

1 Introduction to process design

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Introduction

At the core of chemical engineering is design, frequently of continuous processes. A food process plant will consist of a series of process units, each of which carries out some specific job, such as mixing, fermentation, sterilization, or separation. Each of these units is designed using physical and chemical principles; later chapters of this book will consider the principles which underpin these designs. However, to produce an efficient process it is necessary to consider the whole process, to understand the way in which material moves around the plant and to calculate the heating and cooling duties needed.

Chemical engineers begin design by constructing a **flowsheet** for a plant, on which a **Material Balance** can be carried out to define all the flows in and out of the system and individual units. This balance enables a preliminary idea of the best flowsheet to be obtained; for example, if only 5% of the inputs in a process unit are actually used, then it will probably be necessary to add a recycle stream to return unreacted material to the unit. In addition to the mass balance, an estimate of the heating and cooling loads on the plant, the **Thermal Balance**, can be developed. Material and thermal balances can be carried out before going into detail about the sizes of individual units; the preliminary flowsheet incorporates all the key elements of the process without specifying the details of the design, such as the size of any pumps, pipes and heat exchangers needed.

This chapter introduces techniques for the analysis of flowsheets and processes which will be used throughout this book. It also introduces the key problem of food process engineering, of ensuring that the process is economically viable. The profitability of a given process is, in practice, very difficult to estimate. However, the use of ideas such as the net present value of a project can be used both to estimate the success of the project and to compare it to possible other investments. A series of examples are provided to illustrate the concepts developed in this chapter; these will be taken up and developed in depth in the rest of the book.

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The aim of design is to arrive at a precise specification of all the material and energy requirements, and the equipment, pipework, instrumentation and control schemes necessary for a process to be constructed and operated efficiently, safely and economically. This involves consideration of the whole process and of the individual units that comprise it. The first stage in process design is to generate possible schemes that might meet the requirements of the process in question. This involves considering alternative **operations** (such as direct or indirect sterilization, filtration or centrifugation, co- or counter-current spray drying) and **sequences** of these operations. It results in a qualitative process description, which is usually presented as a schematic diagram, or flowsheet, of the whole process. For example, Fig. 1.1 shows a simplified outline of a hypothetical process for semi-batch extraction from a solid using supercritical carbon dioxide. In this case, the engineer would certainly consider other alternatives with a view to improving energy efficiency and process economics.

In many ways flowsheet development is the most creative part of the design process and the most difficult to pin down in terms of standard or rote procedures. Here, we won't focus on this preliminary phase of overall process design, although we shall consider some alternatives, and how to evaluate them, on the basis of selected examples. First, however, consider how alternative flowsheets could be evaluated. The first point, clearly, is to determine whether the process is technically feasible. It may not be feasible for a variety of reasons: for example, one of the process operations might be fraught with difficulties, or require unrealistically large material or energy inputs. Invariably there will be several technically feasible options, but some will certainly be more efficient – in technical terms – than others, and in order to discriminate between them it is necessary, in the next stages of evaluation, to estimate the flows of materials and energy. A further stage in the appraisal process would be to consider the relative economic merits of the various alternatives. All these stages of process design and evaluation are quantitative, even if they do not involve very accurate calculations early on in the design process. Some of the methods that underpin these stages

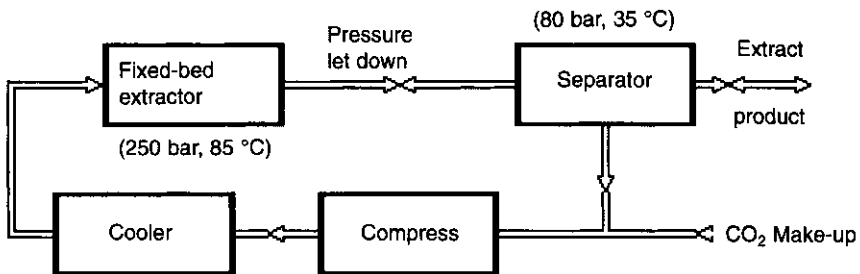


Fig. 1.1 Simplified flowsheet of semi-batch extraction with supercritical carbon dioxide.

will be developed in this chapter, which is divided into three sections dealing with the quantification of the flows of material, energy and cash respectively.

Chapter 11 outlines a more extended design of an integrated cheese-making plant. This is presented as a problem to be worked through; the solution will be found to draw heavily on material from this chapter. Readers are strongly urged to attempt to solve this problem. A simplified spreadsheet solution of this problem is also given in the computer disk attached to this text.

1.1 Material requirements and flows

1.1.1 Mass balances

We first consider the ideas and techniques of ‘mass balancing’, which are used at the design stage to estimate material flows throughout a process. The same principles have another important application in their use to check, from operating data, that processes are operating as desired. Figure 1.2 shows a simplified flowsheet of a milk spray drying plant. In order to specify the process equipment units it is necessary, *inter alia*, to estimate the flows of dried product and gaseous exhaust per tonne or m³ of milk fed to the process. We can confidently assert that, in spite of any chemical or biochemical changes, matter is neither formed nor destroyed during the process so that, provided all the flows in and out of the process – or in and out of an individual process unit – are accounted for, we can, in principle, set up a material balance.

Consider a time interval t of process operation. Then the total mass of material accumulated within the process will be the net difference between all the flows into and out of the process during the time interval:

$$\text{Accumulation} = \Sigma(\text{Inlet flows}) - \Sigma(\text{Outlet flows})$$

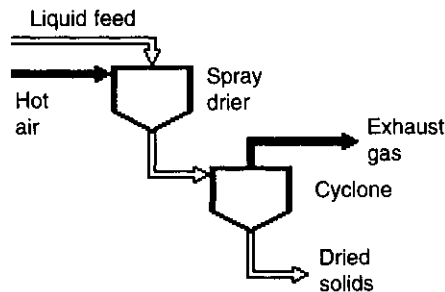


Fig. 1.2 Schematic of spray drier.

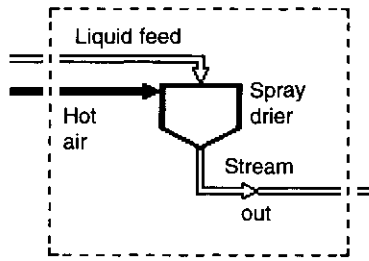


Fig. 1.3 Spray drier unit and system boundary.

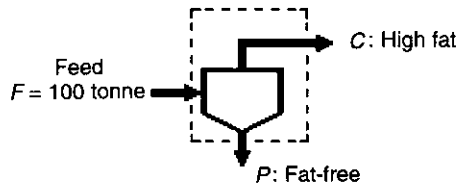


Fig. 1.4 Example 1.1: fat separator.

where Σ indicates summation. For example, a balance over the spray drier unit (Fig. 1.3) would start from

$$\text{Accumulation in drier} = \text{Milk in} + \text{Hot air in} - \text{Hot stream out}$$

Similarly, a balance over the cyclone would start from:

$$\text{Accumulation in drier} = \text{Hot stream in} - \text{Dry milk out} - \text{Gas stream out}$$

Often the accumulation term will be zero. There should be no build-up of product inside a continuously operating spray drier, for example. Thus, if we consider a *steady* continuous process:

$$w_1 = w_2 \quad (1.1)$$

where w_1 and w_2 are the total material flows in and out respectively. This equation also holds for a batch process, where w_1 and w_2 are identified with the totals of the starting and final materials. It also holds for a steady process if w_1 and w_2 are average flowrates (e.g. in kg s^{-1}) rather than total flows (i.e. in kg). Note that in general this equation is only true for **mass** flows. With liquids and where density changes are small it may hold in volumetric units (e.g. in m^3); where gas flows are involved, changes in the conditions between the inlet and outlet mean that volumetric flows are rarely appropriate. For example, there is no reason in general why the volumetric flows of milk and air into the spray drier should equal the volumetric flows of dried product and exhaust air. Nor, where there

are chemical changes, will overall balances written in molar units satisfy equation (1.1).

If there are no chemical/biochemical changes, equation (1.1) will also apply to **individual components** or **compounds** in the process streams. For example, the flow of milk solids into the drier must balance the flow of solids in the dried product and any losses in the gas exhaust.

As it is often necessary to convert between different measures, a few basic definitions are summarized in Appendix 1.A.

1.1.2 Choosing a basis

In order to carry out a material balance calculation it is necessary to define a basis, such as an operating time period or a reference quantity. Suppose you are designing a plant that produces 10000 140 g pots of yoghurt per day; it isn't hard to see that for calculation purposes this might not be the most convenient starting point. It would probably be easier to take a defined quantity of milk (that is, a starting material) and then to scale the results to the real operating conditions at the end of the calculation.

The following three rules will be found useful:

- Choose the basis that is most convenient for calculation.
- Specify the basis explicitly.
- Don't change the basis during the calculation.

The following example illustrates some of the basic principles mentioned above.

EXAMPLE 1.1

Consider a separator in which a liquid containing 5 wt% fat is concentrated to 35 wt%; the other product stream, P, is to be fat-free. The separator produces 195 t day⁻¹ of the high-fat product, C. What are the flows of the streams involved?

Basis: 100 tonne of feed. This is chosen for convenience of calculation; we shall subsequently convert the result to correspond to the specified product flow. The process is represented in Fig. 1.4.

Thus an overall balance gives

$$F = 100 = P + C \quad (1.2)$$

A balance on fat gives

$$0.05F = 5 = 0.35C \quad (1.3)$$

and solving equations (1.2) and (1.3) gives

$$C = 14.29\text{t}$$

and

$$P = 85.71 \text{ t}$$

In other words, for every 100t of feed, there are 14.29 and 85.71 t of high-fat and fat-free product respectively.

However, the 100t feed assumed for the calculation doesn't correspond to the daily production of 195t of product C. To convert the answer to a daily basis we must multiply all the streams by 195/14.29 (= 13.646), to give the daily flows through the plant:

	In (tonnes)	Out (tonnes)
<i>F</i>	1364.6	–
<i>C</i>	–	195.0
<i>P</i>	–	1169.6
Total	1364.6	1364.6

Note that, considering the feed to comprise fat and fat-free liquid, we could write another equation by setting up a balance on the fat-free liquid (on the original basis):

$$0.95F = 95 = 0.65C + P \quad (1.4)$$

However, adding equations (1.3) and (1.4) gives equation (1.2), so that the additional equation is redundant. The reason is that as *F* is specified, there are only two unknowns (*P* and *C*) and thus there can be only two independent equations in the set (1.2)–(1.4). Once two of these are solved, the third is automatically satisfied. In some cases the choice of which independent equations to use makes a considerable difference to the ease of calculation.

EXAMPLE 1.2: MULTICOMPONENT SEPARATION

Suppose that in Example 1.1 the aqueous phase contained some dissolved components, such as lactose and salts. How would these components be distributed following separation? Let us suppose that they are not bound to the fat in any way; in this case they should be distributed in the same proportions in the water phase of the two outlet streams as in the inlet. In particular, suppose that in addition to the fat, the inlet stream contains 5% lactose and 2% salt.

If, as suggested, there is no preferential fractionation of the lactose and salt between the fat-rich and fat-free streams, we can take advantage

of the fact that the lactose, salt and water must therefore be in the same proportions (5:2:88) throughout, by eliminating fat from the calculation. The table below shows the composition of the feed on two different bases:

	Mass (kg)	Mass fraction	Mass fraction (fat-free basis)
Fat	5	0.05	—
Lactose	5	0.05	0.0526
Salt	2	0.02	0.0211
Water	88	0.88	0.9263

On a fat-free basis the total flows of feed, streams *C* and *P* are thus 95, 9.29 (= 14.29 – 5), and 85.71 tonnes respectively. The fractions of lactose, salt and water in each of these are given in the table above. Therefore, for example, the quantity of lactose in stream *C* must be $0.0526 \times 9.29 = 0.489$ t.

On a fat-free basis, the compositions of streams *F*, *C* and *P* are (in kg):

Stream	<i>F</i>	<i>C</i>	<i>P</i>
Lactose	5	0.489	4.511
Salt	2	0.196	1.804
Water	88	8.605	79.395
Total	95	9.290	85.710

Note that this summary table allows one to check that all the component and total balance requirements are satisfied.

A further example will help to illustrate some other closely related concepts, and in particular it will show the way in which many problems can conveniently be solved algebraically.

EXAMPLE 1.3: ALGEBRAIC FORMS, WET AND DRY BASIS, TIE SUBSTANCES

Consider a fruit from which the juice is extracted by pressing. The fruit enters with a juice content of 70 wt% and soluble sugars comprise 15% of the juice. At the end of the pressing process the pressed solid (pomace) contains 10% juice and the clear extract juice contains 15.5% sugars. All

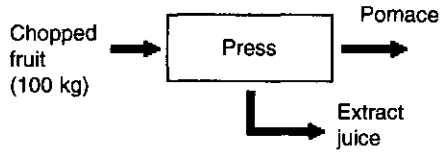


Fig. 1.5 Example 1.3: juice extraction.

percentages are on a weight basis. We wish to complete the mass balance around the extractor.

Basis: 100 kg fruit

There are several unknowns, and it is convenient to denote each by an algebraic symbol. Then a table of inputs and outputs is:

	In (kg)	Out (kg) Pomace	Out (kg) Juice
Insoluble dry matter	30	T	0
Juice			
Soluble sugars	10.5	a	x
Water	59.5	b	y
Total	100	$T + a + b$	$x + y$

We now proceed to calculate T , a , b , etc., using the information on compositions and the same principles as before. In particular, for each component, the input (that is, the entry in the second column) must equal the sum of the outputs (the entries in columns 3 and 4). Note that as there are five unknown variables, five independent equations or relationships will be needed for a unique solution.

1. As the insoluble dry matter can only appear in the pomace, $T = 30$. A component such as this, which is carried unchanged across a process, often provides a useful check or vehicle for establishing a mass balance. It is called a **tie substance**.
2. As the pomace contains 10% juice (i.e. soluble sugars and water):

$$\frac{a + b}{30 + a + b} = 0.1 \quad (1.5)$$

i.e.

$$a + b = 3.333 \quad (1.6)$$

3. Balances on sugar and water:

$$10.5 = a + x \quad (1.7)$$

$$59.5 = b + y \quad (1.8)$$

and

$$70 = a + b + x + y \quad (1.9)$$

The three independent equations (1.6), (1.7) and (1.8) are insufficient to solve uniquely for a , b , x and y . Equation (1.9) is not independent, as it is the sum of (1.7) and (1.8), and therefore does not provide any further information.

