(e) The thermal mass of the vessel can be included with the thermal mass of its contents. (This implies also that all resistance to heat transfer in the jacket/coils is on the service side.)

5.2 Basic Equations

The basic equations which describe the thermal performance of the system are the same for all cases considered. They involve the use of certain intermediate functions denoted by the letters *B, E* and *D* which are functions of the different systems, but, provided that the assumptions listed above hold, these functions are constant for any given system. Details of the derivations of these equations are given in Appendix A, where appropriate sub-scripts are used for the different systems.

The batch time is related to the initial and final temperatures of the batch by the equation:

$$S = B.W.\ln\left(\frac{\theta_0 - t_1}{\theta_S - t_1}\right) \qquad (5.1)$$

where

S	is the batch time	(s)
W	is the thermal mass of the batch and vessel	($J.K^{-1}$)
t_1	is the inlet temperature of the service fluid	(K)
θ_0	is the initial temperature of the batch	(K)
θ_S	is the final temperature of the batch	(K)
B	is a function of the system (see Table 1)	($K.s.J^{-1}$)

The thermal mass of the batch and vessel is given by:

$$W = M_B.C_B + M_V.C_V$$

where

M_B	is the mass of the batch	(kg)
M_V	is the mass of the vessel	(kg)
C_B	is the specific heat of the batch	($J.kg^{-1}.K^{-1}$)
C_V	is the specific heat of the vessel	($J.kg^{-1}.K^{-1}$)

The variation of batch temperature with time is given by:

$$\theta = t_1 + (\theta_0 - t_1).\exp\left(-\frac{s}{B.W}\right) \qquad (5.2)$$

where q is the batch temperature (K) at time *s* seconds.

The variation of heat load with time is given by:

$$q = \frac{\theta - t_1}{B} \qquad (5.3)$$

where q is the heat load (W) at time s.

Note:
For these equations, the heat load is positive if the vessel contents are being cooled, and negative if they are being heated.

For cases where there is an intermediate fluid between the batch and the service fluid, the temperature of this intermediate fluid entering the service (external) exchanger is given by:

$$T_1 = t_1 + D.q \qquad (5.4)$$

where:

T_1	is the temperature of the intermediate fluid	(K)
D	is a function of the system (see Table 1)	$(K.s.J^{-1})$

Other temperatures in the system may be derived by a heat balance as follows:

For a single phase service fluid, the outlet temperature is given by:

$$t_2 = t_1 + \frac{q}{m.c} \qquad (5.5)$$

where

m	is the mass flowrate of the service fluid	$(kg.s^{-1})$
c	is the specific heat of the service fluid	$(J.kg^{-1}.K^{-1})$

For the batch fluid circulated through an external exchanger, the outlet temperature from the external exchanger is given by:

$$\theta_2 = \theta - \frac{q}{M.C} \qquad (5.6)$$

where

M	is the mass flowrate of the batch fluid	($kg.s^{-1}$)
C	is the specific heat of the batch fluid.	($J.kg^{-1}.K^{-1}$)

For an intermediate fluid circulated through an external exchanger, the outlet temperature from the external exchanger is given by:

$$T_2 = T_1 - \frac{q}{M.C} \qquad (5.7)$$

where

M	is the mass flowrate of the intermediate fluid	($kg.s^{-1}$)
C	is the specific heat of the intermediate fluid.	($J.kg^{-1}.K^{-1}$)

The functions *B* and *D* are functions of the flow rates and specific heats of the various fluids and the heat transfer coefficients. They are defined for the various cases in Table 1. In order to simplify the equations, in many cases further intermediate functions *E* are also defined. Provided that the assumptions listed in 5.1 apply, these functions are constant for a given system.

The various terms in Table 1 are as follows:

a	the heat transfer surface of the vessel jacket and/or coil	(m^2)
A	the heat transfer surface of the external heat exchanger	(m^2)
c	the specific heat of the service fluid	($J.kg^{-1}.K^{-1}$)
C	(i) the specific heat of the batch fluid (external exchanger)	($J.kg^{-1}.K^{-1}$)
	(ii) the specific heat of the intermediate fluid (indirect system)	
m	the mass flowrate of the service fluid	($kg.s^{-1}$)
M	(i) the mass flowrate of the circulating batch fluid or,	($kg.s^{-1}$)
	(ii) the mass flowrate of the intermediate fluid	
r	the ratio $m.c/M.C$	
u	the overall heat transfer coefficient for the vessel jacket/coil	($W.m^{-2}.K^{-1}$)
U	the overall heat transfer coefficient for the external exchanger	($W.m^{-2}.K^{-1}$)

