



PDHonline Course K135 (3 PDH)

Estimating the Vaporization Time in Batch Reactors

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Estimating the Vaporization Time in Batch Reactors

Edward H. Steve, P.E.

Introduction

Often the operating cycle of an agitated jacketed batch reactor includes a step that reduces the volume of the contents by vaporization at either atmospheric or reduced pressure to concentrate a dissolved product. Alternately it could be the first step in the replacement of one solvent with another.

This course provides the practicing process engineer with the equations needed to easily and quickly estimate the time required to remove a defined amount of liquid from a jacketed batch reactor by vaporization. The course develops equations for both steam and heat transfer fluid (HTF) used as the heating medium.

The step-by-step derivations serve as mathematics refreshers for those who have not used this skill recently.

Before beginning his or her study, the student should become familiar with the definitions and the associated units of the items in the NOMENCLATURE list that appears at the end of the course.

Basis of the Derivations

Figure 1 depicts an agitated jacketed batch reactor used in a vaporization operation with steam in the jacket. Figure 2 represents the same operation with a liquid heat transfer fluid (HTF) in the jacket.

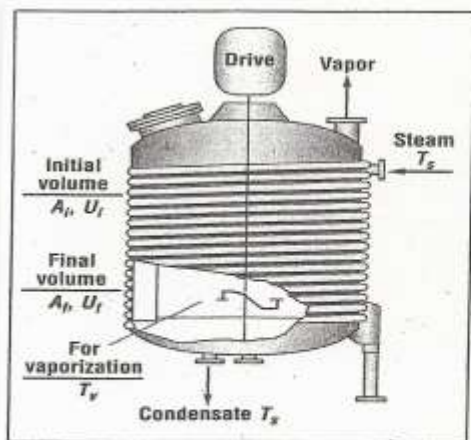


FIGURE 1. Steam provides heat at constant temperature with top-down flow

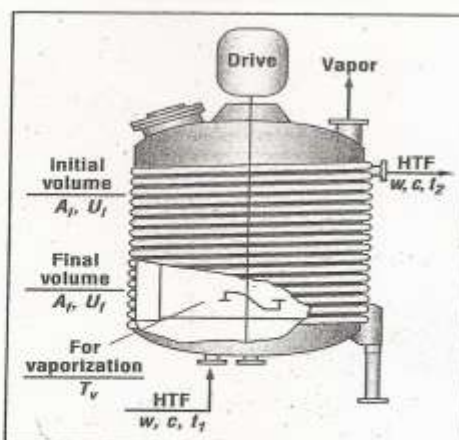
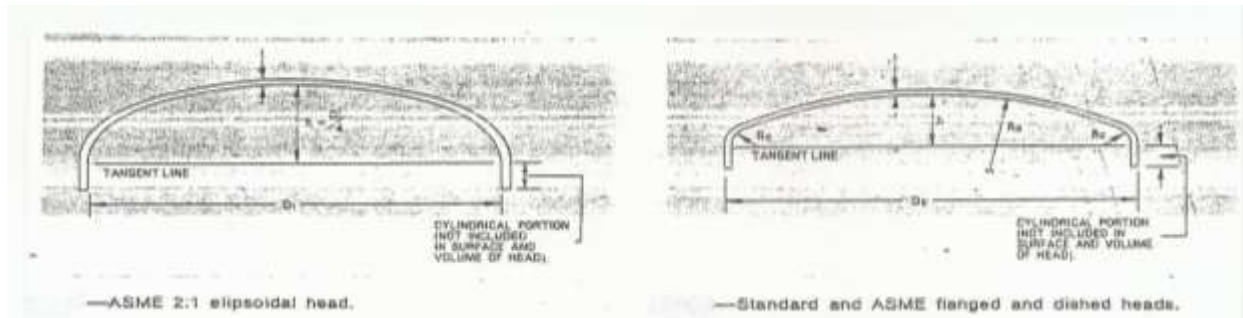


FIGURE 2. Liquid HTF provides heat at varying temperature in an upward flow
(Note: $t_1 > t_2$)

(Figures are from “Estimating the Stripping Time in Batch Reactors”, *Chemical Engineering*, December 2001.)

The reactor geometry considered in this course is a vertical cylindrical shell with a “dished” head on each end. The “dished” shapes considered here are the ASME 2:1 Elliptical head and the ASME Flanged & Dished (F&D) head, both shown below by figures from a classic article by William Dimoplon, Jr. Other reactor and head geometries are not considered in this course. The overall height of the reactor shell extends between the tangent lines of the top and bottom heads (i.e., T-T) so that area and volume calculations for the shell capture the small cylindrical portions not considered in the formulae for the heads.



(Figures are from “How to Determine the Geometry of Pressure Vessel Heads”, *Hydrocarbon Processing*, August 1974.)

Because the wall thicknesses of the shell and the heads are small as compared to the vessel diameter, the math in this course uses the internal reactor diameter (D) in all the derivations.