A further equation may be written, as the extract juice is known to contain 15.5% sugars, or

$$0.155 = \frac{x}{x + y} \quad (1.10)$$

so that

$$x = 0.1834y \quad (1.11)$$

From equations (1.9) and (1.6):

$$x + y = 66.667$$

so that

$$x = 10.33$$

and

$$y = 56.337$$

From (1.7) and (1.8):

$$a = 0.27$$

$$b = 3.063$$

It will be seen that these values satisfactorily complete the input/output table:

	In (kg)	Out (kg) Pomace	Out (kg) Juice
Insoluble dry matter	30	30	0
Juice			
Soluble sugars	10.5	0.27	10.33
Water	59.5	3.063	56.337
Total	100	33.333	66.667

In Example 1.2 we showed how the compositions might be defined on a fat-free basis. In a similar way we can distinguish here between a **wet**

and a **dry** basis. For example, in the problem statement the pomace juice was defined as a percentage of the total pomace: that is, on a **wet basis**. On this basis the juice is 10%, which is of course consistent with the final table, column 2: $3.333/33.333$. On a dry, juice-free, basis its fraction is $3.333/30 = 0.111$.

In the general case where a stream contains a , b , c and w kg of components A, B, C and water respectively the mass fractions on an overall (wet) and dry basis are summarized in the table below. It is often convenient to be able to convert between different bases in this way.

	Mass (kg)	Mass fraction	Mass fraction (dry basis)
A	a	$a/(a + b + c + w)$	$a/(a + b + c)$
B	b	$b/(a + b + c + w)$	$b/(a + b + c)$
C	c	$c/(a + b + c + w)$	$c/(a + b + c)$
Water	w	$w/(a + b + c + w)$	–

In example above, the percentage of juice in the pomace on a wet basis is 10%:

$$\frac{a + b}{30 + a + b} = 0.1$$

From this we can readily calculate its composition on a dry basis:

$$\frac{a + b}{30} = 0.1/0.9 = 0.111$$

Many problems are more complex than the ones considered so far. Sometimes there are many components to account for, as in processes to recover complex flavour components. Sometimes the topology of the process is more complex. Figure 1.1 includes an additional complication over the first three examples because solvent (the carbon dioxide) is recycled; recycle streams and complex linkages between process units are very common in the process industry. Often the individual components of the feed are not conserved in the same form over the process. In cheese-making, for example, a series of microbial or enzymatic processes lead to the transformation of milk into cheese, butter, ethanol etc. In this latter case we need to know something about the stoichiometry of the process, while recognizing that this is invariably more complex with bioprocesses than with chemical processes. Before considering this latter aspect, let us first consider some of the issues concerned with the process topology.

1.1.3 The system boundary

In the examples above it was tacitly assumed that the separation took place in one unit. However, it wouldn't make any difference to the overall answer if several concentration and separation stages were involved to give the same result. In other words, the boundary box shown in Fig. 1.4 (Example 1.1) merely defines the system over which the material balance is established. Whether the 'box' contains one or several process stages is immaterial provided the boundary is drawn correctly so as to cut all entering and leaving streams. Nor does it matter how the stages within the box are connected to each other. We could, then, draw a system boundary around the whole of a flowsheet, and provided all the material flows into and out of the process (but not necessarily those within the process) are correctly represented on the flowsheet we could then use this to set up an overall balance.

EXAMPLE 1.4

Suppose that the fat separation process in Example 1.1 was carried out in two stages, as illustrated in Fig. 1.6; the intermediate concentrate S contains 25% fat. Calculate the unknown streams and their compositions.

Three possible 'systems' over which balances could be established are identified in Fig. 1.6 by the dotted lines defining the system boundaries. In particular, boundary A delineates the overall process: the only streams relevant are F , C and P . Boundaries B and D define the boundaries appropriate to balances over the individual units, from which S , P_1 and P_2 can, in principle, be calculated.

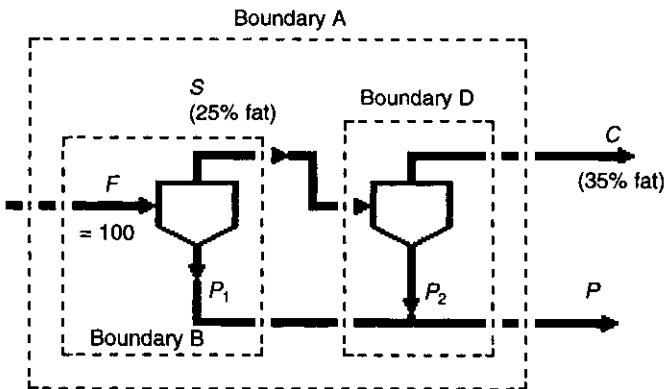


Fig. 1.6 Example 1.4: two-stage separation.

Basis: 100 tonnes F

1. Overall balance (i.e. boundary A):

Two balances only are needed to yield the flows C and P . Here we use the total and one component balances:

Total flows:

$$F = 100 = P + C \quad (1.12)$$

Fat:

$$0.05F = 5 = 0.35C \quad (1.13)$$

so that

$$C = 14.29$$

$$P = 85.71$$

which is, of course, identical to the solution of Example 1.1. This confirms the point made above about the irrelevance of the internal structure to the overall balance.

2. Balance over first separator (i.e. boundary B):

Again, as the input is specified, there are two unknowns only, S and P_1 , and thus two balances or relations are needed:

Total flows:

$$F = 100 = S + P_1 \quad (1.14)$$

Fat:

$$0.05F = 5 = 0.25S \quad (1.15)$$

so that:

$$S = 20$$

$$P_1 = 80$$

3. Balance over second separator (boundary D):

This is formally identical to the problem posed by the first separator, as the input S is now known. The solution is straightforward:

Total:

$$20 = C + P_2 \quad (1.16)$$

Fat:

$$5 = 0.35C \quad (1.17)$$

so that:

$$C = 14.29$$

$$P_2 = 5.71$$

Note however that there is some redundancy here, as C was already calculated from the overall balance, and

$$P_2 = P - P_1 = 5.71 \quad (1.18)$$

In this example the topology was not complex: the calculations were straightforward, as it was possible to complete the solution by marching forward from the inlet. However, an attempt to solve the problem 'backwards', by solving around separator 2 first, would be unsuccessful: it is often found preferable for the directions of the material and information flows to coincide. Note that the balances on the individual units must always be consistent with the overall balance.

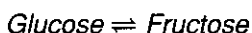
1.1.4 Recycles

Recycle streams are very common in process technology. They are used for various reasons and, in particular, to conserve material and to increase process efficiency. The carbon dioxide loop in Fig. 1.1 is a good example; note, too, that the solvent may also recycle valuable extracted components. In a similar way, the efficiency of a continuous fermenter (as used in ethanol production, for example) can often be increased, for example by recycling cells and unconsumed nutrients.

We illustrate the effects of recycling and the method of solving material balance problems with recycle in the next example.

EXAMPLE 1.5

One important bioprocess where recycling allows significant improvements in process efficiency is the enzymatic isomerization of glucose:



This reaction is reversible, and the equilibrium constant is close to 1. Thus the best that can be achieved is a product stream containing 50% each of glucose and fructose. However, fructose and glucose can be partially separated (by using a chromatograph, for example), so that the process flowsheet in Fig. 1.7 may allow higher yields of fructose by recycling unreacted glucose to the reactor.

In practice the glucose feed is always contaminated with a small percentage of inert oligosaccharides, and this has an important bearing on the recycle process.

As an example consider a simplified process in which the fresh feed contains 98% glucose and 2% oligosaccharides; all percentages are on a weight basis.

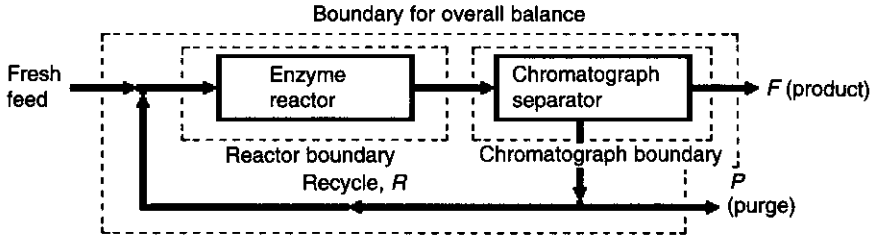


Fig. 1.7 Example 1.5: glucose isomerization process.

The reaction products are at equilibrium. The chromatograph is assumed to achieve perfect separation of the fructose and glucose: that is, the product stream is glucose-free; the recycle is fructose-free; all the oligosaccharide leaves the separator in the glucose stream. We now consider how the process yield varies with recycle, R.

Basis: 100 kg fresh feed

At steady state, there is no change in any composition or flow; then an overall balance (see Fig. 1.7) where the system boundary is cut only by the feed, product and purge streams, gives

$$100 = F + P \tag{1.19}$$

and an overall balance on inerts yields

$$2 = (1 - x)P \tag{1.20}$$

where x is the fraction of glucose in stream P .

Notice that, without the purge stream, inert oligosaccharides would build up in the process.

Specifying x fixes P and F . Thus if $x = 0.9$ (i.e. the inerts comprise 10% of the stream), $P = 20$ and $F = 80$ kg. If $x = 0.95$, $P = 40$ and $F = 60$ etc. In order to see what this implies for the recycle we must consider what happens inside the process.

First consider a balance over the reactor (Fig. 1.7). The flows of glucose, fructose, and inerts (all in kg) are:

	In	Out
Glucose	$98 + 0.9R$	$49 + 0.45R$
Fructose	0	$49 + 0.45R$
Inert	$2 + 0.1R$	$2 + 0.1R$
Total	$100 + R$	$100 + R$

where the equilibrium condition (i.e. that the glucose and fructose concentrations are equal) has been used to calculate the glucose and fructose

exit concentrations in column 3. Note that, as in the previous examples, the overall total acts as a check on the calculation.

Although this balance doesn't itself yield the recycle (in fact it holds for all possible values of R) we can follow through one or more of the components to check that the internal and overall balances coincide, and to complete the solution of the problem. That is, the solution must ensure that the flows of all components in the outlet stream from the reactor equate to their flows in the exit stream from the chromatograph, and thus to the flows in the purge and recycle. The easiest component to use is fructose, as the fructose leaving the reactor all ends up in stream F after the separator. Thus a balance on fructose over the chromatograph (see boundary illustrated in Fig. 1.7) gives

$$49 + 0.45R = F = 80 \quad (1.21)$$

so that $R = 68.9$ kg.

There is only one value of the recycle flow consistent with the predetermined value of x . You can readily check that as x , the fraction of glucose in the recycle stream, decreases so must R increase. The object of recycle in this case was to increase the yield of fructose on glucose. In the absence of recycle the fractional conversion of glucose would be 0.5. Here the fractional conversion is

$$y = \frac{80}{98} = 0.816$$

Again you can check that increasing the recycle rate (which must be increasingly dilute in glucose) would give an increased conversion of glucose. For example, at $x = 0.2$, $R = 485$ kg, and $y = 0.995$.

Of course, this increased conversion is not realized at zero cost: there is an increasingly large volume of material to recirculate and the reactor must be redesigned to achieve the chosen efficiency (which here is to reach equilibrium).

Finally, return to the balance over the separator (Fig. 1.7). The glucose and inerts entering from the reactor enter the recycle stream and a purge split is then taken to maintain the inerts balance. The mass balance on glucose and inerts over the split must satisfy the requirements imposed. Thus:

	Leaving separator	Leaving in P	Recycle
Glucose	$49 + 0.45R$	$0.1P$	$0.1R$
Inerts	$2 + 0.9R$	$0.9P$	$0.9R$

which, since $F = 100 - P$, are both consistent with equation (1.21).

You should check that all the individual and total flows in and out of each process unit balance.

1.1.5 Solving problems that include recycles

Invariably, the first step in trying to solve any problem should be to establish an overall balance, as was done in Example 1.5 by equations (1.19) and (1.20). As the example shows, problems involving recycle loops are sometimes tractable analytically. Sometimes, however, it is then necessary to resort to trial-and-error methods, and many computer-aided design packages incorporate efficient algorithms for this.

In Example 1.5 the recycle flow necessary to reconcile the component balances could be arrived at by such a process: that is, by repeated trials with different values of R . The method is illustrated below.

EXAMPLE 1.6: NUMERICAL SOLUTION OF RECYCLE PROBLEM

The same values of the feed flow (100 kg) and glucose concentration in the purge ($x = 0.9$) are assumed as in Example 1.5. Thus, from the overall balance (equations (1.19) and (1.20)), $P = 20$ kg and $F = 80$.

The calculation procedure is as follows:

1. Guess R .
2. With $x = 0.9$, calculate glucose (g) and inerts (i) in recycle (= A in Table 1.1).
3. Using feed content 98 kg glucose and 2 kg inerts, calculate g and i at entry to reactor (= B in Table 1.1).
4. Using equilibrium condition, calculate g and f at reactor exit (= C in Table 1.1).
5. Calculate fructose product, F_c , and compare with target stream $F (= 80)$.
6. Calculate g and i leaving separator (= D).
7. Calculate g and i in recycle from $D - P$ and compare with target (= A).

If the calculated values do not match with the design or assumed values (i.e. in steps 5 and 7) try a new R and repeat until answers converge.

The procedure is illustrated in Table 1.1 for two iterations. The correct result can be converged on readily using a simple algorithm.

1.1.6 Reaction stoichiometries

Although Example 1.5 involves a reaction, it is relatively simple to handle because of the simplicity of the reaction stoichiometry: one mole (or kg) of glucose gives one mole (or kg) of fructose. Thus it is easy to keep track of the flows.

Table 1.1 Example 1.6First iteration, $R = 50$

	A	B	C	F_c	F	D	P	D-P
<i>g</i>	45	143	71.5	0	0	71.5	18	53.5
<i>f</i>	0	0	71.5	71.5	80	0	0	0
<i>i</i>	5	7	7	0	0	7	2	5
T	50	150	150	71.5	80	78.5	20	58.5

Result: Calculated fructose product (F_c) < Design valueCalculated glucose in recycle ($D-P$) > Assumed value \therefore Try higher R Second iteration, $R = 80$

	A	B	C	F_c	F	D	P	D-P
<i>g</i>	72	170	85	0	0	85	18	67
<i>f</i>	0	0	85	85	80	0	0	0
<i>i</i>	8	10	10	0	0	10	2	8
T	80	180	180	85	80	95	20	75

Result: Calculated fructose product (F_c) > Design valueCalculated glucose in recycle ($D-P$) < Assumed value \therefore R too high: try new value in range $50 < R < 80$

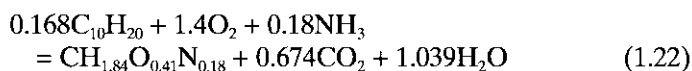
Many situations, however, are more complex. In food and bioprocess operations involving more than blending, the raw materials are transformed (bio)chemically into new products, and these processes may be too complicated to represent by a simple chemical equation. Consider for example the processes involved in transforming milk into cheese and whey, or the set of reactions involved in extrusion cooking. Nonetheless, however complex the chemical processes, we can be sure that:

1. a total overall mass balance must close;
2. balances on the chemical elements (C, N etc.) must close;
3. a balance on inert components must also close.

