. It is also assumed that no flooding of the heat transfer surface occurs and that the jacket is adequately steam-trapped; heat transfer coefficients in a flooded region may be several times smaller than in a well-drained gravity-control region. It is felt that the general use of the gravity-control correlations is justified for design purposes.

#### Gravity Control Flow, Vertical Ducts

We follow the analysis of Butterworth (Handbook of Heat Exchanger Design, Hemisphere, 1983)

The dimensionless average heat transfer coefficient in the gravity control region from  $z = 0$  to  $z = z$  is defined as

$$h^+(0,z) = (h/k) \cdot (\mu_L^2 / (g \rho_L (\rho_L - \rho_V)))^{0.33}$$

$h$  = average coefficient from  $z = 0$  to  $z = z$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

The Reynolds Number is based on the liquid flowrate at  $z = z$

$$Re = Re(z) = 4W(z)/\mu_L P$$

$W(z)$  = liquid flowrate at  $z$

$z$  = co-ordinate in flow direction

$P$  = width of condensing surface

$$\text{For } Re < 30, \quad h^+(0,z) = 1.47 Re^{-0.333}$$

$$\text{For } 30 < Re < 1600, \quad h^+(0,z) = Re/(1.08 Re^{1.22} - 5.2)$$

$$\text{For } Re > 1600, \quad h^+(0,z) = Re/(8750 + 58 Pr^{-0.5} (Re^{0.75} - 253))$$

The average coefficient over any interval of  $z$  can be calculated from these expressions.

### Stratified Flow, Horizontal Ducts

Butterworth gives the following expression for the local coefficient,

$$h = a (k^3 \rho_L g H_V (\rho_L - \rho_V)/(\mu_L d_e \Delta T_S))^{0.25}$$

$H_V$  = latent heat of vaporization

$\Delta T_S$  = temperature differential between bulk steam and condensing surface

$a = 0.728 e^{0.75}$  (Kern gives average of  $a = 0.612$ )

$e$  = void fraction =  $1/(1 + (1 - X)(\rho_V/\rho_L)^{0.67/X})$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.11 Heat Transfer and Pressure Drop in Dimple Jackets

#### Introduction

Madison Technical Software (Garvin, 2001) has published design correlations for heat transfer and pressure drop in dimple jackets. These correlations have been implemented in Delta T and are summarised here.

#### Dimple Jacket Geometry

The following notation is used here:

$A_{min}$  = minimum flow area between adjacent dimples

$A_{max}$  = maximum or unrestricted flow area between dimples

$w$  = dimple center-to-center transverse distance

$x$  = dimple center-to-center distance parallel to flow

$z$  = internal height of dimple

$d_1$  = dimple diameter (1)

$d_2$  = dimple diameter (2)

$d_o$  = mean dimple diameter =  $(d_1 + d_2)/2$

$f$  = Fanning friction factor

$j$  = Colburn heat transfer factor =  $Nu/RePr^{1/3}$

$K$  = friction coefficient =  $\Delta P_t / (\rho V_{max}^2 / 2)$

$\rho$  = fluid density

$\mu$  = viscosity

$V_{max}$  = fluid velocity at minimum flow area

$\Delta P_t$  = pressure drop per dimple row

$Re$  = Reynolds Number =  $d_o V_{max} \rho / \mu$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### Heat Transfer Coefficient

Dimple jackets are constructed like conventional jackets but are dimpled and plug-welded to the outer vessel surface on a rectangular or staggered pattern. The presence of the plug-weld supports makes for a sturdy jacket while allowing relatively light jacket material to be used. The presence of the plug-welded dimples also provides a source of turbulence and thus generates enhanced heat transfer. Published correlations by Madison Technical Software (Garvin, 2001) derived from published data on a wide range of non-uniform flows give design estimates of the heat transfer coefficient.