TABLE 1 DEFINITIONS OF FUNCTIONS

Case	Description	B	D	E
1	Service fluid in jacket or coil. Isothermal service fluid.	$B_1 = \frac{1}{u.a}$		
2	Service fluid in jacket or coil. Single phase service fluid.	$B_2 = \frac{E_2}{m.c.(E_2 - 1)}$		$E_2 = \exp\left(\frac{u.a}{m.c}\right)$
3	External heat exchanger. Isothermal service fluid.	$B_3 = \frac{E_3}{M.C.(E_3 - 1)}$		$E_3 = \exp\left(\frac{U.A}{M.C}\right)$
4	External heat exchanger. Single phase service fluid.	$B_4 = \frac{r.E_4 - 1}{m.c.(E_4 - 1)}$		$E_4 = exp\left(\frac{U.A.(r-1)}{m.c}\right)$
5	External heat exchanger. Single phase service fluid. Special case for equal flowing heat capacities (r = 1).	$B_5 = \frac{M.C + U.A}{M.C.U.A}$		
6	Indirect system. Isothermal service fluid.	$B_6 = \frac{B_3.M.C.(1-E_6) - 1}{M.C.(1-E_6)}$	$D_6 = B_3$	$E_6 = exp\left(\frac{u.a}{M.C}\right)$
7	Indirect system. Single phase service fluid.	$B_7 = \frac{B_4.M.C.(1-E_6) - 1}{M.C.(1-E_6)}$	$D_7 = B_4$	
8	Indirect system. Single phase service fluid. Special case for equal flowing heat capacities (r = 1)	$B_8 = \frac{B_5.M.C.(1-E_6) - 1}{M.C.(1-E_6)}$	$D_8 = B_5$	

6 APPLICATION OF THE METHOD

6.1 Determining the Behavior of an Existing System

If the system is completely defined in terms of the mechanical details of the equipment and the flow rates and properties of the fluids, determination of the batch time is straight forward:

(a) Determine the performance of the heat transfer equipment at the start and end of the temperature cycle. For an external heat exchanger, either used directly on the process fluid or as part of an intermediate system, this can usually be done using a suitable computer program, following the recommendations of **GBHE-PEG-HEA-502.** For heat transfer between the vessel contents and a jacket or coil, the best recommendations available at present are given in the HTFS Design Report. The situation is rather

more complicated if there is an intermediate fluid between the vessel and the service fluid, as in Cases 6 to 8, as the temperature of this fluid entering the external exchanger is needed. It is necessary to adjust this temperature until the heat duty between the vessel and the intermediate fluid matches that between the intermediate fluid and the service fluid.

(b) If the values of the heat transfer coefficients for the jacket/coil and the external heat exchanger are reasonably constant over the cycle, calculate the value of *B* for the appropriate case from Table 1. If the values are not constant, go to (d).

(c) Calculate the heating or cooling time from Equation 5.1 and the variation of heat load and temperatures with time, if required, from Equations 5.2 to 5.7.

(d) If the overall coefficients calculated in (a) are shown to vary significantly between the start and end of the batch, a rough estimate of the batch time may be obtained by calculating the value of *B* for the mean conditions.

A more accurate estimate of the time can be obtained by performing a series of heat transfer calculations for a range of batch temperatures through the batch cycle. If the batch temperature is then plotted against the reciprocal of the heat duty, the area under this graph will be the cycle time.

6.2 Specifying the Heat Transfer Duty for a New System

Often, when designing a batch system, the desired time to heat or cool the vessel contents is fixed, and it is required to specify the heat exchanger that will enable this time to be achieved.

The suggested procedure for specifying the exchanger is as follows:

(a) Determine the thermal mass of the vessel and contents, *W,* the required cycle time, *S*, and the initial and final temperatures, θ_0 and θ_S. Then, using Equation 5.1 determine the required value of the function *B*.

(b) Determine the mean temperature of the batch fluid, θ_m. As the batch fluid temperature falls towards the service inlet temperature with an exponential decay, as shown by Equation 5.2, the best value to use for this is that corresponding to the LMTD between the start and end of the cycle:

$$\theta_m = t_1 + \frac{\theta_0 - \theta_S}{\ln\left(\frac{\theta_0 - t_1}{\theta_S - t_1}\right)} \qquad (6.1)$$

(c) Calculate the heat duty at this temperature from Equation 5.3, using the value of *B* calculated in (a).

(d) Calculate the other temperatures in the system from Equations 5.4 to 5.7 as appropriate.

(e) These temperatures, together with the physical properties of the fluids, define the required heat transfer duties, and enable the exchangers to be designed using appropriate methods. See **GBHE-PEG-HEA-502** for recommendations on suitable computer programs for the design of heat exchangers, or HTFS Design Report for methods for the estimation of heat transfer to agitated vessels.

(f) Rate the designs at conditions corresponding to the start and finish of the cycle and compare these calculations with the estimates obtained assuming a constant value of *B* in the equations in 5.2*.* If reasonable agreement is obtained, the process is complete.