For example, in a typical microbial process we have

C-, N-, H-, O-, etc. sources + cells = more cells and products

The usual approach taken in attempting to describe these processes is to write an overall pseudo-chemical equation. For example, the production of single cell protein (SCP) from an n -alkane carbon source (assuming an average composition $C_{10}H_{20}$) has been described by:



Note that, while this equation does not pretend to give a mechanistic description, it must satisfy various consistency requirements, as follows.

Each element should balance on the left- and right-hand sides of the equation. Thus:

	LHS	RHS
C	1.68	1.674
H	3.90	3.878
O	2.8	2.797
N	0.18	0.18

It will be seen that, to a fair degree of accuracy, the balance is achieved.

The total **mass** on the right- and left-hand sides of the equation must also be equal. If the individual elemental balances are satisfied then the overall balance must also be automatically satisfied. Thus:

$$\begin{aligned} \text{LHS} &= 0.168 \times 140 + 1.4 \times 32 + 0.18 \times 17 = 71.38 \\ \text{RHS} &= 22.92 + 0.674 \times 44 + 1.039 \times 18 = 71.28 \end{aligned}$$

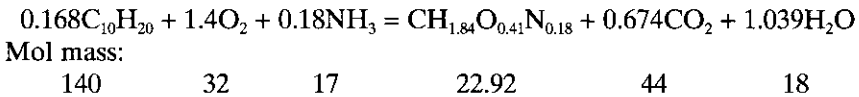
Here the 'molecular mass' of the microbial cells is 22.92: to avoid ambiguity it is conventional to define the molecular mass of a 'carbon mole' of cells: that is, of cells defined with the number of C atoms set arbitrarily to 1. Note that the overall cell composition simply represents the relative proportions between the elements. Different organisms or the same organism under different growth conditions will have (slightly) different compositions.

In general, **moles** are not conserved, where (bio-)reactions occur. In the example above there is an increase of almost one mole over the reaction. Usually, therefore, in dealing with biological processes it is more convenient to work in mass units. It must be emphasized that all components that are not transformed in the process (i.e. elements or inerts) are conserved.

It is noteworthy that the closure of the mass balance in this example is not perfect. One reason is that the overall stoichiometry does not have the same fundamental significance as a typical single chemical equation, such as $\text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3$. The equation quoted above is the net result of many simultaneous and parallel reactions, not just one; moreover, a C-mole of cells is a very different concept from a mole of a chemical or biochemical compound, and must be empirically determined. In practice, instrument errors and inaccuracies, variations in flows and hold-ups in a process conspire to make the accurate closure of material balances extremely difficult. Nevertheless, the use of experimental data to attempt to establish elemental or overall material balances is a most important diagnostic tool for the process engineer.

1.1.7 Stoichiometric and yield coefficients

The premultipliers in the stoichiometric equation (1.22) (0.168, 1.4 etc.) are the **stoichiometric coefficients**. They represent the molar proportions between the various components involved in the reaction. By convention the coefficient of one of the reagents or products is set to 1: it is immaterial which is chosen. Thus in section 1.1.6, 1.4 moles of oxygen are consumed per C-mole of cells produced (and per 0.18 moles of ammonia consumed, etc.). Given the molecular masses of the components these coefficients are readily transformed into mass units. Consider equation (1.22):

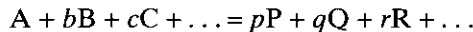


The mass of cells per unit mass of C-source is

$$Y = \frac{22.92}{0.168 \times 140} = 0.974 \quad (1.23)$$

Y is known as a **yield coefficient** and has the units of kg kg^{-1} (here, kg cells kg^{-1} n -alkane). Yield coefficients can be defined for each pair of products and substrates.

Thus for the reaction



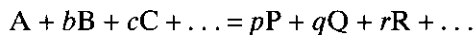
we can write the yield coefficient between product P (molecular mass M_P) and substrate B (molecular mass M_B):

$$Y_{PB} = \left(\frac{p}{b} \right) \left(\frac{M_P}{M_B} \right) \quad (1.24)$$

The stoichiometric and yield coefficients represent the ratios between components **consumed and produced**; it is quite rare for all the components to be fed in the same proportions as their coefficients (that is, in stoichiometric proportions), and care must be taken in handling these real problems.

1.1.8 Use of stoichiometric and yield coefficients in design

Consider a complex process:



where A, B etc. represent the compounds participating as substrates in the reaction. For convenience suppose that P is the primary product. Yield coefficients are defined, for example:

$$Y_{PA} = \text{kg P produced kg}^{-1} \text{ A consumed } (= p \cdot M_P / M_A),$$

$$Y_{PB} = \text{kg P produced kg}^{-1} \text{ B consumed } (= p \cdot M_P / bM_B) \text{ etc.}$$

Table 1.2 Use of stoichiometric and yield coefficients in design

	In (kg)	In (kmol)	Out (kmol)	Out (kg)
A	w_A	w_A/M_A	$(1-x)w_A/M_A$	$(1-x)w_A$
B	w_B	w_B/M_B	$w_B/M_B - xbw_A/M_A$	$w_B - xbw_A M_B/(M_A)$
...				
P	0	0	xpw_A/M_A	$xpw_A M_P/(M_A)$
Q	0	0	xqw_A/M_A	$xqw_A M_Q/(M_A)$
Σ	$w = w_A + \dots$			w

Now consider a process with feed comprising w_A, w_B, \dots kg of A,B etc. Suppose a fraction x of A is converted by the reaction above: what are the quantities of A,B, ... P,Q, ... leaving in the product streams?

We illustrate how an overall balance can be arrived at in terms of the stoichiometric coefficients: from the reaction stoichiometry, w moles of A react with (wb) moles of B (etc.) to produce wp moles of P, etc.; similarly, y kg of A react with ym_B/M_A kg of B. Thus we can construct a table of inputs and output. In Table 1.2 the calculation sequence goes from left to right across the columns. The totals of columns 1 and 4 must balance.

The fractional conversions of the feed components are equal (i.e. to x) only when their molar flows are in the same ratio as the stoichiometric coefficients: that is, they are fed in stoichiometric proportions. This can be seen by considering the entries for component B in the table above. The fractional conversion z is defined by $(1-z)(\text{column 2}) = (\text{column 3})$:

$$\frac{(1-z)w_B}{M_B} = \frac{w_B}{M_B} - \frac{xbw_A}{M_A}$$

so that

$$(1-z) = (1-x)$$

when

$$\frac{w_B}{M_B} = \frac{bw_A}{M_A}$$

In many processes of practical importance the feed components are not fed in stoichiometric proportions; the substrate that would first disappear if the process went to completion is called the **limiting reagent**. (This is not necessarily the limiting substrate in the language of fermentation technology.)

The same type of calculation as shown in Table 1.2 can be carried though using yield rather than stoichiometric coefficients, as illustrated in the following example.

EXAMPLE 1.7

We take as an example the (BP) process for SCP production based on *n*-alkanes. Details are summarized below. The aim is to establish a complete mass balance over the whole process.

Basis: 100 kg *n*-alkane

Data

C-source: C-10 (i.e. C₁₀H₂₀)

O-source: air; supplied in 20% excess over stoichiometric requirement

N-source: ammonia; supplied in 5% excess over the stoichiometric requirement

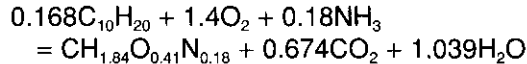
Salts: added in aqueous solution, neglect in balance

Cell concentration in product stream: 30 g l⁻¹

Yield: 90% of alkane converted

Yield coefficients

On the basis of the stoichiometry above (equation (1.22)):



the yield coefficients (Table 1.3) are readily calculated from equation (1.24), which in its most general form is

$$Y_{ij} = \left(\frac{a_i}{a_j} \right) \left(\frac{M_i}{M_j} \right) (\text{kg component } i)(\text{kg component } j)^{-1}$$

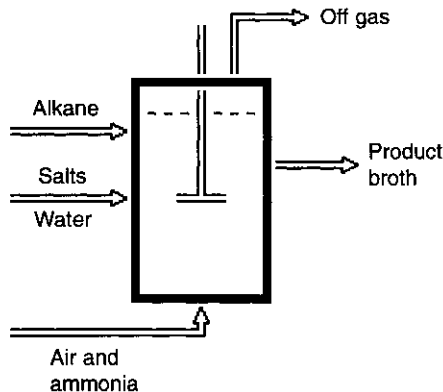


Fig. 1.8 Example 1.7: fermenter.

Table 1.3 Example 1.7: Yield coefficients

Compound	Molecular mass	Stoichiometric coefficient	Cell yield coefficient, Y_{xi} (kg cells) (kg compound i) ⁻¹
<i>n</i> -Alkane	140	0.168	0.9745
Oxygen	32	1.40	0.5116
Ammonia	17	0.18	7.49
Carbon dioxide ^a	44	0.674	0.7729
Water ^a	18	1.039	1.226
Cells	22.92	—	—

^aDenotes product

Table 1.4 Example 1.7: Calculation of mass balance

Component	In: feed (kg)	Consumed or produced (kg)	Out in product Stream (kg)
Alkane	100	99	1
Oxygen	200	188.6	11.4
Nitrogen ^a	658.4	—	658.4
Ammonia	13.66	12.87	0.79
Cells	—	96.48	96.48
Carbon dioxide	—	124.74	124.74
Water ^b	—	78.71	78.71
Total	972.06	0.54	971.52

^a Assuming air to be 23.3 wt % oxygen

^b Excluding water added to fermenter

where a_i , M_i and a_j , M_j are the stoichiometric coefficients and molecular masses associated with 'i' and 'j'.

The ratio of quantities consumed or produced between any pair of substrates and products i and j is given in terms of the cell yield coefficients in Table 1.3 by

$$Y_{ij} = \frac{Y_{xj}}{Y_{xi}} (\text{kg } i)(\text{kg } j)^{-1}$$

For example, between oxygen and alkane:

$$Y_{oa} = \frac{0.9745}{0.5116} = 1.905 \text{ kg oxygen (kg alkane)}^{-1}$$

On the basis of 100 kg *n*-alkane the theoretical requirements for oxygen and ammonia can be calculated:

$$\text{Theoretical oxygen requirement} = 1.905 \times 100 = 190.5 \text{ kg}$$

$$\text{Theoretical ammonia requirement} = 0.130 \times 100 = 13.0 \text{ kg}$$

The actual flows are 1.2 and 1.05 times these values, respectively. As 99 kg alkane are consumed per 100 kg fed to the fermenter, the actual masses of oxygen and ammonia consumed are 0.99 times the theoretical requirements. The amounts of cells, carbon dioxide and water produced are calculated in a similar way to give the results in Table 1.4. The slight errors in the table reflect the inaccuracy in the stoichiometric equation.

This calculation does not include the water added to the fermenter. The final cell concentration in the aqueous phase is 3 wt%: the broth therefore is 3216 kg, which implies addition of 3039.81 kg of water in the feed. Neglecting the solubility of the gases in water and assuming the gas product stream is dry, the overall balance can be represented (after rounding):

In (total)	4012 kg
Out	
Gas	795 kg
Liquid	3216 kg
Total	4011 kg

1.1.9 Algebraic representation

In order to generalize these results it is often convenient to represent the balances in algebraic form. Indeed, other chapters in this book, particularly that on reactor design (Chapter 8), use this method.

Consider a continuous steady process with feed and outlet flowrate w and inlet and outlet concentrations of a chosen species s_i and s_o . For a particular species, the amount of that species consumed per unit time is

$$w(s_i - s_o) \quad (1.25)$$

Considering the fermenter process above, for example, we can write balances on substrate and cells, with concentrations s and x respectively, in terms of the yield coefficient of cells Y_{xs} on substrate, as:

$$\text{Cells produced} = Y_{xs} (\text{Substrate consumed})$$

to give

$$w(x_o - x_i) = Y_{xs} w(s_i - s_o) \quad (1.26)$$

or, as x_i is often zero (corresponding to a sterile feed):

$$x_o = Y_{xs} (s_i - s_o) \quad (1.27)$$

1.1.10 Conclusions

In this section we have introduced some of the basic ideas of mass balances and their application to design and operational control in the process indus-

try. Today many of the calculation procedures mentioned above are carried out routinely by computer, using one of the many flowsheeting or design programs that are now available. We should not allow ourselves to be mystified by the apparent sophistication and power of these methods: the fundamental principles are based on the laws of conservation, which have been introduced here. From a consideration of the conservation of mass we next move on to the conservation of energy.

1.2 Energy balances

1.2.1 Introduction

Energy is a vital and often expensive input into the process industries. The simpler sorts of question that commonly arise in the context of process design or operation are to calculate the heating or cooling requirements for a thermal process, such as sterilization, or the power requirements for a mixing or pumping operation. Sometimes energy will be required in the form of heat (typically as process steam) or sometimes as shaft power from a motive or electrical source. From a conceptual point of view, the energy source or sink may not be important, but it will have a considerable bearing on the process efficiency. This brings us to the second sort of question: is a particular method of heating or cooling the most efficient method? What is the best option? How can the energy efficiency of a process or part of a process be maximized?

Many of the more elementary, but none the less important, questions of the first type can be answered on the basis of the first law of thermodynamics. Others, such as the calculation of theoretical limits, may need the second law. Here we will confine ourselves to the first law, which is essentially a statement that energy is conserved. The second law analysis of processes is outlined in Chapter 6. The first task is to clarify what we mean by energy.

1.2.2 Energy: units and datum levels

In a system with basic units of mass, length and time there are three important derived units: **force**, **energy** (or **work**, as these are synonymous) and **power**. In the SI system, where the unit of force, with the dimensions of mass times acceleration, is the newton (N), defined as 1 kg m s^{-2} , energy or work has the units of joules (J) where $1 \text{ J} = 1 \text{ Nm}$; power, which is the rate of doing work, is defined in watts, where $1 \text{ watt (W)} = 1 \text{ J s}^{-1}$.