For values of Reynolds Number of 1,000 through 50,000

$$j = 0.0845 (w/x)^{0.368} (A_{\min}/A_{\max})^{-0.383} \text{Re}^{-0.305}$$

### Friction Factor

The pressure drop in a dimple jacket is derived here in the following way. We define a friction coefficient K by,

$$\Delta P_t/\rho = K (V_{\max}^2/2)$$

Published data by Madison Technical Software (Garvin, 2001) give the following expression for the flow coefficient K for  $\text{Re} > 5000$

$$K = 0.135 + 0.937(w/z)^{0.575} (A_{\min}/A_{\max})^{-2.10} \text{Re}^{-0.33}$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.12 Pressure Drop in Closed, Curved Channels

#### Pressure Drop in Laminar Flow

Define,

$$Re_1 = 15000 \quad \text{for } d_e/d_c > 0.30706$$

$$Re_1 = 2000(1+13.2(d_e/d_c)^{0.6}) \quad \text{for } d_e/d_c < 0.30706$$

Laminar flow exists if  $Re < Re_1$

For straight and curved tubes and channels,

$$\Delta P = 2f.L.V^2.\rho/d_e$$

$$f = (16/Re).(1 + 0.007386 B^{1.175})^{0.40}$$

$$B = Re.(d_e/d_c)^{0.5}$$

#### Pressure Drop in Turbulent Flow

Define,

$$Re_2 = 15000 \quad \text{for } d_e/d_c > 0.0006$$

$$Re_2 = 4000 \quad \text{for } d_e/d_c < 0.0006$$

The flow is turbulent for  $Re > Re_2$

$$\Delta P = 2f.L.V^2.\rho/d_e$$

for straight tubes and channels,

$$1/(4f)^{0.5} = -2 \log_{10}(e/(3.7 d_e) + 2.51/(Re.(4f)^{0.5}))$$

with  $e$  = Absolute Roughness (typically = 0.00015 ft). For curved tubes and channels, add  $0.01(d_e/d_c)^{0.5}$  to the straight-tube friction factor.

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.13 Vessel Time-Temperature Functions

In Time-Base Output, vessel temperature and other quantities are presented as a function of time. This section presents the basic formulas used.

Define,

$$R = UA/wc$$

$$f = \text{Exp}(-R) \text{ for an unmixed jacket} \\ = 1/(1+R) \text{ for a well-mixed jacket}$$

U = Overall Heat Transfer Coefficient  
A = Heat Transfer Area  
w = Mass Flowrate through Jacket  
c = Specific Heat of Jacket Fluid

The case of a well-mixed jacket occurs with a conventional jacket fitted with agitation nozzles. The other jacket designs available as options in Delta T are best modelled as unmixed jackets.

For cooling duties, a well-mixed jacket is characterised by,

$$T_{j2} = T_{jm} > T_{j1}$$

and an unmixed jacket is characterised by,

$$T_{j2} > T_{jm} > T_{j1}$$

$T_{j2}$  = Jacket Exit Temperature  
 $T_{j1}$  = Jacket Entry Temperature  
 $T_{jm}$  = Mean Jacket Temperature

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

The jacket exit temperature at any time is given by,

$$T_{j2} = T_{j1} + (T_v - T_{j1}) \cdot (1 - f)$$

where,  $T_v$  = Vessel Temperature

The time-dependent solution is derived from the following equation

$$dT_v/dt = F(T_v) = -(wc/B_e) \cdot (T_{j2} - T_{j1}) + (q_{ex} + q_a)/B_e$$

$q_{ex}$  = exotherm rate

$q_a$  = absorbed agitator power

$B_e$  = equivalent thermal bulk of vessel and contents

This equation becomes,

$$dT_v/dt = F(T_v) = -(wc/B_e) \cdot (T_v - T_{j1}) \cdot (1 - f) + (q_{ex} + q_a)/B_e$$

The fourth order Runge-Kutta solution is,

$$T_{v,n+1} = T_{v,n} + (k_0 + 2k_1 + 2k_2 + k_3)/6$$

$$k_0 = h \cdot F(T_v)$$

$$k_1 = h \cdot F(T_v + k_0/2)$$

$$k_2 = h \cdot F(T_v + k_1/2)$$

$$k_3 = h \cdot F(T_v + k_2)$$

The error of the method is approximately  $h^5/120$  where  $h$  is the magnitude of the computation step.