An external jacket forms an annular space for steam or a hot HTF to supply heat to the contents of the reactor. The jacket physically covers the T-T dimension and as much of the bottom head as possible. For this course, the jacket is the only source of heat. Design details of the jacket are not important for using steam as long as condensate removal is efficient; those details are important if the flow of HTF is not known and must be calculated (these calculations are not within the scope of this course).

During vaporization, the reactor contents decrease from an initial volume (V_i) to a final (lesser) value (V_f). The mathematics in this course assumes that:

1. The maximum initial volume does not rise above the tangent line of the top head.
2. The minimum final volume does not fall below the tangent line of the bottom head. For this reason, the minimum volume in the reactor is the volume contained in the bottom head (V_h).

For vaporization to occur, heat flows from the jacket through the area of the vessel wall covered by the contents of the reactor (A). In general, this area is the sum of the area of the bottom head (A_h) and some portion of the area of the cylindrical (straight) side of the vessel (A_s).

EQ-1: $A = A_h + A_s$

Bottom head area

Because the minimum volume in the reactor is limited to the tangent line of the bottom head, the bottom head is always full of liquid and, therefore, A_h is a constant in the derivations that follow.

The area of the bottom head removed to accommodate nozzles is usually small compared to the total area of the head. In addition, the heat conduction property of the material provides temperature uniformity over the entire bottom head area. For these reasons the math in this course assumes that the total area (A_h) is available for contributing to the transfer of heat to the contents.

For the bottom head, A_h can be estimated closely by the general expression:

$$\text{EQ-2: } A_h = a D^2$$

The value for the parameter “a” in EQ-2 is specific to the shape of the bottom head:

- 0.931 for the ASME F&D head.
- 1.084 for the ASME 2:1 ellipsoidal head.

Notice that for any given vessel diameter, the ratio of the “a” values shows that the 2:1 head provides 16.4% more surface area than the F&D head.

Straight side area

If the total volume in the reactor at any time (V_c) exceeds the volume of the bottom head, the difference in volume is contained within the cylindrical portion of the reactor (V_s).

$$\text{EQ-3: } V_s = V_c - V_h.$$

For the straight cylindrical side, the area covered by the contents (A_s) at any time is given by:

$$\text{EQ-4: } A_s = \pi D H_s$$

The term H_s is the height of straight side contacted by the contents. The derivation of the equation used to calculate H_s directly starts by considering volume of liquid (gallons) contained in that height:

$$\text{EQ-5: } V_s = (\pi D^2/4) H_s 7.48 \text{ gal/ft}^3$$

Because the bottom head contains a portion of the reactor contents, the total liquid volume in the reactor at any time is given by rearranging EQ-3 and substituting EQ-5:

$$\text{EQ-6: } V_c = [(\pi D^2/4) H_s 7.48 \text{ gal/ft}^3] + V_h$$

Rearranging EQ-6 gives the expression of the height of straight side contacted by the

contents of the reactor at any time:

$$\text{EQ-7: } H_s = [4 (V_c - V_h)] / [(\pi D^2) 7.48]$$

Because the bottom head is always full of liquid, the volume (V_h) is a constant and can be estimated closely by the general expression:

$$\text{EQ-8: } V_h = b D^3$$

Similar to the expression for the area of the bottom head, the value for the parameter “b” in EQ-8 is also specific to the type of head:

- 0.606 for the ASME flanged and dished head.
- 0.9793 for the ASME 2:1 ellipsoidal head.

Notice that for any given vessel diameter, the ratio of the “b” values shows that the 2:1 head contains 61.6% more volume than the flanged and dished head.

Substituting EQ-8 into EQ-7 and clearing the fraction refines the expression for H_s :

$$\text{EQ-9: } H_s = 0.53476(V_c - [b D^3]) / (\pi D^2)$$

Substituting EQ-9 into EQ-4 gives the expression for calculating A_s directly:

$$\text{EQ-10: } A_s = 0.53476(V_c - [b D^3]) / D$$

Initial heat transfer area

Before vaporization begins, the initial contents of the reactor (V_i) contact an initial heat transfer area (A_i). To derive an expression that can be used to directly calculate the initial heat transfer area, EQ-2 and EQ-10 are substituted into EQ-1 to give the following result:

$$\text{EQ-11: } A_i = a D^2 + \{0.53476 (V_i - [b D^3]) / D\}$$

Because EQ-11 contains constants, the terms in the equation can be grouped with a few steps to shorten the equations that will be developed later.

$$\text{EQ-12: } A_i = a D^2 + (0.53476 (V_i / D) - (0.53476 b D^3 / D))$$

$$\text{EQ-13: } A_i = [a D^2 - (0.53476 b D^2)] + (0.53476 V_i / D)$$

$$\text{EQ-14: } A_i = [D^2 (a - 0.53476 b)] + (0.53476 V_i / D)$$

To shorten the equation even further, constants can be grouped into terms named β and γ :

$$\beta = [D^2 (a - 0.53476 b)]$$

$$\gamma = (0.53476 / D)$$

The final refined expression for A_i is, therefore:

$$\text{EQ-15: } A_i = \beta + \gamma V_i$$

If the initial amount of material in the reactor is expressed by weight (M_i , lbs) it can easily be converted to volume by using the density (R , lbs/gal):

$$\text{EQ-16: } V_i = M_i/R$$

Change in heat transfer area

When a volume of material boils off during vaporization (V), the loss creates a reduction in heat transfer area (A_r). The relationship between the lost area and the lost volume can be expressed mathematically with a few steps.