Consider an object of mass 1 kg held stationary 1 m above the floor. This object then has a potential energy of 9.81 J. Note that it is necessary to define a reference level: in this case the floor. If some other reference or

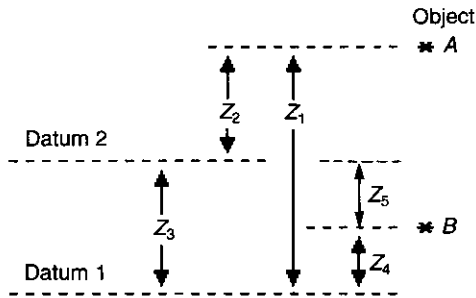


Fig. 1.9 Energy datum levels.

datum level had been chosen the energy of the object would of course be different. However, it is straightforward to relate the various energy levels to one another as illustrated by Fig. 1.9, in which *A* and *B* indicate two positions of the object. The table below summarizes the potential energies of the 1 kg objects with reference to various datum levels:

Object	Datum	Energy
<i>A</i>	1	$E(A,1) = 9.81Z_1$
<i>A</i>	2	$E(A,2) = 9.81Z_2 = 9.81\{Z_1 - Z_3\}$
<i>B</i>	1	$E(B,1) = 9.81Z_4$
<i>B</i>	2	$E(B,2) = -9.81Z_5 = 9.81\{Z_4 - Z_3\}$
<i>A</i>	<i>B</i>	$E(A,B) = 9.81\{Z_1 - Z_4\}$
<i>B</i>	<i>A</i>	$E(B,A) = 9.81\{Z_4 - Z_1\}$

Note, for example, that $E(A,B) = E(A,1) - E(B,1)$ or $E(A,2) - E(B,2)$; $E(A,B) = -E(B,A)$. The signs associated with the E -values are important. A negative sign corresponds to an object whose energy level is *below* the datum. Provided the datum levels are defined unambiguously, the calculation of energy levels with respect to other datum levels is a trivial matter. Moreover, the route by which the object reaches its stationary level *A* or *B* is irrelevant: energy is a function of **state** and not of path.

This brief discussion has been in terms of the very familiar concept of **potential energy**, whose application to many thermal problems in process engineering is relatively limited. Materials and objects have energy as a result of attributes other than position, such as velocity, temperature, pressure, physical state and chemical composition. Just as with potential energy, it is important to define datum levels unambiguously; energy is always a function of state and the simple rules of additivity etc. seen above can be transferred whatever the form of energy involved. Of course it is also important to work in the same and consistent units: then the question as to whether heating comes from an electrical source or steam, say, becomes

irrelevant to the energy balance (but not to efficiency or cost). This still begs the question of how we define energy levels for the situations relevant to process engineering. We shall return to that issue after considering a more abstract formulation of the laws of energy conservation.

1.2.3 Conservation of energy

While we believe that energy is conserved in all cases of practical importance in the food and biological process industries, there are of course several important constraints, many of which derive from the ways in which energy can be converted from one form to another. In flow problems a mechanical energy balance is adequate when the interconversion of thermal and mechanical energy is negligible: Bernoulli's equation (equation (2.5)) is then the appropriate form of the energy balance. In other situations the interchange may be represented as a loss term, even though energy is not really 'lost'. In mixing vessels the shaft power to drive the process is converted into motion and, ultimately, through viscosity into heat. Thermal energy or heat can only be transferred down a temperature gradient, so that while a cooling water stream may retrieve the energy being dissipated from a high-temperature process vessel, the energy will be low quality because of its temperature, and it will require ingenuity and money to upgrade its quality (see Chapter 6). Many of these very important features are concealed by the first law of thermodynamics, which simply asserts that energy is conserved across all these processes of transformation. In the real world many of the transformation processes are irreversible (it is easier to convert mechanical energy into heat than vice versa).

1.2.4 Application of the laws of conservation of energy

As with material balances it is important to have a clear definition of the system over which the balance is constructed. We must also differentiate between systems that are **closed** and those that are connected to the wider environment by material flows, such as the thermal sterilizing system in Fig. 1.10, which is an example of an **open** system. An example of a closed system would be a batch mixing vessel, such as a butter maker, in which the only transfers of energy across the boundary of the system during operation are in the non-material forms of heat and shaft power. In an open system the flowing streams have work done on them in entering, and do work on the fluid ahead in leaving. (see Chapter 2, section 2.2.3).

For a **closed system** the formal statement of the first law is very simple. Consider a process operated over a given time interval (Fig. 1.11), in which the total net flows of heat and work are $Q_T (= Q_{T1} + Q_{T2} - Q_{T3})$ and W (defined positive for flows **into** the system). Then the increase (decrease) in

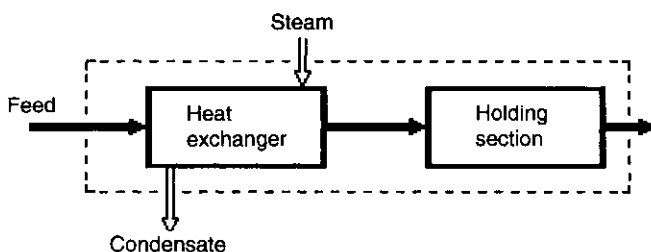


Fig. 1.10 Steam sterilization by indirect exchange: an open system.

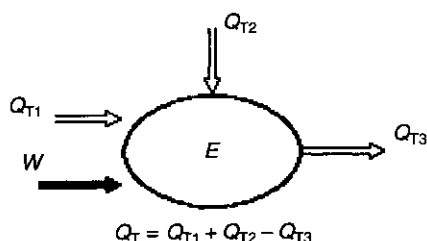


Fig. 1.11 Closed system.

energy stored in the system must, because of the conservation rule, equal the net transfer of energy into (out of) the system, or

$$\Delta E = Q_T + W \quad (1.28)$$

If ΔE is not zero then the final system contents must differ from the starting contents in some way, such as changed composition, temperature, physical state or internal surface area. For example, if the system represented a device for stirring and heating a liquid, the increase in energy resulting from stirring would be entirely accounted for by an increase in temperature of the contents. For a butter maker, however, chemical and physical changes including the generation of an emulsion would need to be accounted for. Clearly, equation (1.28) will only be really useful when ΔE can be related to these physical and chemical changes.

In the limit, equation (1.28) can also be written in terms of the **rates** of energy change and transfer so that instantaneously

$$\frac{dE}{dt} = Q + w \quad (1.29)$$

where Q and w are the instantaneous rates of input of energy and work into the system, (i.e. $\frac{dQ_T}{dt}$ and $\frac{dW}{dt}$) so that the right-hand side of equation

(1.28) is the net power input. Equation (1.28) will normally have the units of joules, while (1.29) will be in watts.

Note that by writing these equations in terms of energy **changes** there is no need to define an explicit datum level from which to measure the stored energy in the system.

Now consider the more general case of an **open system**, which we represent in an abstract way (Fig. 1.12). Here m represents a flowrate; Q and w are the net rates (normally in watts) of heat and work input (i.e. power as heat and mechanical energy). M , Q_T and W represent total (integrated) quantities over a period of time.

The net change in stored energy within the system boundary over a given period of operation must, if energy is conserved, exactly balance the net energy input by heat and work and the net energy difference between all the inflowing and outflowing streams. Thus, if we call the energy per unit mass of each stream E_1 , E_2 , etc. (where the energy levels must now be defined with reference to consistent datum levels) the energy balance becomes

$$\Delta E_s = Q_T + W + (M_1 \times E_1 + M_2 \times E_2 + \dots) - (M_{O1} \times E_{O1} + M_{O2} \times E_{O2} + \dots) \quad (1.30)$$

where ΔE_s is the **change** in stored system energy over the operating period in question. As before, equation (1.30) can be written in terms of instantaneous rates in the form

$$\frac{dE_s}{dt} = Q + w + (m_1 \times E_1 + m_2 \times E_2 + \dots) - (m_{O1} \times E_{O1} + m_{O2} \times E_{O2} + \dots) \quad (1.31)$$

In what follows we shall write more compactly:

$$\sum_{\text{in}} ME = (M_1 \times E_1 + M_2 \times E_2 + \dots) \quad (1.31a)$$

$$\sum_{\text{out}} mE = (m_{O1} \times E_{O1} + m_{O2} \times E_{O2} + \dots) \quad (1.31b)$$

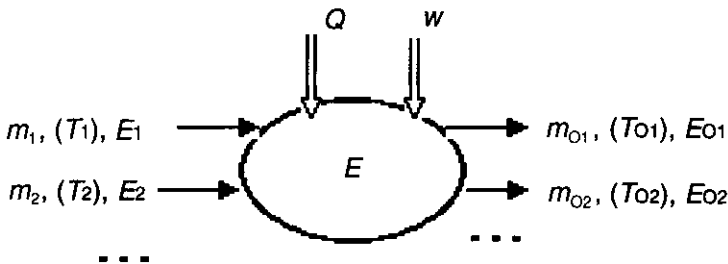


Fig. 1.12 A generalized open system.

etc.

Equations (1.30) and (1.31) represent the general and abstract case of an **unsteady open system**: unsteady because they include changes in the stored energy of the system with time. The start-up of a liquid heater would be unsteady while the contents build up and the temperatures are established. However, once the system has achieved a steady state in which all flows and temperatures are constant with time, the stored energy is then constant so that equations (1.30) and (1.31) become respectively

$$Q_T + W + \sum_{\text{in}} ME - \sum_{\text{out}} ME = 0 \quad (1.32)$$

and

$$Q + W + \sum_{\text{in}} mE - \sum_{\text{out}} mE = 0 \quad (1.33)$$

which are the general equations for a **steady open system**.

1.2.5 Stored and internal energy, enthalpy

As we have noted before, the stored energy within a process stream includes contributions from a variety of sources, such as kinetic and potential energies, electrical and magnetic potential, surface energy, the temperature, composition, physical conditions and state of the stream. In any particular situation some or most of these terms will be negligible: thus, in situations involving only a single phase, surface forces can be forgotten. It is important to remember that all the contributions must be measured with respect to a defined but usually arbitrary datum.

In many applications we can work in terms of the specific enthalpy of a component or mixture of components. The **enthalpy** (which is simply a measure of energy content) is the sum of **internal energy** U (reflecting temperature, physical state, etc. in relation to a defined datum), and a **flow work** term PV (where P is pressure and V is volume), also in joules. The origin of this term is discussed in Chapter 2 (section 2.2.3). This term is only relevant to **open** systems.

Values of the internal energy U and enthalpy h of pure components are readily calculated and are often tabulated, always with respect to a defined datum. For example, the steam tables tabulate the internal energies and enthalpies of water as liquid and vapour over a wide range of conditions, with reference to liquid water at its triple point. These tabulated values do not include the contribution to the internal energy of water that comes from its chemical composition. This latter term is only relevant if water is decomposed or generated by a chemical reaction during the process. If this term were to be included we would need to change the datum from liquid water to its elements.

Values of specific enthalpy are usually given the symbol h (kJ kg^{-1}); in chemical and biochemical applications enthalpies are often defined per mole. Specific enthalpy is defined by

$$h = U + PV$$

where U is the specific internal energy and V is the specific volume (i.e. $1/\rho$).

In summary, the integrated form of the first law for a closed system containing total mass M is:

$$Q_T + W = M[U_{\text{final}} - U_{\text{start}}] \quad (1.34)$$

and for a steady open system:

$$Q_T + W + \sum_{\text{in}} Mh - \sum_{\text{out}} Mh = 0 \quad (1.35)$$

1.2.6 Values of enthalpy

We now briefly consider some simple situations where internal energy and enthalpy values can be readily calculated.

Pure component with no change of phase. The specific heat capacities at constant volume and pressure c_v and c_p are defined as the energy required for a single degree change in temperature; in particular,

$$c_p = \frac{\partial h}{\partial T} \quad (1.36)$$

where the derivative is taken at constant pressure. Thus the enthalpy of a pure component at T_2 with reference to itself in the same physical state at T_1 is

$$h_{21} = \int_{T_1}^{T_2} c_p dT = \bar{c}_p (T_2 - T_1) \quad (1.37)$$

where \bar{c}_p is the mean specific heat capacity over the temperature range T_1 to T_2 .

Thus, for example, liquid water has a mean heat capacity of $4.19 \text{ kJ kg}^{-1} \text{ K}^{-1}$ over the range $0\text{--}100^\circ\text{C}$; taking its enthalpy as zero at 0°C , the enthalpy of water at 50°C is thus approximately $50 \times 4.19 = 209.5 \text{ kJ kg}^{-1}$. The energy to heat 100 kg of water from 25 to 50°C is, from equation (1.37):

$$Q_T = 100 \times 4.19 \times (50 - 25) = 104750 \text{ kJ}$$

This assumes that the mean heat capacity over the temperature ranges in question remains constant; it is not constant, but the errors involved here are small.

Pure component with change of phase. A phase change occurring at a given temperature and pressure invariably requires or liberates an amount of energy: the specific latent heat or enthalpy. Consider a pure component with enthalpy datum T_1 , liquid phase. The component evaporates at T_2 and

is then superheated to T_3 . The heat capacities of the liquid and vapour over the temperature ranges in question are c_f and c_g respectively; then the enthalpy at T_3 is

$$h_{3,1} = \int_{T_1}^{T_2} c_f dT + h_{fg}(T_2) + \int_{T_2}^{T_3} c_g dt \quad (1.38)$$

$$= h_{f2,1} + h_{fg}(T_2) + h_{g3,2} \quad (1.39)$$

where $h_{fg}(T_2)$ is the specific latent heat at T_2 , and the other two terms are the enthalpy of the liquid at T_2 with reference to liquid at T_1 and of vapour at T_3 with reference to vapour at T_2 .

Because energy and enthalpy are state functions it will be seen that in fact the final enthalpy is independent of the path between the reference at T_1 and the final state at T_3 ; in other words, the temperature T_2 need not correspond to the actual temperature at which the phase change occurs.

EXAMPLE 1.8

Consider the continuous sterilization process illustrated in Fig. 1.13 with the temperatures indicated. The process is to handle $36\,000\text{ kg h}^{-1}$ of liquid medium. All heat losses may be neglected. Energy is to be supplied by condensing steam at 180°C ; there is no subcooling of the condensate, i.e. the condensed steam leaves at 180°C . Assume the mean specific heat capacity of the liquid = $4.2\text{ kJ kg}^{-1}\text{ K}^{-1}$ and assume that the liquid has the same properties as liquid water.

Calculate:

- the rate of heat transfer between steam and medium, and the required steam flowrate;
- the rate of heat transfer between the liquid and the cooling water, and the required cooling water flow.

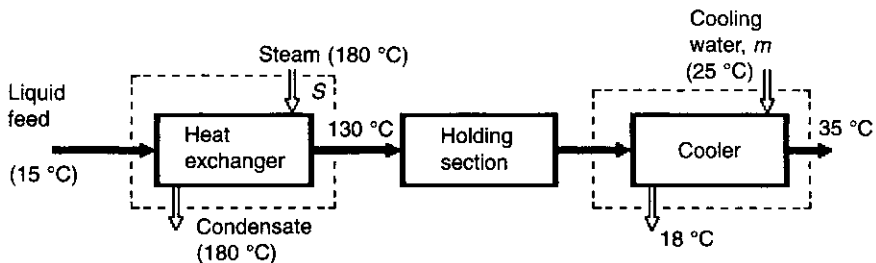


Fig. 1.13 Example 1.8: steam sterilization with product cooling.

From steam tables:

T (°C)	h_f (kJ kg ⁻¹)	h_{fg} (kJ kg ⁻¹)	h_g (kJ kg ⁻¹)
180	763.1	2014.9	2778.0

where h_f and h_g have the same datum and (see equation (1.39)) $h_g = h_f + h_{fg}$.