Note that when the jacket temperature is uniform as in the case of steam heating, the appropriate form for  $F(T_v)$  is,

$$F(T_v) = -(UA/B_e)(T_v - T_j) + (q_{ex} + q_a)/B_e$$

# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

### 10.14 References

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# The new batch reactor heat transfer and chemical properties calculator



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## 10 TECHNICAL REFERENCE (continued)

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# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS

### 11.1 Enhanced Database

Air	
Ar	argon
BCl <sub>3</sub>	boron trichloride
Br <sub>2</sub>	bromine
Cl <sub>2</sub>	chlorine
SiCl <sub>4</sub>	silicon tetrachloride
TiCl <sub>4</sub>	titanium tetrachloride
D <sub>2</sub> O	deuterium oxide
F <sub>2</sub>	fluorine
He	helium
Hg	mercury
I <sub>2</sub>	iodine
NO	nitric oxide
NO <sub>2</sub>	nitrogen dioxide
N <sub>2</sub>	nitrogen
N <sub>2</sub> O	nitrous oxide
Ne	neon
O <sub>2</sub>	oxygen
SO <sub>2</sub>	sulfur dioxide
O <sub>3</sub>	ozone
SO <sub>3</sub>	sulfur trioxide
HBr	hydrogen bromide
HCl	hydrogen chloride
HF	hydrogen fluoride
HI	hydrogen iodide
H <sub>2</sub>	hydrogen
H <sub>2</sub> O	water
H <sub>2</sub> S	hydrogen sulfide
NH <sub>3</sub>	ammonia
PH <sub>3</sub>	phosphine
N <sub>2</sub> H <sub>4</sub>	hydrazine
SiH <sub>4</sub>	silane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

CBrClF <sub>2</sub>	bromochlorodifluoromethane
CBrCl <sub>3</sub>	bromotrichloromethane
CBr <sub>2</sub> F <sub>2</sub>	dibromodifluoromethane
CBrF <sub>3</sub>	trifluorobromomethane
CClF <sub>3</sub>	chlorotrifluoromethane
CCl <sub>2</sub> F <sub>2</sub>	dichlorodifluoromethane
COCl <sub>2</sub>	phosgene
CCl <sub>3</sub> F	trichlorofluoromethane
CCl <sub>4</sub>	carbon tetrachloride
CF <sub>4</sub>	carbon tetrafluoride
CO	carbon monoxide
COS	carbonyl sulfide
CO <sub>2</sub>	carbon dioxide
CS <sub>2</sub>	carbon disulfide
CHBr <sub>3</sub>	tribromomethane
CHClF <sub>2</sub>	chlorodifluoromethane
CHCl <sub>2</sub> F	dichloromonofluoromethane
CHCl <sub>3</sub>	chloroform
CHF <sub>3</sub>	fluoroform
HCN	hydrogen cyanide
CH <sub>2</sub> Br <sub>2</sub>	dibromomethane
CH <sub>2</sub> BrCl	bromochloromethane
CH <sub>2</sub> Cl <sub>2</sub>	dichloromethane
CH <sub>2</sub> F <sub>2</sub>	difluoromethane
COH <sub>2</sub>	formaldehyde
CO <sub>2</sub> H <sub>2</sub>	formic acid
CH <sub>3</sub> Br	methyl bromide
CH <sub>3</sub> Cl	methyl chloride
CH <sub>3</sub> F	methyl fluoride
CH <sub>3</sub> I	methyl iodide
CH <sub>3</sub> NO	formamide
CH <sub>3</sub> NO <sub>2</sub>	nitromethane
CH <sub>4</sub>	methane
CH <sub>4</sub> O	methanol
CH <sub>4</sub> S	methyl mercaptan
CH <sub>5</sub> N	methyl amine
C <sub>2</sub> BrF <sub>3</sub>	bromotrifluoroethylene
C <sub>2</sub> Br <sub>2</sub> ClF <sub>3</sub>	1,2-dibromo-1-chlorotrifluoroethane
C <sub>2</sub> Br <sub>2</sub> F <sub>4</sub>	1,2-dibromotetrafluoroethane
C <sub>2</sub> ClF <sub>3</sub>	chlorotrifluoroethylene
C <sub>2</sub> ClF <sub>5</sub>	chloropentafluoroethane
C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub>	1,1-dichlorotetrafluoroethane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C2Cl2F4	1,2-dichlorotetrafluoroethane
C2Cl3F3	1,2,2-trichlorotrifluoroethane
C2Cl4	tetrachloroethylene
C2Cl4F2	1,1,2,2-tetrachlorodifluoroethane
C2F3N	trifluoroacetonitrile
C2F4	perfluoroethylene
C2F6	perfluoroethane
C2N2	cyanogen
C2HClF2	1-chloro-2,2-difluoroethylene
C2HClF4	chloro-1,1,2,2-tetrafluoroethane
C2HCl3	trichloroethylene
C2HCl5	pentachloroethane
C2HF3O2	trifluoroacetic acid
C2H2	acetylene
C2H2Cl2	1,1-dichloroethylene
C2H2Cl2	cis-1,2-dichloroethylene
C2H2Cl2	trans-1,2-dichloroethylene
C2H2Cl4	1,1,1,2-tetrachloroethane
C2H2Cl4	1,1,2,2-tetrachloroethane
C2H2F2	1,1-difluoroethene
C2H2O	ketene
C2H3Cl	vinyl chloride
C2H3ClF2	1-chloro-1,1-difluoroethane
C2H3ClO	acetyl chloride
C2H3Cl3	1,1,1-trichloroethane
C2H3Cl3	1,1,2-trichloroethane
C2H3F	vinyl fluoride
C2H3F3	1,1,1-trifluoroethane
C2H3N	acetonitrile
C2H3NO	methyl isocyanate
C2H4	ethylene
C2H4Br2	1,2-dibromoethane
C2H4Cl2	1,1-dichloroethane
C2H4Cl2	1,2-dichloroethane
C2H4F2	1,1-difluoroethane
C2H4O	acetaldehyde
C2H4O	ethylene oxide
C2H4O2	acetic acid
C2H4O2	methyl formate
C2H5Br	ethyl bromide
C2H5Cl	ethyl chloride
C2H5F	ethyl fluoride

