# **18 Modeling of Heat and Mass Transfer in SSF Bioreactors**

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### **18.1 Introduction**

Chapters 22 to 25 present case studies in which mathematical models are used to explore the design and operation of various SSF bioreactors. Chapters 18 to 20 address the basic principles of the balance/transport sub-models of these bioreactor models.

The various phenomena that need to be described by the balance/transfer submodel, such as conductive and convective heat transfer, were covered in a qualitative manner in Chap. 4. The current chapter shows the mathematical expressions that are used to describe these phenomena. The aim is not to teach heat and mass transfer principles to a depth that will allow readers to construct the appropriate mathematical expressions themselves. Rather, it is to enable readers to inspect a mathematical model of an SSF bioreactor and recognize which transport phenomena are described by the model, on the basis of the various terms that appear within the model equations. These terms include various system, thermodynamic, and transport parameters. Chapters 19 and 20 quote some typical values that have been used for these parameters and give some general advice as to how they might be determined experimentally. However, please note that detailed experimental instructions are not provided.

# **18.2 General Forms of Balance Equations**

The transport/balance part of a mathematical model of a bioreactor consists of mass and energy balance equations. Such an equation expresses how a key system variable changes over time and includes terms that describe various phenomena that affect that variable.

Regardless of what the units of the variable of interest are, the balance equation should initially be written in such a way that all of its terms have units of either kg  $h^{-1}$ , in the case of a mass balance, or J  $h^{-1}$ , in the case on an energy balance. After this the equation can be rearranged if necessary to isolate the variable of interest.

As an example, an energy balance will appear in the form:

$$
m_{bed} C_{Pbed} \frac{dT_{bed}}{dt} = \pm Q_A \pm Q_B \pm Q_C + ... + r_Q,
$$
 (18.1)

where  $m_{bed}$  is the mass of the bed (kg),  $C_{Pbed}$  is the overall heat capacity of the bed (J kg<sup>-1</sup> °C<sup>-1</sup>),  $T_{bed}$  is the bed temperature (°C),  $r_Q$  is the rate of metabolic heat production (J h<sup>-1</sup>) (see Eq. (17.1)), and  $Q_A$ ,  $Q_B$ , and  $Q_C$  represent expressions that describe the rates at which different heat transport phenomena occur (all in J  $h^{-1}$ ). Whether they are added or subtracted will depend on whether they tend to increase or decrease the energy of the bed. The current chapter addresses the question of how these various "*Q*-terms" can be written mathematically. Equation (18.1) says that the rate of change in the amount of energy stored within the bed (in J  $h^{-1}$ ), which is represented by the left hand side of the equation, depends on the rates of the various processes that either add energy to the bed or remove energy from it. Equation (18.1) is written in terms of energy, because this is a conserved quantity, whereas temperature is not. Later on, this equation will be rearranged to leave only  $dT_{bed}/dt$  on the left hand side, since this is actually the system variable of interest.

The construction of the left hand side of Eq. (18.1) can be understood by assuming that initially a substrate bed is at a temperature  $T_{initial}$ , and during the fermentation a part of the metabolic heat released by growth remains in the bed, increasing its temperature. The amount of "extra energy" held within the substrate bed due to this increase in temperature is given by the product of the mass of the bed, the heat capacity of the bed and the temperature difference:

"
$$
\text{``Extra Energy''} = m_{bed} C_{Pbed} (T_{bed} - T_{initial}),\tag{18.2}
$$

which can be shown by determining the units of the result of the calculation (i.e.,  $kg \times J kg^{-1}$  °C<sup>-1</sup> × °C simplifies to give J).

On the other hand, a mass balance, for example, a balance on the water in the bed, will appear in the form:

$$
\frac{dM_{\text{water}}}{dt} = \pm R_A \pm R_B \pm R_C + ... + r_W, \qquad (18.3)
$$

where  $M_{water}$  is the overall mass of water in the bed (kg),  $r_W$  is the rate of metabolic water production (kg h<sup>-1</sup>) (See Eq. (17.2)), and  $R_A$ ,  $R_B$ , and  $R_C$  represent the rates of various mass transfer phenomena that involve water (all in kg  $h^{-1}$ ). Whether they are added or subtracted will depend on whether they tend to increase or decrease the amount of water in the bed. The current chapter addresses the question of how these various "*R*-terms" can be written mathematically. Equation (18.3) says that the rate of change in the mass of water in the bed (in kg h<sup>-1</sup>), which is represented by the left hand side of the equation, depends on the rates of the various processes that either add water to the bed or remove water from it.