Basis: 36 000 kg h⁻¹ = 10 kg s⁻¹

Datum: Liquid water/medium at 0 °C.

Energy balance around the first unit

Assume steady conditions. Considering the whole heat exchanger, there are no flows of heat or power other than those associated with the material flows, so that

$$\sum_{\text{in}} m \times h = \sum_{\text{out}} m \times h$$

where:

$$\text{Inputs: } \sum_{\text{in}} m \times h = 10 \times 4.2 \times 15 + S \times 2778 \text{ (kW)}$$

$$\text{Outputs: } \sum_{\text{out}} m \times h = 10 \times 4.2 \times 130 + S \times 763.1 \text{ (kW)}$$

whence:

$$10 \times 4.2 \times 115 = S \times 2014.9 \quad (= S \times h_{fg})$$

so that

$$S = 2.397 \text{ kg s}^{-1}$$

The rate of heat exchange between the condensing steam and the liquid medium is $2.397 \times 2014.9 = 4829.7 \text{ kW}$. Notice that in this case the energy balance states that the change in enthalpy of the liquid stream exactly balances the change in enthalpy on the steam side; the datum values disappear from the calculation.

The balance is summarized in the table below:

Stream in	Flow (kg s ⁻¹)	T (°C)	$m \times h$ (kW)	Stream out	Flow (kg s ⁻¹)	T (°C)	$m \times h$ (kW)
Water	10	15	630	Water	10	130	5460
Steam	2.397	180	6658.9	Cond.	2.397	180	1829.1
Total	12.397		7288.9		12.397		7289.1

It would have been possible to draw system boundaries around the two separate streams (Fig. 1.14). In this case it would be necessary to solve first for q ($= 4830 \text{ kW}$) before completing the calculation of the steam flow.

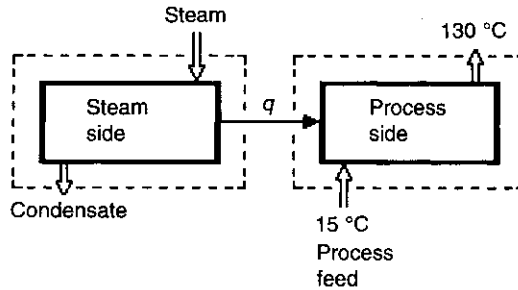


Fig. 1.14 Example 1.8: indirect steam sterilization (alternative representation).

Energy balance around the cooler (Fig. 1.13)

This is very simple. Using the same method as above we obtain

$$10 \times 4.2 \times (130 - 35) = m \times 4.2 \times (25 - 18)$$

so that the cooling water flowrate m is

$$\frac{10 \times 95}{7} = 135.7 \text{ kg s}^{-1}$$

with rate of transfer to the coolant stream $= 135.7 \times 4.2 \times 7 = 3989.6 \text{ kW}$.

Generalizing to a heat exchanger at steady state with no heat losses in which stream 1, flowrate m_1 , undergoes a temperature change ΔT_1 and stream 2, flowrate m_2 , undergoes a change ΔT_2 :

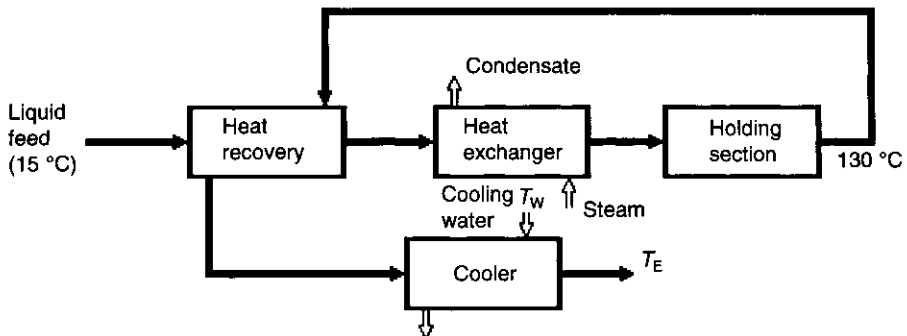


Fig. 1.15 Example 1.8: steam sterilization with heat recovery.

$$m_1 c_{p1} \Delta T_1 = m_2 c_{p2} \Delta T_2$$

where c_{p1} and c_{p2} are the mean specific heat capacities.

The flowsheet used in this problem is very inefficient from an energy conservation point of view, as the energy transferred from the steam is rejected into the cooling water stream at a temperature of only 25 °C, with no attempt at recovery. A more efficient scheme might be as shown in Fig. 1.15. Note that in practice there can never be complete recovery, as there must always be a finite driving force for heat transfer, so that the exit and inlet temperatures on the heat exchanger may approach to within typically 10 °C. Further discussion of this point is given in Chapter 6.

1.2.7 Enthalpies of mixtures

In practice most process streams comprise mixtures of components, whether dissolved or suspended. Sometimes these mixtures are far from ideal, so that enthalpy and other data must be gathered from the literature or measured directly. Usually, a reasonable first approximation in the situations that arise in the context of food and bioprocessing is to assume ideal behaviour: that is, that the enthalpy of a mixture is the weighted sum of the specific enthalpies of the various components, just as adding mixtures of mass m_1 and m_2 with solute concentrations c_1 and c_2 gives a total solute quantity equal to $m_1 c_1 + m_2 c_2$. This assumption will often break down where there are strong solutions, or significant heat effects on mixing etc. Three heat effects in particular can invalidate the assumption of ideality: due to dissolution, mixing and dissociation. In many cases it is reasonable and justifiable for the purposes of establishing an energy balance to treat a complex stream as if it were a single component with empirically determined physical and thermodynamic properties.

1.2.8 Chemical and biochemical reactions

So far all this discussion of energy balances has been concerned with essentially physical changes. Clearly, however, there are many situations of great importance where chemical or biochemical changes occur. We now consider how the treatment may be extended to cover such eventualities. Consider an energy balance about a biscuit-baking line. Suppose the datum level is taken as the raw material ingredients (flour, fat, water etc.) at 0 °C. The materials fed to the dough mixer will then have positive enthalpy values because their temperatures will generally be greater than the datum. (Sometimes enthalpies deriving only from temperature effects are called 'sensible' enthalpies.) At the end of the dough-making cycle the dough will also have a positive 'sensible' enthalpy by virtue of its temperature, but its enthalpy or energy value must also reflect the fact that the dough is not simply an ideal mixture of the datum ingredients. In practice some of the

energy input into the mixer will have gone into the creation of new chemical bonds, and the dough's enthalpy will reflect this. Indeed, if we wished to measure the standard enthalpy of formation of dough from its ingredients we would carry out an experiment in which the ingredients would start at 25°C, the dough would be made, while monitoring the net energy input by mixing and cooling, until the end of the process when the dough would be returned to 25°C. The net energy input over this whole process would be the enthalpy of the final product with respect to the starting materials under isothermal conditions. This would be the standard enthalpy or heat of formation of the dough; the sign convention adopted is that **exothermic** processes have a **negative** heat of formation or reaction, corresponding to the removal of heat from the process to maintain isothermal conditions.

In principle, food and biological operations can be handled in just the same way as chemical reactions, for which the necessary thermodynamics is well established. In practice, as with complex mixtures, many unknown transformations may occur, in which case the process can be handled as a pseudo-reaction (compare the brief description of the stoichiometry of biochemical processes in section 1.1.6 above); alternatively it may be possible to identify the most important or limiting processes to help quantification.

We shall confine ourselves here to a steady continuous system as sketched in Fig. 1.16. Here, m_{j_i} , m_{k_o} are mass flowrates (kg s^{-1}); n_{j_i} , n_{k_o} are the corresponding molar flowrates (kmol s^{-1}); T_{j_i} etc. are temperatures (K or °C); and h_{j_i} are the corresponding specific enthalpies (kJ kg^{-1}) (see below for the datum levels). Subscripts i and o refer to input and output streams respectively.

Non-reacting system. Datum: 25°C; all components in their standard states.

Then from equation (1.35)

$$\sum_j m_{j_i} \times h_{j_i} + Q + w = \sum_k m_{k_o} \times h_{k_o} \quad (1.40)$$

(\sum_j implies that the summation is carried out over all inputs, i.e. $j = 1, 2, \dots$)

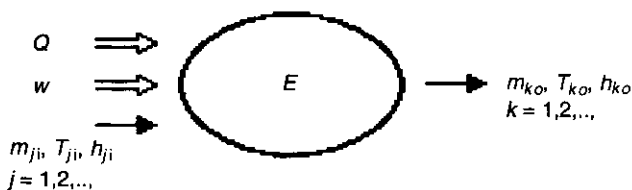


Fig. 1.16 Steady continuous open system.

Reacting systems. First we must clarify the definition of standard enthalpies of formation and reaction.

By convention standard heats or enthalpies are defined at 25°C (298 K); the physical states of all reagents and products **must** be specified.

The standard enthalpy of formation of a compound is the change in enthalpy when 1 kmol of the compound is formed from its elements in stoichiometric proportions, beginning and ending at 25°C and 1 bar (10⁵ Pa), with specified states of the elements and compound.

In this case the enthalpy datum is the **elements** at 25°C.

The standard enthalpy of any reaction is defined in an exactly corresponding way as the enthalpy change that results from a reaction beginning and ending at 25°C and 1 bar; again, the physical states of all the reagents must be specified.

In this case the change in enthalpy is defined with respect to the **reagents** at 25°C.

By virtue of the fact that enthalpies are function of state we can readily relate the standard heats of **formation** of the reagents and products (ΔH_{fr} , ΔH_{fp}) to the standard heat or enthalpy of **reaction**, ΔH_R° :

$$\Delta H_R^\circ = \sum a \Delta H_{fp} - \sum b \Delta H_{fr} \quad (1.41)$$

where a , b are the stoichiometric coefficients of products and reagents respectively. Thus for the reaction



$$\Delta H_R^\circ = \Delta H_{fc} - x\Delta H_{fa} - y\Delta H_{fb} \text{ per kmol C} \quad (1.42)$$

We now consider how these definitions can be used in setting up energy balances.

Energy balance over a reacting system. The balance can be written in various complementary ways, depending on the choice of datum. It is possible to write the balance using the **elements** as the datum level, in which case all enthalpies of reagents and products must be defined relative to their elements (i.e. to include contributions from the heat of formation and the 'sensible' enthalpy). For complex biological processes this is usually less convenient than choosing the **inputs** (i.e. reagents and other feed materials) as the datum. As the qualitative discussion of the dough-making process illustrates, in this latter case:

- the enthalpy of the input stream(s) is simply the sum of the sensible enthalpies of all the feed materials, i.e. allowing for temperature and possibly phase changes from the standard state taken as datum;
- the enthalpy of the output stream(s) has two components that are to be added:
 - (a) the 'sensible' enthalpy, which measures the enthalpy of the output materials with respect to themselves at 25°C (to account for the fact that the output streams are not at the datum temperature), and

- (b) the enthalpy of the output compounds at 25°C with respect to the feed materials, also at 25°C. This second term is of course the standard enthalpy of reaction. For a single reaction in which x kmol of product are formed this latter term will be $x\Delta H^\circ_{\text{R}}$; in the general case we can write the overall energy balance

$$\sum_j n_{j_i} \times h_{j_i} + Q + w = \sum_r x \times \Delta H^\circ_{\text{R}} + \sum_k n_{k_o} \times h_{k_o} \quad (1.43)$$

where the summations are carried out over all inputs ($j = 1, 2, \dots$), all reactions ($r = 1, 2, \dots$) and all outputs ($k = 1, 2, \dots$) respectively. The specific enthalpies h are all measured/calculated relative to the same compound at 25°C as datum (i.e. the h terms are the 'sensible' enthalpies referred to above).

As equation (1.43) is written in terms of flowrates, Q and w will be in kW; the balance can of course be written in terms of quantities, in which case Q_T and W will be in energy units.

It will be seen that equation (1.43) reduces trivially to the earlier balances for non-reacting systems (i.e. equation (1.40)).

In the chemical industry it is relatively rare to encounter reactors in which the work input (w) is significant in comparison with the thermal input or output, but this is not the case in the food and biotechnology sectors. Extrusion cookers and many fermenters involve considerable work inputs, which must be included in the energy balance.

EXAMPLE 1.9

Torula yeast (C. utilis) is a food grade yeast that can be produced by fermentation of complex sugars. The yeast is produced continuously in a fermenter of capacity 50 m³ operating at 35°C. The liquid feed contains 10 wt% substrate and is fed at 50 kg min⁻¹. The yeast yield is 0.5 kg/kg substrate fed. The oxygen requirement is 0.6 kg/kg yeast consumed and is supplied as air at twice that rate.

The conditions in the fermenter are indicated in Fig. 1.17. The mixer has a power drive of 100 kW: neglecting losses in the motor and shaft we assume that 100 kW of (shaft) work is put into the fermenter contents. The overall apparent enthalpy of the reaction (which, being aerobic, is highly exothermic) is $-16000 \text{ kJ (kg yeast formed)}^{-1}$. Assume the respiratory quotient (moles CO₂/O₂) = 1. With the data below calculate the cooling requirements for the fermenter.

Data

Assume the medium and broth have the same specific heat capacity as water = $4.2 \text{ kJ kg}^{-1} \text{ K}^{-1}$.

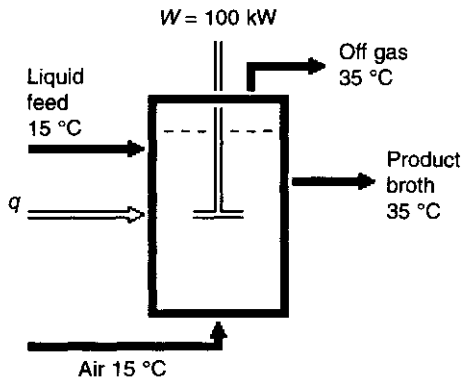


Fig. 1.17 Example 1.9: yeast fermenter.

Air:

Assume comprises 21 vol% (23 wt%) oxygen,
 Mean density: 1.29 kg m^{-3} ,
 Mean specific heat capacity: $1 \text{ kJ kg}^{-1} \text{ K}^{-1}$.

Water vapour at 35°C :

Saturated vapour pressure: 0.062 bar,
 Enthalpy: 2450 kJ kg^{-1} referred to liquid water at 25°C ,
 Density: 0.804 kg m^{-3} .

Solution

Basis: feed rate of 50 kg min^{-1}

Datum: 25°C ; inputs at their standard states; liquid water.