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 1

## 11 LIST OF COMPOUNDS (continued)

C2H5I	ethyl iodide
C2H5NO	acetamide
C2H6	ethane
C2H6O	dimethyl ether
C2H6O	ethanol
C2H6O2	ethylene glycol
C2H6S	ethyl mercaptan
C2H6S	dimethyl sulfide
C2H7N	ethyl amine
C2H7N	dimethylamine
C2H7NO	monoethanolamine
C2H8N2	ethylenediamine
C3CIF5O	chloropentafluoroacetone
C3F6O	perfluoroacetone
C3F8	perfluoropropane
C3H3F3	trifluoropropene
C3H3F5	1,1,1,2,2-pentafluoropropane
C3H3N	acrylonitrile
C3H3NO	oxazole
C3H3NO	isoxazole
C3H4	propadiene
C3H4	methyl acetylene
C3H4O	acrolein
C3H4O2	acrylic acid
C3H4O2	vinyl formate
C3H5Cl	allyl chloride
C3H5Cl3	1,2,3-trichloropropane
C3H5N	propionitrile
C3H6	cyclopropane
C3H6	propylene
C3H6Cl2	1,2-dichloropropane
C3H6O	acetone
C3H6O	allyl alcohol
C3H6O	propionaldehyde
C3H6O	1,2-propylene oxide
C3H6O	1,3-propylene oxide
C3H6O	vinyl methyl ether
C3H6O2	propionic acid
C3H6O2	ethyl formate
C3H6O2	methyl acetate
C3H7Cl	propyl chloride
C3H7Cl	isopropyl chloride

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C3H8	propane
C3H8O	1-propanol
C3H8O	isopropyl alcohol
C3H8O	methyl ethyl ether
C3H8O2	methylal
C3H8O2	1,2-propanediol
C3H8O2	1,3-propanediol
C3H8S	methyl ethyl sulfide
C3H9N	n-propyl amine
C3H9N	isopropyl amine
C3H9N	trimethyl amine
C4F8	perfluorocyclobutane
C4F10	perfluorobutane
C4H4	vinylacetylene
C4H4O	furan
C4H4S	thiophene
C4H5Cl	chloroprene
C4H5N	allyl cyanide
C4H5N	pyrrole
C4H6	1-butyne
C4H6	2-butyne
C4H6	1,2-butadiene
C4H6	1,3-butadiene
C4H6O2	vinyl acetate
C4H6O3	acetic anhydride
C4H6O4	dimethyl oxalate
C4H6O4	succinic acid
C4H7N	butyronitrile
C4H6O2	methyl acrylate
C4H8	1-butene
C4H8	cis-2-butene
C4H8	trans-2-butene
C4H8	cyclobutane
C4H8	isobutylene
C4H8O	n-butyraldehyde
C4H8O	isobutyraldehyde
C4H8O	methyl ethyl ketone
C4H8O	tetrahydrofuran
C4H8O	vinyl ethyl ether
C4H8O2	n-butyric acid
C4H8O2	isobutyric acid
C4H8O2	1,4-dioxane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C4H8O2	ethyl acetate
C4H8O2	methyl propionate
C4H8O2	n-propyl formate
C4H8S	tetrahydrothiophene
C4H9Cl	1-chlorobutane
C4H9Cl	2-chlorobutane
C4H9Cl	tert-butyl chloride
C4H9N	pyrrolidine
C4H9NO	morpholine
C4H10	n-butane
C4H10	isobutane
C4H10N2	piperazine
C4H10O	1-butanol
C4H10O	2-butanol
C4H10O	isobutanol
C4H10O	tert-butanol
C4H10O	diethyl ether
C4H10O	methyl propyl ether
C4H10O	methyl isopropyl ether
C4H10O2	1,2-dimethoxyethane
C4H10O2	1,3-butanediol
C4H10O2	1,4-butanediol
C4H10S	diethyl sulfide
C4H10S2	diethyl disulfide
C4H11N	n-butyl amine
C4H11N	isobutyl amine
C4H11N	diethyl amine
C5F12	perfluoropentane
C5H2F6O2	hexafluoroacetylacetone
C5H4O2	furfural
C5H5N	pyridine
C5H6N2	2-methyl pyrazine
C5H6O	2-methyl furan
C5H8	cyclopentene
C5H8	1,2-pentadiene
C5H8	cis-1,3-pentadiene
C5H8	trans-1,3-pentadiene
C5H8	1,4-pentadiene
C5H8	1-pentyne
C5H8	isoprene
C5H8	3-methyl-1,2-butadiene
C5H8O	cyclopentanone