Note that it may be desirable to have an equation that expresses directly the rate of change of the water content of the bed  $(W, kg\text{-water kg-dry-solids}^{-1})$ , and not the total mass of water in the bed. Even in this case, the equation should initially be written in the form shown in Eq. (18.3). The term *W* can then be separated out by realizing that the total amount of water in the bed is the product of the water content *W* and the total mass of dry solids in the bed  $(D, kg-dry-solids)$ . In other words, "kg-water kg-dry-solids<sup>-1</sup>  $\times$  kg-dry-solids" simplifies to give units of "kgwater". Of course, since both the water content and the total mass of dry solids in the bed are changing over time, *W* must be isolated using the product rule of differentiation:

$$
\frac{dM_{\text{water}}}{dt} = \frac{d(WD)}{dt} = D\frac{dW}{dt} + W\frac{dD}{dt}.
$$
 (18.4)

Substituting the right hand side of Eq. (18.4) into the left hand side of Eq. (18.3) and rearranging gives:

$$
\frac{dW}{dt} = \frac{1}{D} \left( \pm R_A \pm R_B \pm R_C + \dots + r_W - W \frac{dD}{dt} \right). \tag{18.5}
$$

Note that the solution of the problem, which will be done by numerical integration, is not unduly complicated by the appearance of the variable *W* and the differential term *dD*/*dt* on the right hand side of the equation.

The aim of this chapter is therefore to give an insight into how the rates of the various different heat and mass transfer phenomena that appear within these balance equations can be expressed mathematically. Once you are able to recognize the mathematical forms, it is possible to inspect a bioreactor model and deduce which heat and mass transfer processes it describes. This section will show that the same phenomenon can appear in slightly different mathematical forms, depending on where in the bioreactor it is occurring. For example, the expressions describing heat conduction in a static bed and heat conduction between the bed and the wall have different forms. Note that equations will not be given for  $O<sub>2</sub>$ balances, since they will not appear in the modeling case studies presented later. In any case, the mathematical forms of the terms of an  $O<sub>2</sub>$  balance are similar to those that will be presented for water balances.

These mathematical expressions include various parameters. The values of these parameters will need to be known in order to be able to use the mathematical model of the bioreactor to make predictions about how the bioreactor will perform. Chapters 19 and 20 will give advice about how the values of these parameters can be estimated.

The sections below will talk in terms of the typical directions of transfer during the rapid growth phase, namely when both heat and water are being removed from the bed. However, the processes are freely reversible: The direction in which they occur simply depends on the direction of the driving force. This is taken into account automatically in the form of the equations, since the driving force calculated will be either positive or negative, and the sign will determine the direction of transfer.

# **18.3 Conduction**

Conduction occurs in several places within subsystems of SSF bioreactors:

- $\bullet$  within the solid bed (both within the solid and gas phases of the bed);
- within the headspace gas;
- across the bioreactor wall, usually treated as occurring only directly from the inside surface to the outside surface of the wall and not along the wall.

The mathematical forms for describing these processes are presented below.

### **18.3.1 Conduction Across the Bioreactor Wall**

The rate of heat transfer across the bioreactor wall  $(Q_{cond}$ , J h<sup>-1</sup>) depends on:

- the difference in temperature between the bed in contact with the wall and the phase on the other side of the wall  $(^{\circ}C)$ ;
- the area of the wall across which heat transfer is taking place  $(A, m^2)$ ;
- the heat transfer coefficient for conduction through the wall, representing the Joules of energy that will be transferred per unit of time per area of wall per degree of temperature difference (i.e., J h<sup>-1</sup> m<sup>-2</sup>  $^{\circ}C^{-1}$ );
- the heat transfer coefficients for transfer from the bed to the inner surface of the wall and for transfer from the outer surface of the wall to the surroundings (i.e.,  $J h^{-1} m^{-2} C^{-1}$ ).

It is common to treat the three steps in heat removal (that is from the bed to the wall, through the wall, and from the wall to the surroundings) as a single overall process (Fig. 18.1). In this case, the rate of heat transfer is written as:

$$
Q_{cond} = h A (T_{bed\ outer\ surface} - T_{surroundings}), \qquad (18.6)
$$

where *h* is the "overall heat transfer coefficient". The temperatures are selfexplanatory. On the other hand, if the bioreactor wall is treated as a different subsystem, then for transfer from the bed to the inner surface of the wall we write:

$$
Q_{\text{cond1}} = h_1 A_1 (T_{\text{bed outer surface}} - T_{\text{wall inner surface}}),
$$
 (18.7)

where  $h_1$  is the heat transfer coefficient between the bed and the inner surface of the wall and  $A<sub>l</sub>$  is the area of contact between the bed and wall.

For transfer across the bioreactor wall we can write:

$$
Q_{cond2} = h_2 A_2 (T_{wall\ inner\ surface} - T_{wall\ outer\ surface}),
$$
\n(18.8)

where  $h_2$  is the heat transfer coefficient for transfer within the material of the bioreactor wall and  $A_2$  is the area of the wall.