(a) Mass balance (approximate)

Assuming complete conversion of the carbon source:

Yeast production rate = 2.5 kg min^{-1}

Gas feed:

Oxygen consumed = $0.6 \times 2.5 = 1.5 \text{ kg min}^{-1}$

As the actual supply rate is twice the demand,

air supplied = $(2 \times 1.5)/0.23 = 13.0 \text{ kg min}^{-1}$

and, as the RQ = 1,

carbon dioxide produced = $1.5 \times 44/32 = 2.06 \text{ kg min}^{-1}$

Gas exit stream:

Total dry gas leaving = $13.0 - 1.5 + 2.06 = 13.56 \text{ kg min}^{-1}$

Assuming this gas is saturated with moisture:

Water in exit gas $\approx 0.062 \times 13.56 \times 0.804/1.39$

$= 0.486 \text{ kg min}^{-1}$

Liquid stream out $\approx 50 - 2.5 - 0.5 = 47 \text{ kg min}^{-1}$ (assuming all substrate consumed).

(b) Energy balance

(i) Enthalpy of inlet streams (datum = 25 °C):

$$\frac{-(50 \times 4.2 \times 10 + 13 \times 10)}{60} = -37.17 \text{ kW}$$

(ii) Sensible enthalpy of outlet streams (datum = 25 °C):

This comprises respectively (i) the liquid product, (ii) the 'sensible' enthalpy of the gas stream, and (iii) the latent heat of the water vapour in the outlet gas stream:

$$\frac{47.0 \times 4.2 \times 10 + 13.56 \times 10 + 0.486 \times 2450}{60} = 55 \text{ kW}$$

(c) Net heat of reaction

$$\frac{2.5 \times 16000}{60} = 666.7 \text{ kW}$$

(d) Overall balance (here written in mass units; compare equation (1.43))

$$\sum_j m_j \times h_j + Q + w = \sum x \times \Delta H^\circ_R + \sum_k m_{k_o} \times h_{k_o}$$

substituting from above:

$$-37.2 + Q + 100 = -666.7 + 55.0$$

so that

$$Q = -674.5 \text{ kW}$$

The results of the calculation are summarized in the table below, with the same datum of 25 °C and the reagents.

Input	Flow (kg s^{-1})	T (°C)	Enthalpy (kW)	Output	Flow (kg s^{-1})	T (°C)	Enthalpy (kW)
Liquid	0.833	15	-35	Liquid	0.783	35	32.9
Air	0.217	15	-2.17	Gas	0.226	35	22.1
Mixer			100	Cooling			674.5
ΔH°_R			666.7				
Total			729.53				729.5

EXAMPLE 1.10

As a second example we consider the glucose isomerization process whose material balance implications were discussed in Example 1.5. Here we consider the reactor only. Glucose enters in 40% aqueous solution at 60 °C; there is no recycle. The reactor is operated adiabatically (i.e. $Q = 0$). It is assumed that the specific heat capacity of the liquid stream is the same as water ($c_p = 4.18 \text{ kJ kg}^{-1} \text{ K}^{-1}$). Heat-of-solution effects are neglected. The standard enthalpy of the isomerization reaction at 25 °C, ΔH°_R , is $5730 \text{ kJ kmol}^{-1}$; the equilibrium constant for the reaction (which is 1.04 at 60 °C) follows the van't Hoff equation (Atkins, 1990, p. 219):

$$\frac{d(\ln K)}{dT} = \frac{\Delta H^\circ_R}{R_g T^2} \quad (1.44)$$

or

$$\frac{d(\ln K)}{d(1/T)} = -\frac{\Delta H^\circ_R}{R_g}$$

where $R_g = 8314 \text{ J kmol}^{-1} \text{ K}^{-1}$; T is in K.

Assuming that the products are in equilibrium at the end of the reactor we wish to calculate the temperature and composition of the product stream.

The special feature of this problem is that the mass balance cannot be calculated *ab initio*, because the exit composition depends on the equilibrium constant, which itself depends on temperature through equation (1.44). As the reaction is (mildly) endothermic, the exit temperature will presumably be below 60 °C; moreover, the heat absorbed by the reaction depends on the number of moles of glucose isomerized, so the equations for conservation of mass and energy are coupled together.

Basis: 1 kmol glucose in the feed.

Datum: 25 °C; liquid water; glucose in solution.

(a) Material flows and composition

As the inlet stream contains 40wt% glucose the total inlet flow corresponding to the chosen basis is $180/0.4 = 450 \text{ kg}$.

Let the fractional conversion of glucose = f . Then the outlet stream contains $1 - f$ kmol glucose and f kmol fructose respectively.

By definition

$$\frac{f}{1-f} = K(T) \quad (1.45)$$

where $K(T)$ may be deduced from equation (1.44).

(b) Equilibrium constant, K

Integrating equation (1.44):

$$\ln K = -\frac{\Delta H^\circ_R}{R_g T} + C \quad (1.46a)$$

where C is the constant of integration.

Using the fact that $K = 1.04$ at 60°C gives $C = 2.109$. Thus

$$\ln K = -\frac{5730}{R_g T} + 2.109 \quad (1.46b)$$

(c) Energy balance

As the reactor is operated adiabatically, $Q = 0$, and equation (1.43) becomes

$$\text{Total enthalpy of inlet stream} = \text{Net enthalpy of reaction} + \text{Total enthalpy of output stream} \quad (1.47)$$

where the enthalpy terms in equation (1.47) are

Inputs: $450 \times 4.18 \times (60 - 25)$

Reaction: $5730 \times f$

Outputs: $450 \times 4.18 \times (T - 25)$

whence:

$$T = 60 - \frac{5730 \times f}{450 \times 4.18} \quad (1.48)$$

The exit conditions from the reactor, i.e. f and T , are given by solving equations (1.45), (1.46b) and (1.48) simultaneously or by trial and error. This can be represented graphically (Fig. 1.18).

Solving by trial and error gives:

$$T = 58.45^\circ\text{C}$$

$$f = 0.5073$$

$$K = 1.03$$

The result – that the temperature is so close to the inlet of 60°C and the equilibrium constant is very close to 1.04 – is not surprising, as the reaction here is only weakly endothermic, and there would be little loss of accuracy in assuming that the system was isothermal and adiabatic.

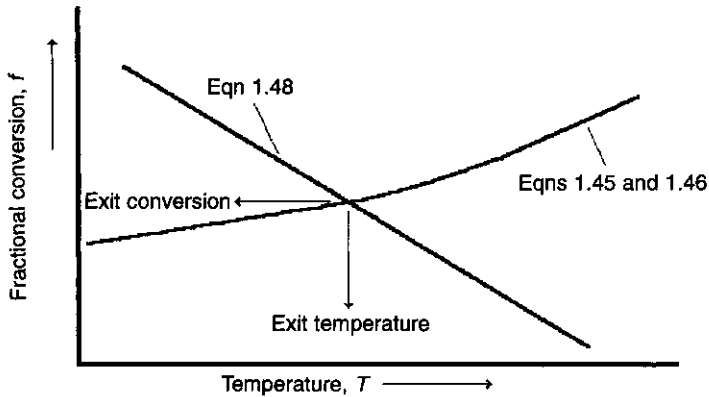


Fig. 1.18 Example 1.10: mass and energy balance solution.

1.2.9 Coupled heat and mass balances

Example 1.10 illustrates the fact that mass and energy balances cannot always be carried out independently, by computing first a mass balance and then an energy balance. In practice many processes depend on the simultaneous resolution of the two balances. The final example of a spray drier exemplifies the issues involved, this time in a system without reaction.

EXAMPLE 1.11

100 kg h⁻¹ of spray milk powder containing 4% moisture are produced in a continuous cocurrent spray drier. The feed solution contains 45 wt% milk solids and enters at 15 °C. Atmospheric air with humidity $\mathcal{H} = 0.005$ kg water/kg dry air is heated to 150 °C before entering the drier.

The air stream leaves the drier at 95 °C, and the solids product leaves at 70 °C.

Neglecting any heat losses, calculate the inlet liquid flow, the air flow and the exit humidity of the air stream.

Set up an overall summary mass and energy balance.

Data

Mean specific heat capacity of dry air = 1 kJ kg⁻¹ K⁻¹

Mean specific heat capacity of water vapour = 1.67 kJ kg⁻¹ K⁻¹

Mean specific heat capacity of dry solids = 1.6 kJ kg⁻¹ K⁻¹

Mean specific heat capacity of liquid water = 4.2 kJ kg⁻¹ K⁻¹

Latent heat of evaporation of water at 0 °C = 2500 kJ kg⁻¹

Solution

Basis: 100 kg spray dried product

Datum: 0 °C; liquid water.

Process diagram (Fig. 1.19)

(All flows in kg h^{-1})

L = liquid feedrate

g = **dry** air rate

G_i = total airflow in

G_o = total airflow out

S = product rate = 100 kg h^{-1}

Balance on dry solids

$$\begin{aligned} \text{Solids in} &= \text{Solids out} \\ 0.45L &= 100(1 - 0.04) = 96 \\ L &= 213.3 \text{ kg h}^{-1} \\ \text{Water in feed} &= 0.55L \\ &= 117.3 \text{ kg h}^{-1} \end{aligned}$$

Balance on dry air

$$\text{Dry air in} = g = \text{dry air out}$$

Water balance

$$\text{Water in} = \text{Water out (in exit air + solids)}$$

i.e.:

$$0.005g + 117.3 = \mathcal{H}g + 4$$

where \mathcal{H} = humidity of exit stream. Thus

$$g(\mathcal{H} - 0.005) = 113.3 \quad (1.49)$$

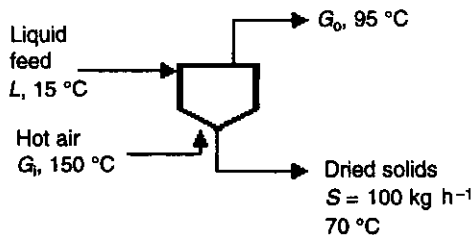


Fig. 1.19 Example 1.11: spray drier.

Enthalpy balance

Neglecting heat losses, the energy balance (equation (1.35)) becomes

$$\text{Enthalpy of } L + \text{Enthalpy of } G_i = \text{Enthalpy of } G_o + \text{Enthalpy of } S$$

where the total enthalpies of these streams are given by:

$$L: (117.3 \times 4.2 + 96 \times 1.6)15 = 9693.9 \text{ kJ}$$

$$G_i: 150g + 0.005g(1.67 \times 150 + 2500) = 163.75g \text{ kJ}$$

$$G_o: 95g + g\mathcal{A}(1.67 \times 95 + 2500) = (95 + 2658.65\mathcal{A})g \text{ kJ}$$

$$S: (96 \times 1.6 + 4 \times 4.2)70 = 11928 \text{ kJ}$$

Thus

$$9693.9 + 163.75g = 11928 + (95 + 2658.65\mathcal{A})g$$

i.e.:

$$g(2658.65\mathcal{A} - 68.75) = -2234.1 \quad (1.50)$$

Solution for g and \mathcal{A}

Equations (1.49) and (1.50) can now be solved simultaneously for g and \mathcal{A} , to give

$$g = 5472.0 \text{ kg dry air h}^{-1}$$

$$\mathcal{A} = 0.025705 \text{ kg kg}^{-1} \text{ dry air}$$

so that

$$G_i = 5472(1 + 0.005) = 5499.4 \text{ kg h}^{-1}$$

$$G_o = 5472(1 + 0.025705) = 5612.7 \text{ kg h}^{-1}$$

Summary of overall mass and energy balances – basis 1 h; datum 0°C

Stream	In (kg)	Enthalpy in (kJ)	Out (kg)	Enthalpy out (kJ)
Liquid, L	213.3	9693.9	–	–
Air, G_i	5499.4	896040	–	–
Air, G_o	–	–	5612.7	893799.8
Solids, S	–	–	100	11928
	5712.7	905733.9	5712.7	905727.8

1.2.10 Conclusions

In this section we have encountered some of the basic principles and methods that can be used to apply the first law of thermodynamics (the principle

of energy conservation) to selected food and bioprocess problems. The discussion has largely centred on problems involving thermal changes and energy inputs in the form of shaft work, such as in mixing. The application of 'mechanical' energy balances is considered in Chapter 2; Chapter 3, on heat transfer and heat exchanger design, also draws implicitly on the material of this chapter. Chapter 6 addresses some questions of energy efficiency and the use of analyses based on the second law of thermodynamics.

Finally, in the following section of this chapter we consider briefly some elementary aspects of process economics.

1.3 Process economics

There is surely no need here to emphasize the importance of economics in determining the viability of a process or product. In just the same way that a fully detailed mass and energy balance can only be elaborated when the detailed process design is complete, so the full details of the process economics will only be revealed when the process is up and running and the product has entered the market. Nevertheless, it is clearly important to be able to make realistic estimates of the process economics during the design and development stages. It is often not fully appreciated how much light an economic analysis can shed on the priorities for research and development and process engineering. In this section we shall very briefly discuss some of the factors that contribute to the cost of a product and then some of the basic concepts of economic appraisal. These concepts can be applied at any stage of the process cycle.

1.3.1 Processes, products and time

No process was ever built in a day; any manufacturing plant in the food industry will be the result of many years of research, development and operating experience. An idealized and simplified picture of the way such a process comes into being would start with the preliminary idea of an integrated plant; an outline preliminary flowsheet and estimates of the main material and energy flows would then be developed with a first very preliminary assessment of the likely economics. There would then be a period – perhaps several years – of research and development and pilot-scale testing, as existing technology is adapted and new technology created. At this stage a detailed design of the whole process can be finalized, leading (assuming the future for the process and its economics still look favourable) to the fabrication, construction and commissioning of the plant. Plant start-up is invariably followed by a period of running-in as bottlenecks are removed and unforeseen problems are resolved. It is usually some time before the

plant reaches anything like its design capacity and its operating phase, which if all goes well ought then to extend over several years.

Figure 1.20 shows, in a simplified way, and not to scale, how the patterns of expenditure and revenue vary during this process development and production cycle.

Another way of representing this flow of expenditure and revenues is in the form of a cumulative cash picture, in which the origin is an arbitrarily chosen date for the start of the project (Fig. 1.21). Among the points that can be made about this picture are the following.

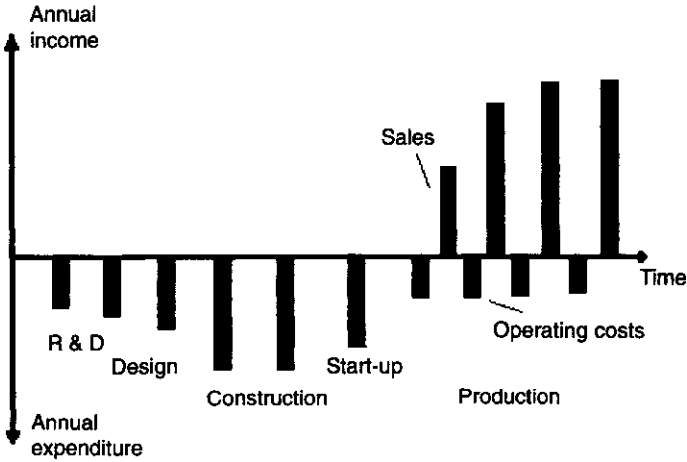


Fig. 1.20 Time profile of income and expenditure.