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C5H8O	dihydropyran
C5H8O2	ethyl acrylate
C5H10	cyclopentane
C5H10	1-pentene
C5H10	cis-2-pentene
C5H10	trans-2-pentene
C5H10	2-methyl-1-butene
C5H10	2-methyl-2-butene
C5H10	3-methyl-1-butene
C5H10O	valeraldehyde
C5H10O	methyl propyl ketone
C5H10O	methyl isopropyl ketone
C5H10O	diethyl ketone
C5H10O	2-methyl tetrahydrofuran
C5H10O	tetrahydropyran
C5H10O2	n-valeric acid
C5H10O2	isovaleric acid
C5H10O2	isobutyl formate
C5H10O2	n-propyl acetate
C5H10O2	ethyl propionate
C5H10O2	methyl butyrate
C5H10O2	methyl isobutyrate
C5H11N	piperidine
C5H12	n-pentane
C5H12	2-methyl butane
C5H12	2,2-dimethylpropane
C5H12O	1-pentanol
C5H12O	2-methyl-1-butanol
C5H12O	3-methyl-1-butanol
C5H12O	3-methyl-2-butanol
C5H12O	2-methyl-2-butanol
C5H12O	2,2-dimethyl-1-propanol
C5H12O	ethyl propyl ether
C5H12O	butyl methyl ether
C5H12O	tert-butyl methyl ether
C6BrF5	bromopentafluorobenzene
C6ClF5	chloropentafluorobenzene
C6Cl2F4	dichlorotetrafluorobenzene
C6Cl3F3	1,3,5-trichlorotrifluorobenzene
C6Cl6	perchlorobenzene
C6F6	perfluorobenzene
C6F12	perfluorocyclohexane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C6F14	perfluoro-n-hexane
C6F14	perfluoro-2-methylpentane
C6F14	perfluoro-3-methylpentane
C6F14	perfluoro-2,3-dimethylbutane
C6HF5	pentafluorobenzene
C6HF5O	pentafluorophenol
C6H2F4	1,2,3,4-tetrafluorobenzene
C6H2F4	1,2,3,5-tetrafluorobenzene
C6H2F4	1,2,4,5-tetrafluorobenzene
C6H4Cl2	o-dichlorobenzene
C6H4Cl2	m-dichlorobenzene
C6H4Cl2	p-dichlorobenzene
C6H4F2	1,4-difluorobenzene
C6H5Br	bromobenzene
C6H5Cl	chlorobenzene
C6H5F	fluorobenzene
C6H5I	iodobenzene
C6H5NO2	nitrobenzene
C6H6	benzene
C6H6O	phenol
C6H7N	aniline
C6H7N	2-methylpyridine
C6H7N	3-methylpyridine
C6H7N	4-methyl pyridine
C6H10	1,5-hexadiene
C6H10	cyclohexene
C6H10O	cyclohexanone
C6H11N	capronitrile
C6H12	cyclohexane
C6H12	methylcyclopentane
C6H12	1-hexene
C6H12	2-hexene,cis
C6H12	2-hexene,trans
C6H12	3-hexene,cis
C6H12	3-hexene,trans
C6H12	2-methyl-1-pentene
C6H12	4-methyl-1-pentene
C6H12	2-methyl-2-pentene
C6H12	3-methyl-2-pentene,cis
C6H12	3-methyl-2-pentene,trans
C6H12	4-methyl-2-pentene,cis
C6H12	4-methyl-2-pentene,trans