$$\text{EQ-17: } V = [\pi D^2/4] H_r 7.48 \text{ gal/ft}^3 = 1.87 \pi D^2 H_r$$

The term H_r in EQ-17 is the reduction in the covered height of straight side due to the loss of V . The corresponding loss in heat transfer area is given by:

$$\text{EQ-18: } A_r = \pi D H_r.$$

But rearranging EQ-17 gives:

$$\text{EQ-19: } H_r = (0.53476 V) / \pi D^2.$$

Substituting EQ-19 into EQ-18 gives the expression for the change in surface area that has occurred:

$$\text{EQ-20: } A_r = \pi D [(0.53476 V) / \pi D^2] = 0.53476 V/D = \gamma V$$

At any time during vaporization, the liquid contacts an effective heat transfer area (A_e) that is the initial area minus the reduction in area:

$$\text{EQ-21: } A_e = A_i - A_r$$

Substituting EQ-15 and EQ-20 into EQ-21 gives the expression for A_e in terms of the volume lost:

$$\text{EQ-22: } A_e = \beta + \gamma V_i - \gamma V = \beta + \gamma (V_i - V)$$

Notice that initially $V = 0$ so $A_e = A_i$ and EQ-22 becomes EQ-15.

If the amount of material removed by vaporization is expressed in weight units (M , lbs),

it also can easily converted to volume:

EQ-23: $V = M/R$

Thermal considerations

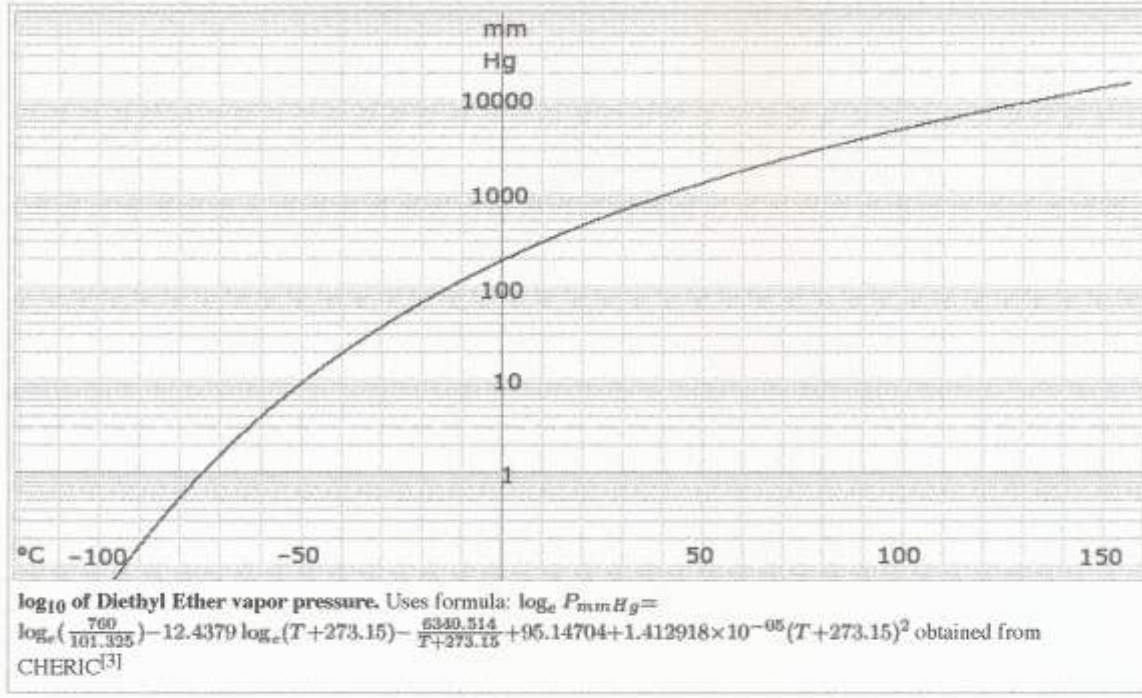
This course assumes that the initial contents of the reactor have been raised to their boiling point before the vaporization operation begins. The derived equations do not predict the time required for that temperature change to occur.

Because the boiling point of a liquid corresponds to the pressure present in the reactor, a vapor pressure chart like the one below for ethyl ether from the Internet could be used to determine the vaporization temperature (T_v) at the proposed operating pressure. The math in this course assumes that the vaporization temperature is constant. If that temperature will change due to, for instance, an increase in the dissolved solids concentration, an average temperature (T_a) should be estimated and used in the equations.