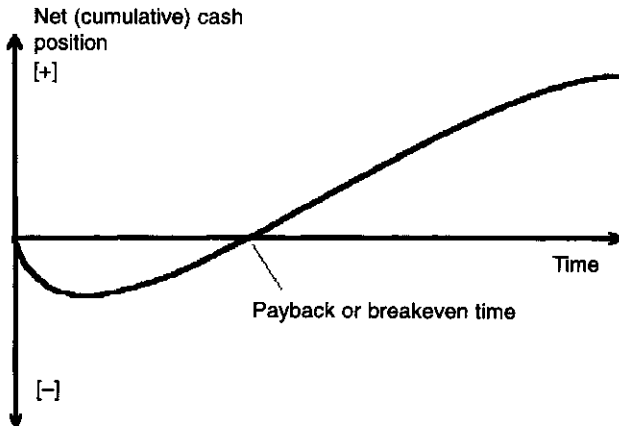


Fig. 1.21 Cumulative cash-flow diagram.

- Flows of expenditure and revenue are spread over considerable periods of time.
- Expenditure and revenue may often be shared with other projects and operations.
- The picture is inherently subject to variations (markets, prices, quality, availability etc.). Apart from the difficulties of forecasting these variations, the accuracy of technical and economic design parameters should improve during the design and development cycle; early projections of plant cost are likely only to be accurate to within around 25–30%, but later projections must be much more accurate.
- Expenditure is likely to be allocated to different heads during the cycle. In the earlier phases it will be allocated to R&D and design. There will be a period of considerable capital expenditure during the construction phase. During the production phase the principal items of expenditure will be on people, materials and services, maintenance and taxes. The allocation of R&D and design expenditure is a matter for industry policy. In what follows we shall assume that the capital costs include an agreed contribution.

We shall consider a simplified picture in which the time origin corresponds with the start of the major capital expenditure. First we consider briefly the ways in which costs are conventionally allocated.

1.3.2 Costs: capital and operating; fixed and variable

Suppose we are designing a cheese-making plant. Among the major costs associated with the process are the following:

1. the cost of the equipment and plant, pipework, instrumentation, buildings etc. (the total installed cost will probably be up to 3.5–4 times the total cost of the major equipment items);
2. the cost of material inputs to the process – milk, starters, etc.;
3. power, steam, cooling water and services;
4. labour;
5. laboratories and other overheads;
6. maintenance;
7. taxes, insurance etc.

Conventionally these costs are often grouped into **capital**-related costs (essentially item 1 above) and **operating** or **running costs**: that is, those costs directly attributable to the day-to-day running of the plant.

An alternative division is between **fixed** and **variable** costs. In this scheme, fixed costs are those that are **necessarily** incurred no matter what the extent of capacity utilization; variable costs are those that depend on the actual scale of production or the capacity utilization. For example, raw

material costs can be expected to depend on the level of production. This division does not generally exactly correspond to that between capital and operating costs; it can be a powerful and useful way of analysing process economics. The first part of the discussion here will use the capital/operating scheme. The use of fixed and variable costs will be illustrated later.

1.3.3 Building up a cost picture

If a process is to be assessed for its viability during the design phase it will be necessary to estimate the capital and operating costs. Capital costs will of course depend on the detailed design and configuration of the equipment. Detailed estimation is a highly specialized job, and we shall assume that acceptably accurate estimates are available. Operating costs depend on the results of the mass and energy balances, which, given unit costs, will permit the calculation of the costs of supplying materials and services. They will also include other costs, such as labour and services. It will also be necessary to estimate the likely market prices for any products and by-products. The same items will, of course, occur in an evaluation carried out during the project lifetime, at which stage they will be available and not estimated.

EXAMPLE 1.12

As an example consider a design study of a fermentation plant to produce ethanol (and feed yeast by-product) from sugar cane juice. The plant is to produce $200\text{ m}^3\text{ day}^{-1}$ of 95% ethanol. It should be noted that the figures used in this example are rather optimistic.

Capital

The total installed cost of the plant is estimated to be around £7.5m. A scrap value at the end of the project of £2.0m is assumed. The plant is assumed to be in full production for 11 years.

Annual costs

The operating costs and revenue on an annual basis at full capacity include the following major elements:

Operating costs	£m
Raw materials (sugar etc.)	21.48
Water, power, steam	3.14
Labour, laboratories, overheads etc.	0.46
Taxes, insurance, maintenance	0.68
Total	<u>25.76</u>

Revenues:	
Ethanol sales (at £390m ⁻³)	27.3
Yeast by-product sales	<u>3.63</u>
Total	30.93

Notes:

- 350 days operation per year are assumed.
- Material, services, products estimated from mass balance and unit costs.

Summary table

	£m
Installed capital cost	7.5
Annual operating costs	25.76
Annual sales revenue	30.93

Annual profile of costs and revenues

Although as we have seen a typical process has several years in gestation and start-up to full production, we shall simplify matters here by assuming that the capital investment period extends over two years only (in two equal instalments) and that the plant comes into full production in the following year. The following year-by-year picture can then be built up (all in £m):

Year	Capital, <i>K</i>	Running, <i>O</i>	Sales, <i>R</i>	Net income, <i>R-O-K</i>	Cumulative income
0	3.75	0	0	-3.75	-3.75
1	3.75	0	0	-3.75	-7.50
2	0	25.75	30.93	5.17	-2.33
3	0	25.75	30.93	5.17	+2.84
4	0	25.75	30.93	5.17	8.01
:	:	:	:	:	
12	(-) 2.0	25.75	30.93	7.17	51.37

The picture above would seem to be very satisfactory: the cumulative cash flow becomes positive between years 2 and 3 of the project, presumably implying that the project would thereafter show a profit. However, a key assumption built into the table is that the net annual surpluses can be added together to give the running cumulative total. We need to consider whether this assumption is correct.

1.3.4 Discounting and the time value of money

The construction of a cumulative total assumes that \$1 or £1 spent or earned in any year is identical in value to \$1 or £1 in any other year. There are two reasons for questioning this: one is inflation, which clearly undermines the value of the currency; the other relates more fundamentally to the potential value of the currency. Consider the assumption that £1 earned today is the same as £1 in 10 years' time. In fact the £1 earned today could be used for investing or lending. If the interest rate were a constant 10% per annum, £1 today invested would yield £1.1 in 1 year, £1.1 × 1.1 in 2 years, and so on. In general, at a constant annual fractional interest rate = i and over a time period of n years:

$$\text{£}X \text{ today} \rightarrow \text{£}X(1+i)^n \text{ in } n \text{ years' time} \quad (1.51)$$

Alternatively

$$\text{£}Y \text{ in } n \text{ years' time} \rightarrow \frac{Y}{(1+i)^n} \text{ today} \quad (1.52)$$

In these relationships, equation (1.51) represents the **future value** (FV) and equation (1.52) the **present value** (PV) of X and Y respectively.

This suggests that to make the annual cash flows commensurable we should work in terms of **either** future **or** present values. The table below shows a simplified example of the application of the formulae for FV and PV, with $i = 0.1$.

Year	Income	FV at end year 3	PV at year 0
0	100	133.1	100
1	100	121	90.91
2	100	110	82.64
3	100	100	75.13
Total	400	464.1	348.68

In practice it is common to work in terms of present values, and we shall conform to that in what follows. The technique is called **discounting**. Clearly our assumption of constant interest rate is not essential; it merely simplifies the arithmetic.

Thus the present value at year zero of a cash flow £ C in year n with a fractional interest or discount rate i is

$$PV = \frac{C}{(1+i)^n} \quad (1.53)$$

Applying the technique of discounting to the alcohol process example (Example 1.12) with values of $i = 0.1$ and 0.2 (i.e. interest rates of 10% and

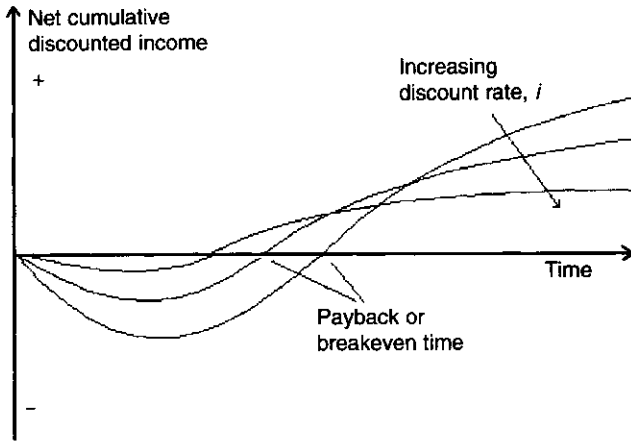


Fig. 1.22 Effect of discounting on cash flow.

Table 1.5 Results of applying discounting to Example 1.12

Year	Net income	PV $i = 0.1$	Σ PV $i = 0.1$	PV $i = 0.2$	Σ PV $i = 0.2$
0	-3.75	-3.75	-3.75	-3.75	-3.75
1	-3.75	-3.41	-7.16	-3.125	-6.875
2	5.17	4.27	-2.89	3.59	-3.285
3	5.17	3.88	0.99	2.99	-0.295
4	5.17	3.53	4.52	2.49	2.195
...
...
12	7.17	2.28	23.98	0.80	11.99
Total	51.37		23.98		11.98

20% p.a.) respectively we obtain the results listed in Table 1.5. The sum of the discounted net revenues (i.e. Σ PV in columns 4 and 6 in the table) is called the **net present value (NPV)** of the project.

Note that the effect of discounting is to reduce the real values of the cash flows and their sums. In general the higher the interest rate, the more significant is the effect of discounting, as is illustrated by Fig. 1.22. The breakeven point (also known as the discounted payback time) is also increased.

1.3.5 Significance

What are the implications and use of the method sketched out above? The interest (or discount) rate is a measure of the rate of return that the owners or managers of the project could realize from an alternative investment.

If it is to be a guide towards the most profitable use of the investment sums, then it should reflect the interest rate that would be realized from the **best** alternative investment: which need not, of course, be in the same sort of project or sector. The discount rate is thus the **opportunity cost** of capital, reflecting the value of the funds to be deployed or the rate of borrowing.

When the market is the only determinant, if the effective return on the project is less than i , it shouldn't go ahead. In other words, provided the correct value of discount rate is used, projects for which $NPV < 0$ should not proceed; projects with $NPV > 0$ should go ahead.

The discount factors $1/(1+i)^n$ that occur in the expression for the NPV can also be regarded as temporal weighting factors: that is, as allocating differential weights to future returns on a project. For example, if I and E are the income and expenditure in any particular year we can write

$$NPV = (I - E)_0 + w_1(I - E)_1 + w_2(I - E)_2 + w_3(I - E)_3 + \dots \quad (1.54)$$

where

$$w_1 = \frac{1}{(1+i)} \quad (1.55)$$

$$w_2 = \frac{1}{(1+i)^2} \quad (1.56)$$

etc.

High values of the discount rate imply a strong preference for early returns; future benefits are given a very low weight as can be seen from the tabulated NPVs in the alcohol project.

With discount rates above 10 or 15% per annum, what happens to the project beyond year 10 becomes relatively unimportant. In assessing industrial projects the lifetime is usually taken in the range 10–15 years.

1.3.6 Internal rate of return (IRR)

Some companies have a preference for using the IRR rather than the NPV as a measure. As the alcohol production example suggests, the value of the NPV at the end of the project (i.e. after 13 years) will become negative at high values of the discount rate. The internal rate of return is defined as the value of the discount rate at which the NPV becomes zero: which usually must be computed by trial and error. If the IRR is greater than the company target (which may be the bank rate, for example) then the project should proceed. If the IRR is lower than the the target, the project should not go ahead. Usually the IRR and NPV methods give the same result in terms of project ranking.

1.3.7 Payback time

Another measure of profitability is the time to recover the investment, or the payback time. On the cumulative cash-flow diagram this is the point at which the curve cuts the axis. Clearly it is important to differentiate between the discounted and undiscounted values of the payback time.

1.3.8 Inflation

It must be emphasized that all the discussion above relates to an inflation-free world; in this picture the time value of money stems from its earning capacity or its cost to the borrower. In the real world inflation does occur and the calculations must be adjusted accordingly so that a reference constant-value currency is adopted. Inflation at a constant annual rate of f further reduces the present value of the unit of currency by $1/(1 + f)^n$. Strictly this should be handled separately from the discounting operation; in practice, if the discount and inflation rates are low, they are sometimes compounded into an effective discount rate $= i + f$.

1.3.9 Risk

New projects always involve a degree of risk. This may be due to over-optimism about the technology, inaccuracies and uncertainties in forecasts of costs and market conditions, and so on. At the very least this implies that any analysis of economic viability should include a study of its sensitivity to the key parameters. In some sectors it is conventional to include some hedging against risk by using artificially high values of the discount rate.

1.3.10 Depreciation

Depreciation should **not** be included as a cost in the calculation of net present value. It does not represent a genuine cost to the project, but only a transfer of funds within the operating entity. It does of course influence the tax regime, and this 'knock-on' effect should be included in the calculations.

1.3.11 Summary of the procedure

When the objective is to calculate the viability of a project or process the procedure outlined above may be summarized as follows.

Given actual or estimated values of:

- capital costs;
- operating costs;
- revenue;
- interest/discount rate;

calculate:

- net annual cost flows;
- NPV;
- if $NPV > 0$, go ahead;
- if $NPV < 0$, do not proceed.

1.3.12 Unit cost of production

Amongst the data needed in the procedure described above is the market cost of the product. Often it is useful to be able to calculate explicitly the actual cost of producing a given amount of product under a defined set of operating conditions. It will be recognized that the same information on capital and operating costs as used above is also needed for this calculation. The net cost of production is the resultant of the contribution of the capital investment, other production costs, and any revenues. The simplest and most direct, but approximate, way of carrying out this calculation is to consider a typical period (say a year) of operation. The annual operating costs and revenues can be calculated as usual; the contribution to the overall cost from the capital investment, which may have been completed several years before, can be estimated by assuming that these costs are spread evenly over the project lifetime. This is equivalent to assuming straight-line depreciation over the project life.

For example, considering the alcohol production process in Example 1.12, the average capital charge per year, neglecting interest payments and the scrap value, is $\text{£}7.5\text{m}/13 = \text{£}0.577\text{m}$ per year, and the net annual cost of production allowing for by-product credits is $\text{£}22.13\text{m}$ per year. Thus, the average net annual cost of production on this basis is $\text{£}(0.577 + 22.13)\text{m}$ or $\text{£}22.707\text{m}$ per year, and the unit cost of production of ethanol is $\text{£}22.707\text{m}/(350 \times 200)$ or $\text{£}324$ per m^3 of product.