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C6H12	2,3-dimethyl-1-butene
C6H12	2,3-dimethyl-2-butene
C6H12	3,3-dimethyl-1-butene
C6H12O	cyclohexanol
C6H12O	ethyl propyl ketone
C6H12O	methyl butyl ketone
C6H12O	methyl isobutyl ketone
C6H12O2	n-butyl acetate
C6H12O2	isobutyl acetate
C6H12O2	ethyl butyrate
C6H12O2	ethyl isobutyrate
C6H12O2	n-propyl propionate
C6H12O2	n-amyl formate
C6H12O2	isoamyl formate
C6H12O3	paraldehyde
C6H14	n-hexane
C6H14	isohexane
C6H14	3-methyl pentane
C6H14	2,2-dimethyl butane
C6H14	2,3-dimethyl butane
C6H14O	1-hexanol
C6H14O	2-hexanol
C6H14O	ethyl butyl ether
C6H14O	methyl amyl ether
C6H14O	dipropyl ether
C6H14O	diisopropyl ether
C6H15N	dipropylamine
C6H15N	diisopropylamine
C6H15N	triethylamine
C7F8	perfluorotoluene
C7F14	perfluoromethylcyclohexane
C7F16	perfluoro-n-heptane
C7H3F5	2,3,4,5,6-pentafluorotoluene
C7H5N	benzotrile
C7H6O	benzaldehyde
C7H6O2	benzoic acid
C7H7Cl	benzyl chloride
C7H8	toluene
C7H8O	anisole
C7H8O	benzyl alcohol
C7H8O	o-cresol
C7H8O	m-cresol

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C7H8O	p-cresol
C7H9N	2,3-dimethylpyridine
C7H9N	2,4-dimethylpyridine
C7H9N	2,5-dimethylpyridine
C7H9N	2,6-dimethylpyridine
C7H9N	3,4-dimethylpyridine
C7H9N	3,5-dimethylpyridine
C7H9N	N-methyl aniline
C7H9N	o-toluidine
C7H9N	m-toluidine
C7H9N	p-toluidine
C7H9N	benzylamine
C7H14	cycloheptane
C7H14	1,1-dimethylcyclopentane
C7H14	1,2-dimethylcyclopentane-cis
C7H14	1,2-dimethylcyclopentane-trans
C7H14	ethylcyclopentane
C7H14	methylcyclohexane
C7H14	1-heptene
C7H14	2,3,3-trimethyl-1-butene
C7H14O	methyl amyl ketone
C7H14O2	n-propyl butyrate
C7H14O2	n-propyl isobutyrate
C7H14O2	isoamyl acetate
C7H14O2	isobutyl propionate
C7H16	n-heptane
C7H16	2-methylhexane
C7H16	3-methylhexane
C7H16	2,2-dimethylpentane
C7H16	2,3-dimethylpentane
C7H16	2,4-dimethylpentane
C7H16	3,3-dimethylpentane
C7H16	3-ethylpentane
C7H16	2,2,3-trimethylbutane
C7H16O	1-heptanol
C8H4O3	phthalic anhydride
C8H7N	indole
C8H8	styrene
C8H8O	methyl phenyl ketone
C8H8O2	methyl benzoate
C8H8O3	methyl salicylate
C8H10	o-xylene