Because the heat of vaporization (λ) can change with temperature as shown in the following chart for a family of ethers (taken from an older classic series of articles by Robert W. Gallant), the value used should be chosen at the selected boiling temperature. The math in this course also assumes that the selected heat of vaporization is constant.

As material is vaporized, the density of the remaining liquid could change. The density value (R) in this course is assumed to be an average value and to remain constant throughout the vaporization process.

Because the inside temperature of a metal (unlined) reactor wall is approximately the same as the outside temperature, the temperature of the heating medium in the jacket may need to be limited if any component of the reactor contents thermally degrades.



[http://en.wikipedia.org/wiki/Diethyl_ether_\(data_page\)](http://en.wikipedia.org/wiki/Diethyl_ether_(data_page))

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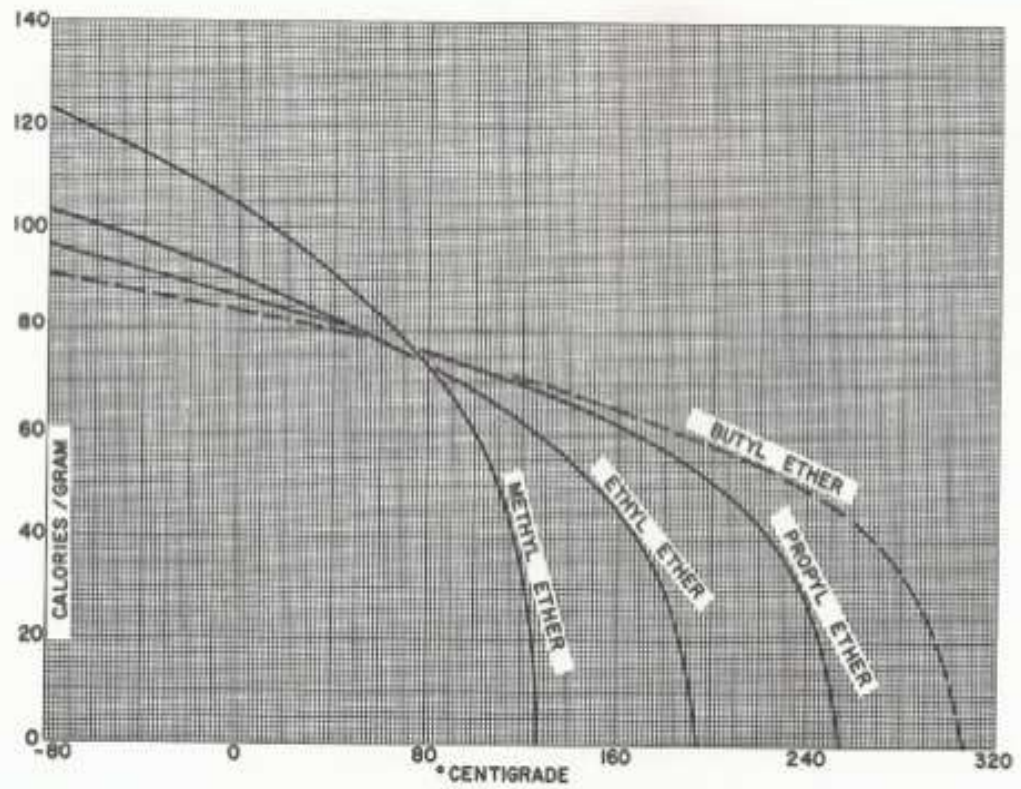


Fig. 28-3—Gives heat of vaporization of ethers from -80°C to $+300^{\circ}\text{C}$.

Figure is from “Physical Properties of Hydrocarbons, Part 28”, *Hydrocarbon Processing*, September 1968.)

The energy for vaporization is supplied by the hot material in the jacket: either by the condensation of steam or by the decrease in temperature of an HTF. This course assumes no loss of heat to the surroundings so every BTU given up by the jacket medium is used to vaporize the contents. The behavioral differences of the heating media are not represented by a common mathematics so each must be treated separately.

Working with steam

When considering steam as the heating medium, this course assumes that the temperature throughout the entire jacket is the steam temperature (T_s). No sub-cooling occurs. The course also assumes that the condensate is removed immediately and completely so that the entire effective heat transfer area is exposed to the steam.

The basic heat balance for the vaporization operation is HEAT OUT = HEAT IN with the units of BTU/hr. The expression that applies to this balance for using steam in the jacket is:

$$\text{EQ-24: } \lambda (dM/d\theta) = U_a A_c (T_s - T_a)$$

The student should recognize the U-term in EQ-24 as the overall heat transfer coefficient with the units of $\text{BTU}/\text{ft}^2\text{-hr-}^\circ\text{F}$. The subscript “a” on that U-term indicates that it too should be an average value due to the possibility that the properties of the contents could change as material is removed by vaporization. Reviewing the data shown in the following table can suggest what average overall heat transfer coefficient is a reasonable selection.