Apart from giving an indication of the operating margin, this type of calculation is also useful in demonstrating interest payments and the relative importance of different cost elements. In this particular example, capital costs are relatively unimportant; the single most important item in the cost of production is the raw material cost. This therefore suggests that a key determinant of economic efficiency will be the yield of product per unit mass of raw material.

1.3.13 Fixed and variable costs

From the example above it will also be clear that some cost elements are independent of the particular conditions of plant operation, and in particular the degree of capacity utilization. For example, the fixed capital investment and many overheads such as labour costs will be the same whether the plant is working at full or 50% capacity. These are called **fixed costs**.

However, other costs – raw materials, medium nutrients, energy, and some taxes – will depend on the particular production level. In the simplest case these **variable costs** will vary directly with the level of production, but in general there is not necessarily a linear relationship between inputs and outputs.

For example, let us drastically simplify the ethanol production example by assuming that the fixed costs comprise the capital costs, labour and overheads, and taxes, insurance and maintenance. It will be assumed that the costs of raw materials and water, power and steam and the revenue from by-products are all variable and directly proportional to the level of production of ethanol.

As before, we take a typical year's production as the basis of the calculation. If the actual scale of production is U m³ ethanol per day (annual production = $350U$) then from the cost data of Example 1.12:

$$\begin{aligned} \text{Annual fixed costs, } F &= \text{Capital cost contribution} \\ &+ \text{Labour etc.} + \text{Taxes etc.} \quad (1.57) \\ &= 0.577 + 0.46 + 0.68 = \text{£}1.717 \text{ m} \end{aligned}$$

Annual variable cost is the product of the marginal variable cost of production, V (assumed constant), and the production level, U .

The annual cost for a plant with capacity 200 m³/day from materials and services is £(21.48 + 3.14)m = £24.62m. Per m³/day of product therefore the marginal cost of production is

$$V = \text{£}24.62\text{m}/200 = \text{£}0.1231 \text{ m}$$

For a plant producing U m³/day, the annual variable cost is:

$$V \times U = \text{£}0.1231 \text{ m} \times U \quad (1.58)$$

and the overall annual cost of production, not including by-product credits, is from equations (1.57) and (1.58)

$$C = F + V \times U = 1.717 + 0.1231 \times U \quad (1.59)$$

Similarly, assuming sales and production levels are always balanced, the **annual sales revenue** from ethanol and by-products is

$$R = S \times U \quad (1.60)$$

where S is the unit income (i.e. annual revenue per m³ of ethanol). Here, assuming a uniform ethanol sales price of £390/m³, and using the fact that the annual sales revenue at the design capacity is £30.93 m (see table of costs and revenues, Example 1.12):

$$R = \frac{30.93 \times U}{200} = 0.15465U \quad (1.61)$$

Clearly, for a plant to remain profitable $R > C$; this condition can be shown graphically by plotting C and R versus the level of production, U , as shown

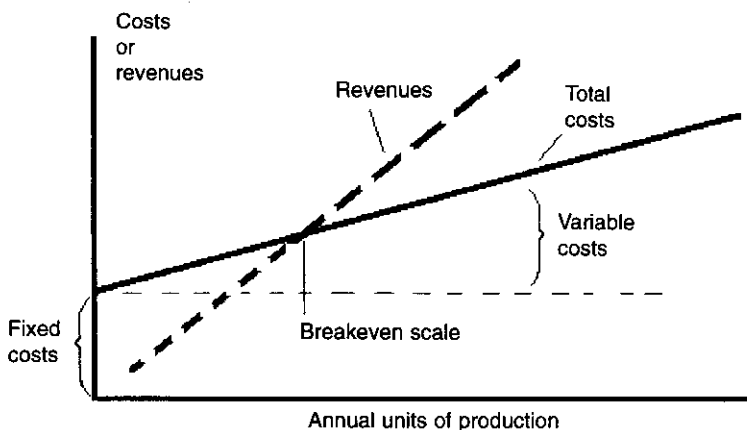


Fig. 1.23 Cost of production and breakeven.

in Fig. 1.23. Breakeven occurs when $R = C$ or, in this example, from equations (1.61) and (1.59), when

$$0.15465 \times U = 1.717 + 0.1231 \times U \quad (1.62)$$

i.e.

$$U = 54.43 \text{ m}^3 \text{ per day}$$

Thus here, where the unit cost of production of ethanol is considerably lower than the assumed market price, a substantial fall in production from the design level could be sustained. Clearly, if the breakeven were very close to the design level, great care would need to be taken before authorizing the project. The problem was simplified by assuming that marginal costs and revenues were independent of the scale of production and market penetration. However, the same principles apply in the more realistic case where the cost and revenue curves are non-linear in scale of production.

1.3.14 Conclusion

It must be stressed that this account of process economics has been drastically simplified. The real world is more complex than the examples here might suggest. However, it is hoped that the discussion will have clarified some of the basic principles. One point that should be stressed is that any estimation of costs and revenues is subject to considerable uncertainty. It is strongly recommended that any economic analysis involves an exploration of the sensitivity of the result to the principal assumptions. Finally, it should be noted that further issues are involved in building up balance sheets from the basic data incorporated in the cash-flow analysis; those issues have not been addressed here.

Appendix 1.A: Some basic definitions*Composition measures*

Consider m kg of a mixture of components A, B, etc., containing m_a kg A, m_b kg B, . . . where A, B have molecular masses M_a , M_b etc. Then

$$m = m_a + m_b + \dots = \sum_i m_i$$

In the SI system the number of kmol of A = m_a/M_a , etc.

Then the mass fraction z_a of A = Mass of A/Total mass

$$\begin{aligned} z_a &= \frac{m_a}{m_a + m_b + \dots} \\ &= \frac{m_a}{\sum_i m_i} \\ &= \frac{m_a}{m} \end{aligned}$$

The mole fraction

$$\begin{aligned} x_a &= \text{kmol A/Total kmol} \\ &= \frac{m_a/M_a}{m_a/M_a + m_b/M_b + \dots} \end{aligned}$$

The mean molecular mass of a mixture, M , is the average in which the weights are the component mole fractions; it is also the ratio between the total mass of the mixture and the number of kmol:

$$\begin{aligned} M &= x_a M_a + x_b M_b + \dots \\ &= \frac{m}{m_a/M_a + m_b/M_b + \dots} \end{aligned}$$

Also

$$\frac{1}{M} = \frac{z_a}{M_a} + \frac{z_b}{M_b} + \dots$$

The mass (molar) concentration is the mass (kmol) of component A per unit volume of mixture. These two measures are related through the molecular mass of A. Concentration measures and mass or mole fractions can be related given the mixture density.

Mixtures: ideal and non-ideal

Although assumptions of ideal behaviour are commonly made, and can drastically simplify calculations, beware that many systems diverge from ideality, particularly at temperatures and pressures different from the ambient.

For example, it can often be assumed that the components of liquid mixtures are additive, so that, for example, the mixture density is estimated as

$$\frac{1}{\rho} = \frac{z_a}{\rho_a} + \frac{z_b}{\rho_b} + \kappa$$

where z_i is the mass fraction of component i . However, even many familiar mixtures deviate from ideality: 50 cm³ of water and 50 cm³ ethanol give a mixture with volume 96.4 cm³.

Gases. Provided ideal behaviour is maintained, the volume and mole fractions of a component in a mixture are identical. Under ideal conditions the partial pressure p can also be directly related to the mole fraction. The partial pressure is defined as the pressure that the individual component would exert at the temperature and total pressure P in question in a defined volume V . For an ideal gas the pressure P is given by

$$PV = nRT$$

where n is the number of moles. With an ideal mixture of ideal gases Dalton's law applies:

$$P = p_a + p_b + \dots$$

where p_a etc. are the partial pressures. Thus we can also write

$$p_a = y_a P$$

and

$$\frac{p_a}{p_b} = \frac{y_a}{y_b}$$

where y_i is the mole fraction of component i in the gas mixture.

The **equilibrium vapour pressure** p° is defined as the pressure that would be exerted in a closed volume in which pure liquid exists in equilibrium with pure saturated vapour. This pressure is a strong function of temperature.

Consider now a closed system containing two totally immiscible liquids. They will therefore evaporate independently: at equilibrium each will exert its equilibrium vapour pressure so that the total pressure P exerted by the mixture is

$$P = p_a^\circ + p_b^\circ$$

Note that P is quite independent of the quantities of the liquid phases present, provided only that both liquids exist at equilibrium. Under these conditions then the partial pressures of A and B are equal to their equilibrium vapour pressures.

A different result is obtained for an ideal solution of two liquids, an ideal solution being one in which the various molecules are so similar that the

solution behaviour is the same as a pure component. The ethanol–water system is not ideal. Under ideal conditions Raoult’s law applies, that is the partial pressure of each component will be proportional to its mole fraction in the liquid, x_i , and the total pressure, being the sum of the partial pressures, is thus

$$P = p_a + p_b = x_a \times p_a^\circ + x_b \times p_b^\circ$$

and the mole fraction of A, say, in the vapour phase is

$$y_a = \frac{x_a \times P_a^\circ}{P}$$

Non-ideal liquid solutions are ones in which the linearity of Raoult’s law between partial pressure and liquid mole fraction does not hold. Usually as one component approaches 100% of the mixture its behaviour will approach Raoult’s law. At low concentrations, Henry’s law often holds:

$$p_a = Hx_a$$

where Henry’s constant, H , depends on the mixture components.

Air/water systems: humidification and drying. There are several common definitions that are particularly useful in the analysis of processes involving water/air mixtures.

In many humidification and drying processes it is convenient to use the quantity of bone-dry air as the basis for calculation, since this is often a tie substance (see Example 1.11). Rather than use mole or mass fractions (which are based on the total mixture) it becomes useful to work in terms of humidity:

$$\text{Humidity, } \mathcal{H} = \frac{\text{Mass of water vapour}}{\text{Mass of bone-dry air}}$$

Similarly, the molar humidity is:

$$\mathcal{H}_m = \frac{p_w}{p_a} = \frac{P_w}{P - p_w}$$

where p_w and p_a are the partial pressures of water vapour and dry air respectively, and P is the total pressure.

Clearly \mathcal{H} and \mathcal{H}_m are related through the molecular masses of air and water respectively:

$$\mathcal{H} = \frac{18 \times \mathcal{H}_m}{29}$$

At saturation the water vapour exerts its equilibrium vapour pressure so that the saturation humidity is

$$\mathcal{H}_s = \frac{P_w^\circ}{P - p_w^\circ}$$

The percentage humidity and relative humidity should not be confused with each other. The percentage humidity is the ratio of the actual and saturation humidities ($\mathcal{H}_m/\mathcal{H}_s$); the relative humidity is the ratio between the partial pressure of the water vapour and its equilibrium vapour pressure, expressed as a percentage.

The temperature at which a particular air–water vapour mixture becomes saturated so that $\mathcal{H}_m = \mathcal{H}_s$ is the saturation temperature or dew-point. Many of these and related thermodynamic properties are available in graphical form.

Conclusions

Although the emphasis in this first chapter on material, energy and economic balances has been towards their use in process design, the same techniques are vital for analysing process performance. Mass balances are needed in order to assess process yields and efficiency. Energy balances allow one to calculate how effectively energy is being used; economic analysis doesn't just reveal whether a process is or is not viable, but can provide considerable insight into the parts of a process which are most critical. In any real process the fact that measurements are subject to error and that process conditions fluctuate and drift must always be remembered when trying to establish these balances.

After reading this chapter you should understand the importance of correctly defining the system boundary, that is, the parts of the process which form the basis of a material or energy balance. You should know the difference between a steady and an unsteady process and should appreciate the significance of assuming that a continuous process is also steady. The principles of setting up – or checking – mass balances based on the total component flows, or on individual components such as the chemical elements, and their appropriateness to different situations have been introduced. Chapter 11 provides an opportunity for you try out these techniques on a realistic process example. A typical process can involve reactions which are so complex that the traditional stoichiometric methods are not applicable, or where recycle and bypass streams complicate matters. You should appreciate some of the ways of handling these complications.

The second part of the chapter dealt with the application of the law of energy conservation to typical processes; the material in this chapter also serves as an introduction to Chapters 3 and 4 on heat transfer. You should understand the importance of establishing a clear reference or datum level for all such balances and recognize the difference between an open and a closed system. The main practical difference between these two is that the first law of thermodynamics for a closed system is most conveniently set up in terms of internal energies, whilst for open systems it is most convenient

to use enthalpies. You should therefore know how these are defined and how they are related. It is worth emphasizing that for liquids and solids the difference between internal energy and enthalpy (or c_p and c_v) is usually small; for gases and vapours, because they are compressible, it is large. After reading this chapter you should be able to solve problems involving energy balances over typical processes, particularly thermal operations. It should also provide a basis for understanding more complicated processes such as compression and refrigeration cycles, and – as outlined in Chapter 6 – the methods of process energy integration.

Like the other sections of this chapter, the methods of economic analysis could themselves be the basis of a whole book. Here we have introduced some very basic ideas, such as the difference between capital and operating (or fixed and variable) costs and how they can be used to construct annual cash flows. One of the most important concepts introduced here is that of discounting, which is the key to ensuring that cash flows in different years can be compared, i.e. made commensurate. Based on these ideas you should understand, and be able to calculate, some of the measures of process viability including the net present value and the internal rate of return. We have not attempted to broach the issues of cost estimation nor of setting up balance sheets and financial statements.

In the real world it is difficult to calculate precise mass, energy and economic balances, because data and measurements are incomplete or error-ridden, or because the future is uncertain. Too often this becomes a counsel of despair and no attempt is made to calculate any balance at all. We hope that, at the end of this book, you will see the importance of carrying out even quite rough calculations: provided the assumptions and uncertainties are recognized, the benefits far outweigh the trouble of doing the calculations. Even when it is not possible to completely solve the material and energy balances, the approach we outline here, of setting a boundary and identifying the flows across it, is always useful. It should be the first stage of every systematic analysis.

Finally, most of the calculations discussed in this chapter are now routinely carried out with spreadsheets or more sophisticated computer-aided design packages. Chapter 11 illustrates a spreadsheet-based procedure. Although some of the calculation algorithms and methods of data generation now available are extremely sophisticated, the basic principles outlined here still apply, and should help you both to check and to understand these more advanced procedures.

Further reading

The material summarized in this chapter is covered at various levels of rigour and comprehensibility in many introductory texts for chemical engineers; one or two food engineering texts also include material on mass and energy balances. Volume 6 of Coulson and Richardson is

particularly useful in that it covers mass and energy balances, some aspects of design and process economics in a single volume. It doesn't, however, consider food engineering applications. This bibliography is divided into three parts. The first covers sections 1.1 and 1.2 of this chapter; the second lists a few books that go into more detail of the process operations typical of the process and food industries; the third covers some books on process economics.

Basic texts

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