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C8H10	m-xylene
C8H10	p-xylene
C8H10	ethylbenzene
C8H10O	o-ethylphenol
C8H10O	m-ethylphenol
C8H10O	p-ethylphenol
C8H10O	ethyl phenyl ether
C8H10O	2,3-xylenol
C8H10O	2,4-xylenol
C8H10O	2,5-xylenol
C8H10O	2,6-xylenol
C8H10O	3,4-xylenol
C8H10O	3,5-xylenol
C8H11N	N,N-dimethyl aniline
C8H11N	N-ethyl aniline
C8H14O4	diethylsuccinate
C8H16	1,1-dimethylcyclohexane
C8H16	1,2-dimethylcyclohexane-cis
C8H16	1,2-dimethylcyclohexane-trans
C8H16	1,3-dimethylcyclohexane-cis
C8H16	1,3-dimethylcyclohexane-trans
C8H16	1,4-dimethylcyclohexane-cis
C8H16	1,4-dimethylcyclohexane-trans
C8H16	ethylcyclohexane
C8H16	1,1,2-trimethylcyclopentane
C8H16	1,1,3-trimethylcyclopentane
C8H16	1,2,4-trimethylcyclopentane-c,c,t
C8H16	1,2,4-trimethylcyclopentane-c,t,c
C8H16	1-methyl-1-ethylcyclopentane
C8H16	n-propylcyclopentane
C8H16	isopropylcyclopentane
C8H16	cyclooctane
C8H16	1-octene
C8H16	2-octene-trans
C8H16O2	isoamyl propionate
C8H16O2	isobutyl butyrate
C8H16O2	isobutyl isobutyrate
C8H16O2	n-propyl isovalerate
C8H18	n-octane
C8H18	2-methylheptane
C8H18	3-methylheptane
C8H18	4-methylheptane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C8H18	2,2-dimethylhexane
C8H18	2,3-dimethylhexane
C8H18	2,4-dimethylhexane
C8H18	2,5-dimethylhexane
C8H18	3,3-dimethylhexane
C8H18	3,4-dimethylhexane
C8H18	3-ethylhexane
C8H18	2,2,3-trimethylpentane
C8H18	2,2,4-trimethylpentane
C8H18	2,3,3-trimethylpentane
C8H18	2,3,4-trimethylpentane
C8H18	2-methyl-3-ethylpentane
C8H18	3-methyl-3-ethylpentane
C8H18	2,2,3,3-tetramethylbutane
C8H18O	1-octanol
C8H18O	2-octanol
C8H18O	4-methyl-3-heptanol
C8H18O	5-methyl-3-heptanol
C8H18O	2-ethyl-1-hexanol
C8H18O	dibutyl ether
C8H18O	di-tert-butyl ether
C8H19N	dibutyl amine
C8H19N	diisobutyl amine
C9H7N	quinoline
C9H7N	isoquinoline
C9H10	indane
C9H10	alpha-methylstyrene
C9H10O2	ethyl benzoate
C9H12	n-propylbenzene
C9H12	isopropylbenzene
C9H12	1-methyl-2-ethylbenzene
C9H12	1-methyl-3-ethylbenzene
C9H12	1-methyl-4-ethylbenzene
C9H12	1,2,3-trimethylbenzene
C9H12	1,2,4-trimethylbenzene
C9H12	1,3,5-trimethylbenzene
C9H13N	N,N-dimethyl-o-toluidine
C9H18	n-propylcyclohexane
C9H18	isopropylcyclohexane
C9H18	1,trans-3,5-trimethylcyclohexane
C9H18	1-nonene
C9H18O	dibutyl ketone

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C9H20	n-nonane
C9H20	2-methyloctane
C9H20	2,2-dimethylheptane
C9H20	2,2,3-trimethylhexane
C9H20	2,2,4-trimethylhexane
C9H20	2,2,5-trimethylhexane
C9H20	3,3-diethylpentane
C9H20	2,2,3,3-tetramethylpentane
C9H20	2,2,3,4-tetramethylpentane
C9H20	2,2,4,4-tetramethylpentane
C9H20	2,3,3,4-tetramethylpentane
C9H20O	1-nonanol
C10F8	perfluoronaphthalene
C10H8	naphthalene
C10H12	1,2,3,4-tetrahydronaphthalene
C10H14	n-butylbenzene
C10H14	isobutylbenzene
C10H14	sec-butylbenzene
C10H14	tert-butylbenzene
C10H14	1-methyl-2-isopropylbenzene
C10H14	1-methyl-3-isopropylbenzene
C10H14	1-methyl-4-isopropylbenzene
C10H14	1,4-diethylbenzene
C10H14	1,2,3,5-tetramethylbenzene
C10H14	1,2,4,5-tetramethylbenzene
C10H14O	thymol
C10H15N	n-butylaniline
C10H18	cis-decalin
C10H18	trans-decalin
C10H18	1,3-decadiene
C10H19N	caprylonitrile
C10H20	butylcyclohexane
C10H20	isobutylcyclohexane
C10H20	sec-butylcyclohexane
C10H20	tert-butylcyclohexane
C10H20	1-decene
C10H20O	menthol
C10H22	n-decane
C10H22	3,3,5-trimethyl heptane
C10H22	2,2,3,3-tetramethylhexane
C10H22	2,2,5,5-tetramethylhexane