TABLE 10-14 Jacketed Vessels: Overall Coefficients

| Jacket fluid | Fluid in vessel | Wall material | Overall U^* | |
|-------------------|------------------|-----------------|-----------------------------|-------------------------|
| | | | Btu/(h·ft ² ·°F) | J/(m ² ·s·K) |
| Steam | Water | Stainless steel | 150–300 | 850–1700 |
| Steam | Aqueous solution | Stainless steel | 80–200 | 450–1140 |
| Steam | Organics | Stainless steel | 50–150 | 285– 850 |
| Steam | Light oil | Stainless steel | 60–160 | 340– 910 |
| Steam | Heavy oil | Stainless steel | 10– 50 | 57– 285 |
| Brine | Water | Stainless steel | 40–180 | 230–1625 |
| Brine | Aqueous solution | Stainless steel | 35–150 | 200– 850 |
| Brine | Organics | Stainless steel | 30–120 | 170– 680 |
| Brine | Light oil | Stainless steel | 35–130 | 200– 740 |
| Brine | Heavy oil | Stainless steel | 10– 30 | 57– 170 |
| Heat-transfer oil | Water | Stainless steel | 50–200 | 285–1140 |
| Heat-transfer oil | Aqueous solution | Stainless steel | 40–170 | 230– 965 |
| Heat-transfer oil | Organics | Stainless steel | 30–120 | 170– 680 |
| Heat-transfer oil | Light oil | Stainless steel | 35–130 | 200– 740 |
| Heat-transfer oil | Heavy oil | Stainless steel | 10– 40 | 57– 230 |
| Steam | Water | Glass-lined CS | 70–100 | 400– 570 |
| Steam | Aqueous solution | Glass-lined CS | 50– 85 | 285– 480 |
| Steam | Organics | Glass-lined CS | 30– 70 | 170– 400 |
| Steam | Light oil | Glass-lined CS | 40– 75 | 230– 425 |
| Steam | Heavy oil | Glass-lined CS | 10– 40 | 57– 230 |
| Brine | Water | Glass-lined CS | 30– 80 | 170– 450 |
| Brine | Aqueous solution | Glass-lined CS | 25– 70 | 140– 400 |
| Brine | Organics | Glass-lined CS | 20– 60 | 115– 340 |
| Brine | Light oil | Glass-lined CS | 25– 65 | 140– 370 |
| Brine | Heavy oil | Glass-lined CS | 10– 30 | 57– 170 |
| Heat-transfer oil | Water | Glass-lined CS | 30– 80 | 170– 450 |
| Heat-transfer oil | Aqueous solution | Glass-lined CS | 25– 70 | 140– 400 |
| Heat-transfer oil | Organics | Glass-lined CS | 25– 65 | 140– 370 |
| Heat-transfer oil | Light oil | Glass-lined CS | 20– 70 | 115– 400 |
| Heat-transfer oil | Heavy oil | Glass-lined CS | 10– 35 | 57– 200 |

*Values listed are for moderate nonproximity agitation. CS = carbon steel.

(Table is from “Perry’s Chemical Engineers’ Handbook, 6th Edition”, McGraw-Hill, NY, 1984.)


CAUTION: If the reactor is glass-lined, the value of $(T_s - T_a)$ should not exceed the published limit determined by the vendor. A chart like the one following should be available from all vendors of glass-lined reactors for use in determining the limiting temperature difference.

Example 1
Charging of the reactor when the glass lined wall or fluid in jacket is at 302 °F. Materials between 32 °F and 482 °F may be safely changed into vessel.

Maximum allowable thermal shock - 3009 glass

Example 2
Introduction of a heating or cooling fluid into the jacket. If the glass lined wall (and the batch) is at 356 °F, the fluid introduced should be between 86 °F and 518 °F.

| Jacket fluid °F | Wall °F | Batch | | Batch °F | Wall °F | Jacket fluid | |
|-----------------|---------|-------|-------|----------|---------|--------------|------|
| | | min. | max. | | | min. | max. |
| -76 | -76 | | 219,2 | -76 | -76 | | 221 |
| -40 | -40 | | 257 | -40 | -40 | | 257 |
| -4 | -4 | | 293 | -4 | -4 | | 293 |
| 32 | 32 | | 329 | 32 | 32 | | 329 |
| 68 | 68 | | 356 | 68 | 68 | | 356 |
| 104 | 104 | | 383 | 104 | 104 | | 383 |
| 140 | 140 | | 410 | 140 | 140 | | 410 |
| 158 | 158 | | 419 | 158 | 158 | | 419 |
| 176 | 176 | | 428 | 176 | 176 | | 428 |
| 194 | 194 | | 437 | 194 | 194 | | 437 |
| 212 | 212 | -76 | 446 | 212 | 212 | | 446 |
| 230 | 230 | -58 | 455 | 230 | 230 | -76 | 455 |
| 248 | 248 | -40 | 464 | 248 | 248 | -49 | 464 |
| 266 | 266 | -22 | 473 | 266 | 266 | -22 | 473 |
| 284 | 284 | 5 | 482 | 284 | 284 | -4 | 482 |
| 302 | 302 | 32 | 482 | 302 | 302 | 23 | 491 |
| 320 | 320 | 59 | 482 | 320 | 320 | 41 | 500 |
| 338 | 338 | 86 | 482 | 338 | 338 | 68 | 509 |
| 356 | 356 | 113 | 482 | 356 | 356 | 86 | 518 |
| 374 | 374 | 140 | 482 | 374 | 374 | 113 | 527 |
| 392 | 392 | 167 | 482 | 392 | 392 | 131 | 536 |
| 410 | 410 | 194 | 482 | 410 | 410 | 158 | 545 |
| 428 | 428 | 221 | 482 | 428 | 428 | 176 | 554 |
| 446 | 446 | 248 | 482 | 446 | 446 | 203 | 558 |
| 464 | 464 | 275 | 482 | 464 | 464 | 221 | 565 |
| 482 | 482 | 302 | 482 | 482 | 482 | 248 | 572 |