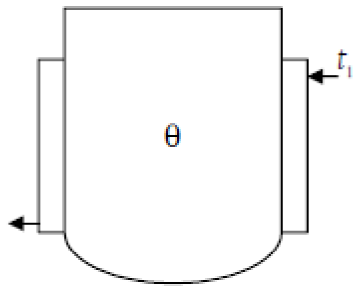
(g) If, due to changes in physical properties during the cycle, the agreement is poor, it will be necessary to carry out detailed rating calculations at a series of temperatures and estimate the cycle time as described in 6.1.

(h) If the estimated cycle time differs from the desired value, estimate a new value of the heat duty at mean conditions by scaling the original value in the ratio of estimated cycle time/desired cycle time, and repeat from (d).

APPENDIX A DERIVATION OF THE EQUATIONS

Note:
The equation numbering system in this section is such that similar equation numbers are used for the same process in each case. This means that in some cases, the numbering is not contiguous.

A1 CASE 1 - ISOTHERMAL FLUID IN JACKET OR COIL



For heat transfer in the jacket or coil, the heat duty is given by:

$$q = u.a.(\theta - t_1) \tag{A1.1}$$

Note that If the vessel has both a jacket and coil, in general both the areas and the coefficients of these will differ. However, as these items always occur as their product a compound value may be used which is given by:

$$u.a = u_j.a_j + u_c.a_c$$

where the subscripts *j* and *c* refer to jacket and coil respectively.

The rate of change of temperature of the batch is given by:

$$\frac{d\theta}{ds} = -\frac{q}{W} = -\frac{u.a.(\theta - t_1)}{W} = -\frac{(\theta - t_1)}{B_1.W}$$

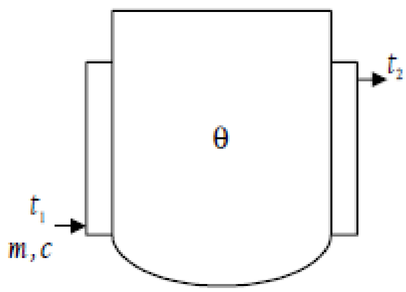
where:

$$B_1 = \frac{1}{u.a}$$

Re-arranging and integrating, with the boundary conditions that the batch temperature is θ_0 at time zero and θ_S at time *S,* gives the batch time:

$$S = B_1 . W . \ln\left(\frac{\theta_0 - t_1}{\theta_S - t_1}\right)$$

A2 CASE 2 - SINGLE PHASE FLUID IN JACKET OR COIL



For heat transfer in the jacket or coil, the heat duty is given by:

$$q = u.a.\frac{(t_2 - t_1)}{\ln\left[\frac{(\theta - t_1)}{(\theta - t_2)}\right]} \qquad \text{(A2.1)}$$

The heat duty is also related to the change in temperature of the service fluid:

$$\text{q} = m.c.(\text{t}_2 - \text{t}_1) \qquad \text{(A2.2)}$$

Hence:

$$\frac{(\theta - t_1)}{(\theta - t_2)} = \exp\left[\frac{u.a}{m.c}\right] = E_2 \quad \text{(say)}$$

Re-arranging:

$$t_2 - t_1 = \left[\frac{E_2 - 1}{E_2}\right].(\theta - t_1)$$

Hence, substituting in Equation A2.2 gives:

$$q = m.c.\left[\frac{E_2 - 1}{E_2}\right].(\theta - t_1) = \frac{(\theta - t_1)}{B_2}$$

where:

$$B_2 = \frac{E_2}{\left[m.c.(E_2 - 1)\right]}$$

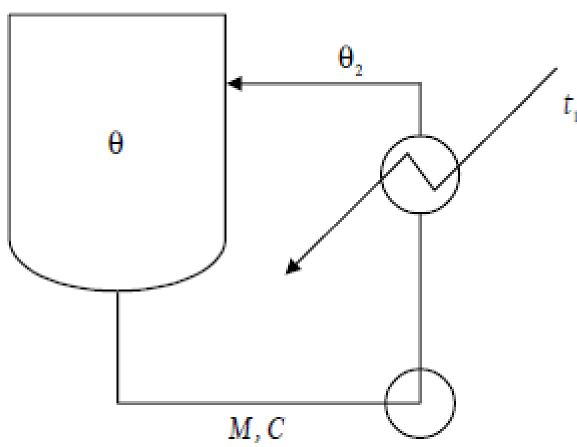
The rate of change of temperature of the vessel contents is given by:

$$\frac{d\theta}{ds} = -\frac{q}{W} = -\frac{(\theta - t_1)}{B_2.W}$$

Rearranging and integrating with the boundary conditions that the batch temperature is θ_0 at time zero and θ_S at time *S,* gives the batch time:

$$S = B_2.W.\ln\left(\frac{\theta_0 - t_1}{\theta_S - t_2}\right)$$

A3 CASE 3 - EXTERNAL HEAT EXCHANGER WITH ISOTHERMAL SERVICE FLUID



The heat lost by the process fluid in the exchanger is:

$$q = M.C.(\theta - \theta_2) \qquad \text{(A3.3)}$$