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C10H22O	1-decanol
C11H10	1-methylnaphthalene
C11H10	2-methylnaphthalene
C11H14O2	butyl benzoate
C11H16	pentamethylbenzene
C11H22	n-hexylcyclopentane
C11H22	1-undecene
C11H24	n-undecane
C12H10	diphenyl
C12H10O	diphenyl ether
C12H18	hexamethylbenzene
C12H24	n-heptylcyclopentane
C12H24	1-dodecene
C12H26	dodecane
C12H26O	dihexylether
C12H26O	dodecanol
C12H27N	tributylamine
C13H12	diphenylmethane
C13H26	n-octylcyclopentane
C13H26	1-tridecene
C13H28	n-tridecane
C14H10	anthracene
C14H10	phenanthrene
C14H12O2	benzyl benzoate
C14H28	n-nonylcyclopentane
C14H28	1-tetradecene
C14H30	n-tetradecane
C15H30	n-decylcyclopentane
C15H30	1-pentadecene
C15H32	n-pentadecane
C16H10	pyrene
C16H22O4	dibutyl-o-phthalate
C16H32	n-decylcyclohexane
C16H32	1-hexadecene
C16H34	hexadecane
C17H34	n-dodecylcyclopentane
C17H36O	heptadecanol
C17H36	n-heptadecane
C18H14	o-terphenyl
C18H14	m-terphenyl
C18H14	p-terphenyl
C18H36	1-octadecene

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

C18H36	n-tridecylcyclopentane
C18H38	octadecane
C18H36O	1-octadecanol
C19H38	1-cyclopentyltetradecane
C19H40	n-nonadecane
C20H40	1-cyclopentylpentadecane
C20H42	n-eicosane
LDB001	calcium chloride 4%
LDB002	calcium chloride 8%
LDB003	calcium chloride 12%
LDB004	calcium chloride 16%
LDB005	calcium chloride 20%
LDB006	calcium chloride 24%
LDB007	calcium chloride 28%
LDB008	Dowtherm A
LDB009	Dowtherm G
LDB010	Dowtherm HT
LDB011	Dowtherm J
LDB012	Dowtherm LF
LDB013	Dowtherm Q
LDB014	ethanol 10%
LDB015	ethanol 20%
LDB016	ethanol 30%
LDB017	ethanol 40%
LDB018	ethanol 50%
LDB019	ethanol 60%
LDB020	ethanol 70%
LDB021	ethanol 80%
LDB022	ethanol 90%
LDB023	ethylene glycol 10%
LDB024	ethylene glycol 20%
LDB025	ethylene glycol 30%
LDB026	ethylene glycol 40%
LDB027	ethylene glycol 50%
LDB028	ethylene glycol 60%
LDB029	ethylene glycol 70%
LDB030	ethylene glycol 80%
LDB031	ethylene glycol 90%
LDB032	methanol 10%
LDB033	methanol 20%
LDB034	methanol 30%
LDB035	methanol 40%

# The new batch reactor heat transfer and chemical properties calculator



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## 11 LIST OF COMPOUNDS (continued)

LDB036	methanol 50%
LDB037	methanol 60%
LDB038	methanol 70%
LDB039	methanol 80%
LDB040	methanol 90%
LDB041	propylene glycol 10%
LDB042	propylene glycol 20%
LDB043	propylene glycol 30%
LDB044	propylene glycol 40%
LDB045	propylene glycol 50%
LDB046	propylene glycol 60%
LDB047	propylene glycol 70%
LDB048	propylene glycol 80%
LDB049	propylene glycol 90%
LDB050	sodium chloride 4%
LDB051	sodium chloride 8%
LDB052	sodium chloride 12%
LDB053	sodium chloride 16%
LDB054	sodium chloride 20%
LDB055	sodium chloride 24%
LDB056	Therminol LT
LDB057	Therminol 44
LDB058	Therminol 55
LDB059	Therminol 59
LDB060	Therminol 60
LDB061	Therminol 66
LDB062	Therminol 75
LDB063	Therminol VP-1
LDB064	Syltherm 800
LDB065	Syltherm XLT