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Substituting EQ-22 into EQ-24, converting from mass to volume units on the left side ($M=VR$) and rearranging give:

$$\text{EQ-25: } dV/d\theta = [U_a / \lambda R] (T_s - T_a) [\beta + \gamma V_i - V]$$

To shorten EQ-25 another group of constants can be defined:

$$g = (U_a / \lambda R) (T_s - T_a)$$

Inserting “g” into EQ-25 and completing another re-arrangement give the differential equation that can be solved for the vaporization time:

$$\text{EQ-26: } \int d\theta = \int dV/g [\beta + \gamma V_i - V]$$

To make the integration easy, EQ-26 can be modified slightly:

$$\text{EQ-27: } \int d\theta = (1/g) \int dV/[(\beta + \gamma V_i) - \gamma V]$$

The integrated solution to the left side of EQ-27 when evaluated with the lower limit of zero gives the vaporization time ($\theta_s - 0 = \theta_s$).

The integrated solution of the right side of EQ-27 is found on a web site such as integrals.wolfram.com (or in a handbook like Tuma, Jan J., Engineering Mathematics Handbook, McGraw-Hill, New York, 1970, page 230):

$$\text{EQ-28: } \int dx / (s + p x) = (1/p) \ln(s + p x).$$

Comparing the variables in EQ-28 with those on the right side of EQ-27 gives the following identities:

$$\begin{aligned} V &= x \\ (\beta + \gamma V_i) &= s \\ -\gamma &= p \end{aligned}$$

The integrated equation before evaluating the right side between the limits of zero and the total volume reduction (V_r) is:

$$\text{EQ-29: } \theta_s = (-1/g\gamma) \ln [(\beta + \gamma V_i) - \gamma V]$$

Evaluating the right side of EQ-29 between the limits of zero and V_r yields the following:

$$\text{EQ-30: } \theta_s = (-1/g\gamma) \ln \{[(\beta + \gamma V_i) - \gamma V_r] - \ln [(\beta + \gamma V_i) - \gamma 0]\}$$

Expressing the subtraction of logs as division (see Tuma, page 4) and clearing the minus sign give the final equation that can be used to estimate the time required to vaporize the volume V_r from a reactor using steam in the jacket:

$$\text{EQ-31: } \theta_s = (1/g\gamma) \ln \{(\beta + \gamma V_i)/[\beta + \gamma(V_i - V_r)]\}$$

Working with HTF

As the hot HTF fluid flows through the jacket of the reactor, it gives up heat that enters the contents through the effective heat transfer area. Because of that loss of heat, the outlet temperature (t_2) of the HTF is less than the inlet temperature (t_1). The jacket-side process is, therefore, non-isothermal.

In terms of the vaporization temperature (T_a) and t_1 , the expression for the jacket outlet temperature (as developed in other sources related to heating and cooling in process vessels) is given by:

$$\text{EQ-32: } t_2 = ([T_a (X - 1)] + t_1)/X$$

CAUTION: If the reactor is glass-lined, the value of ($t_1 - T_a$) should not exceed the published limit determined by the vendor. The chart from the vendor should be used to determine the limiting temperature difference.

The X-term in EQ-32 is a shorthand representation:

$$\text{EQ-33: } X = e^{(U_a A_e / w c)}$$

The U_a and A_e terms in EQ-33 should already be familiar; as the table of overall coefficients shows, however, the value of U_a for HTF may not be the same as that used for steam. The w -term is the flow of HTF (lbs/hr) and the c -term is the heat capacity of the HTF (BTU/lb-°F).

Substituting EQ-22 for A_e in EQ-33 and remembering that subtracted exponents can be expressed as division (see Tuma, page 3) give:

$$\text{EQ-34: } X = e^{U_a/wc [\beta + \gamma V_i - V]} = e^{U_a(\beta + \gamma V_i)/wc - U_a \gamma V/wc} = [e^{U_a(\beta + \gamma V_i)/wc}] / [e^{U_a \gamma V/wc}]$$

EQ-34 can be shortened by defining two additional groups of constants:

$$B = e^{U_a(\beta + \gamma V_i)/wc}$$

$$K = U_a \gamma wc$$

Substituting B and K into EQ-34 gives:

$$\text{EQ-35: } X = B/e^{KV}$$

The basic heat balance with the units of BTU/hr for using a HTF in the jacket is given by:

$$\text{EQ-36: } \lambda (dM/d\theta) = w c (t_1 - t_2).$$

Substituting EQ-32 into EQ-36, converting from mass to volume units on the left side and rearranging give:

$$\text{EQ-37: } dV/d\theta = (wc/\lambda R) (t_1 - \{([T_a (X - 1)] + t_1)/X\})$$

The right side of EQ-37 can be rearranged to form a modified equation:

$$\text{EQ-38: } dV/d\theta = (wc/\lambda R) [(t_1 - T_a) (X - 1)/X]$$

Defining another group of constants will shorten EQ-38:

$$\varepsilon = (wc/\lambda R) (t_1 - T_a)$$

Substituting “ ε ” and EQ-35 into EQ-38 gives:

$$\text{EQ-39: } dV/d\theta = \varepsilon (B/e^{KV} - 1)/(B/e^{KV})$$

By clearing the multiple fractions on the right side of EQ-39, the following equation results:

$$\text{EQ-40: } dV/d\theta = \varepsilon (B - e^{KV})/B$$

The differential equation that can be solved for the vaporization time is then formed by rearranging EQ-40:

$$\text{EQ-41: } \int d\theta = (B/\varepsilon) \int dV/(B - e^{KV})$$

As with steam, the evaluation of the integrated solution for the left side of EQ-41 is the vaporization time (θ_s).

The integrated solution of the right side of EQ-41 is found on a web site such as integrals.wolfram.com (or in the older handbook Perry, J.H., Chemical Engineers' Handbook, 3rd Edition, McGraw-Hill, New York, 1950, page 87):

$$\text{EQ-42: } \int dx / (s + p e^{(n x)}) = (x/s) - [\ln(s + p e^{(n x)})]/sn$$

Comparing the variables in EQ-42 with those on the right side of EQ-41 gives the following identities:

$$V = x$$

$$B = s$$

$$-1 = p$$

$$K = n.$$

The integrated equation before evaluating the right side between the limits of zero and the total volume reduction (V_r) is:

$$\text{EQ-43: } \theta_s = (V/\varepsilon - [\ln(B - e^{KV})]/\varepsilon K)$$

Remembering that $e^0 = 1$ (see Tuma, page 3) and again that subtraction of logs can be expressed as division, completing the evaluation of the right side of EQ-43 yields the following equation that can be used to estimate the time required to vaporize the volume V_r from a reactor using HTF in the jacket:

$$\text{EQ-44: } \theta_s = (V_r/\varepsilon) + (1/\varepsilon K) \ln[(B - 1)/(B - e^{KV_r})].$$

Sample calculations

A 4,000 gallon stainless steel jacketed reactor with 2:1 elliptical heads contains 3,222 gallons of organic solvent with a dissolved organic pharmaceutical product. To enhance crystallization when the contents are subsequently cooled, the batch process requires that 2,222 gallons of solvent be removed by vaporization. The inside diameter of the reactor is 8 feet.

The results of lab testing indicate that the following average process data apply:
vaporization temperature = 194° F, heat of vaporization = 252 BTU/lb and density = 7.91 lb/gal.

For organics in the vessel, the data in the table of overall heat transfer coefficients indicate that average values of 100 for steam in the jacket and of 75 for HTF are reasonable choices.

The product will degrade if it contacts the reactor wall at a temperature greater than 350° F. Steam is available at 75 PSIG (320°F), but the supply temperature of an available HTF can be adjusted to a value equal to or greater than the steam temperature.

The value for the HTF flow (w) is calculated using correlations available in the literature (for conventional jackets, see Steve, Edward, "Simplified Equations for Jacketed-Reactor Design", *Chemical Engineering*, July 1999); the HTF heat capacity (c) is obtained from manufacturers' literature. The values for this sample problem are 26,192 lb/hr flow and 0.9 BTU/lb-°F heat capacity.

The process engineer must estimate the vaporization times for using either steam or the HTF in the jacket. The comparative results will influence the choice of jacket heating medium.

The format of a simple spreadsheet like the following automates the calculations and displays the results for both jacket media.

**SAMPLE CALCULATION FOR ESTIMATING
VAPORIZATION TIME**

1. USING STEAM AS THE HEATING MEDIUM:

| PROCESS DATA | | CALCULATIONS: | |
|--------------|--------|-----------------------------|--------|
| ITEM | VALUE | β | 35.860 |
| a | 1.084 | γ | 0.0668 |
| b | 0.9793 | $T_s - T_a$ | 126 |
| D | 8 | g | 6.32 |
| T_a | 194 | $1/\gamma y$ | 2.37 |
| T_s | 320 | $\beta + \gamma V_i$ | 251.23 |
| U_a | 100 | $\beta + \gamma(V_i - V_r)$ | 102.70 |
| λ | 252 | θ_s | 2.12 |
| R | 7.91 | | |
| V_i | 3222 | | |
| V_r | 2222 | | |

2. USING HTF AS THE HEATING MEDIUM:

| ADDITIONAL PROCESS DATA | | CALCULATIONS: | |
|----------------------------|-------|---------------|----------|
| ITEM | VALUE | B | 2.22 |
| c | 0.9 | K | 0.000213 |
| w | 26192 | $t_1 - T_a$ | 126 |
| t_1 | 320 | ϵ | 1490.06 |
| U_a | 75 | θ_s | 3.64 |

Because the HTF supply temperature can be adjusted, the following spreadsheet repeats the HTF calculations with $t_1 = 350^\circ \text{F}$, the maximum allowable wall temperature. The result indicates that the increased jacket inlet temperature significantly decreases the vaporization time.

Other spreadsheet layouts could consolidate the comparative data and results for several operating alternatives on one page for review and comment.

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| SAMPLE CALCULATION FOR ESTIMATING VAPORIZATION TIME |
|--|

1. USING STEAM AS THE HEATING MEDIUM:

| PROCESS DATA | | CALCULATIONS: | |
|--------------|--------|-----------------------------|--------|
| ITEM | VALUE | | |
| | | β | 35.860 |
| a | 1.084 | γ | 0.0668 |
| b | 0.9793 | $T_s - T_a$ | 126 |
| D | 8 | g | 6.32 |
| T_a | 194 | $1/g\gamma$ | 2.37 |
| T_s | 320 | $\beta + \gamma V_i$ | 251.23 |
| U_a | 100 | $\beta + \gamma(V_i - V_r)$ | 102.70 |
| λ | 252 | θ_s | 2.12 |
| R | 7.91 | | |
| V_i | 3222 | | |
| V_r | 2222 | | |

2. USING HTF AS THE HEATING MEDIUM:

| ADDITIONAL PROCESS DATA | | CALCULATIONS: | |
|----------------------------|-------|---------------|----------|
| ITEM | VALUE | | |
| | | B | 2.22 |
| c | 0.9 | K | 0.000213 |
| w | 26192 | $t_1 - T_a$ | 156 |
| t_1 | 350 | ϵ | 1844.84 |
| U_a | 75 | θ_s | 2.94 |

NOMENCLATURE

- a = bottom head surface area parameter, $\text{ft}^2/\text{diam}^2$
A = vessel wall area covered by contents, ft^2
 A_e = effective heat transfer area, ft^2
 A_f = final heat transfer area, ft^2
 A_h = area of bottom head of the reactor, ft^2
 A_i = initial heat transfer area, ft^2
 A_r = reduction in heat transfer area due to vaporization, ft^2
 A_s = area of straight side of the reactor covered by contents, ft^2
b = bottom head volume parameter, gal/diam^3
B = group of constants, $e^{U_a(\beta + \gamma V_i)/wc}$
c = heat capacity of HTF, $\text{BTU}/\text{lb.}\cdot^\circ\text{F}$
D = inside diameter of reactor, ft.
g = group of constants, $(U_a/\lambda R)(T_s - T_a)$
 H_r = reduction in straight side height covered by content due to vaporization, ft.
 H_s = straight side height covered by contents, ft.
K = group of constants, $U_a\gamma wc$
M = weight of liquid material removed from reactor during vaporization, lb.
 M_i = initial weight of liquid material in the reactor, lb.
R = density of liquid material in the reactor, lb/gal
 t_1 = jacket inlet temperature of HTF, $^\circ\text{F}$
 t_2 = jacket outlet temperature of HTF, $^\circ\text{F}$
 T_a = average vaporization temperature, $^\circ\text{F}$
 T_s = steam temperature, $^\circ\text{F}$
 T_v = vaporization temperature, $^\circ\text{F}$
U = overall heat transfer coefficient, $\text{BTU}/\text{ft}^2\cdot\text{hr}\cdot^\circ\text{F}$
 U_a = average overall heat transfer coefficient, $\text{BTU}/\text{ft}^2\cdot\text{hr}\cdot^\circ\text{F}$
V = volume removed from the reactor by vaporization, gal.
 V_c = total volume of contents in the reactor, gal.
 V_f = final volume of contents in the reactor, gal.
 V_h = volume of bottom head, gal.
 V_i = initial volume of contents in the reactor, gal.
 V_r = total volume removed from the reactor by vaporization, gal.
 V_s = volume contained in straight side of reactor, gal.
w = jacket HTF flow, lb/hr
 $X = e^{(U_a A_e)/(w c)}$
 β = group of constants, $D^2(a - 0.53476 b)$
 γ = group of constants, $(0.53476 / D)$
 ϵ = group of constants, $(wc/\lambda R)(t_1 - T_a)$
 θ = any time during the vaporization, hrs
 θ_s = total vaporization time, hrs
 λ = heat of vaporization, BTU/lb

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