In order to describe transfer from the wall outer surface to the surroundings (*Qcond3*) we would use an term of similar form, but describing convective heat transfer from a surface to a cooling fluid (see Eq. (18.10) in Sect. 18.4.1).



**Fig. 18.1.** Conductive heat transfer across the bioreactor wall, highlighting that it can be treated as consisting of three individual steps or simply as one overall process. Steps: (1) Heat transfer from the outer surface of the substrate bed to the inner surface of the bioreactor wall; (2) Conduction across the bioreactor wall; (3) Convective heat removal from the outer surface of the bioreactor wall to a well-mixed cooling fluid (air or water)

#### **18.3.2 Conduction Within a Phase**

Conduction will also occur within a phase, such as the substrate bed, the headspace gas, or even the bioreactor wall, although the significance of the contribution that it makes to overall heat removal will depend on the presence of other heat removal mechanisms such as convection and evaporation. Conduction will be the dominant mechanism within static beds without forced aeration (Group I bioreactors), that is, within the bed within tray bioreactors. In other bioreactors its contribution to heat removal may be relatively minor.

The rate of transfer of heat by conduction within a static phase  $(Q_{cond}, J h^{-1})$  is determined by:

- the temperature gradient in the phase  $(dT/dx, {}^{\circ}C \text{ m}^{-1});$
- the thermal conductivity of the phase  $(k, J m^{-1} h^{-1} {}^{\circ}C^{-1})$ . This is a property of the material that characterizes how easily it conducts heat, and which will be significantly affected by its composition. In the case of beds of solid particles, it depends on the bed water content, being higher with higher water contents. Note that the bed may be treated as a single pseudo-homogenous phase in which the thermal conductivity is calculated as a weighted average of the thermal conductivities of the solid phase and the inter-particle gas phase;
- the area across which heat transfer is being considered  $(A, m^2)$ . Note that this area term may be cancelled out in the final equation after it is rearranged.

Therefore the term for conductive heat transfer within a phase is given by:

$$
Q_{cond} = -kA \frac{dT}{dz}.
$$
 (18.9)

Depending on the design and operation of an aerated bed, conduction within the bed can occur: (1) co-linearly with the air flow (in which case the transfer by conduction will be in the opposite direction to the air flow); (2) normal to the air flow; or (3) in both the co-linear and normal directions (Fig. 18.2). In other words, an energy balance may contain a term that includes *dT*/*dz*, a term that includes *dT*/*dx*, or two terms, one including *dT*/*dz* and the other including *dT*/*dz.*

Once there is a temperature gradient, conductive heat transfer will occur. Conversely, if conductive cooling is the only heat transfer mechanism in the bed (i.e., in the case of a static unaerated bed) and the surface is being cooled by heat transfer to the surroundings, then temperature gradients will arise in the bed. As shown in Fig. 18.2, conduction occurs "down" the temperature gradient, hence the minus sign on the right hand side of Eq. (18.9). In other words, the flux of heat is positive in the direction in which the temperature gradient is negative.

During the rearrangements made in simplifying the energy balance for a static bed, Eq. (18.9) is often divided by the volume of the bioreactor (volume being given by an axial distance, *z*, multiplied by a cross-sectional area, *A*). This has two consequences: firstly, the area term cancels out and, secondly, the axial distance (*z*) that is left over combines with the term *dz* to make the derivative a secondorder derivative. That is, the conductive term will often appear as " $kd^2T/dz^2$ ".



**Fig. 18.2.** Conductive heat transfer within aerated static beds. Note that conduction normal to the direction of air flow can be promoted by the presence of water jackets. It is important in thin beds but in wide beds its contribution to overall heat removal may be small. The graph on the upper right shows how conduction occurs down a temperature gradient. For the case where the temperature gradient is uniform,  $dT/dx = \Delta T/\Delta x$ 

# **18.4 Convection**

Convective cooling, that is, cooling by transfer of heat to a moving fluid, which then transports the heat away due to bulk flow, occurs in various situations in SSF bioreactors that we might like to describe within bioreactor models:

- at the bioreactor wall, the removal of heat to flowing water in a water jacket, or to flowing air, which might either be forcefully agitated or be undergoing natural convection;
- $\bullet$  at a bed surface in which there is a cross-flow of air;
- within a forcefully aerated bed, in which heat is removed from the solid phase to the flowing air phase between the particles and then removed from that location by the flow of air through the bed.

### **18.4.1 Convection at the Bioreactor Wall**

The rate of heat removal by convection  $(O_{conv}, J h^{-1})$  at a surface in contact with a fluid depends on (Fig. 18.3):

- the coefficient of convective heat transfer  $(h, J m^2 h^{-1} {}^{\circ}C^{-1})$ . This depends on the velocity of the fluid flow because there is a layer of stagnant fluid at the solid surface, and heat transfer through this stagnant layer is limited to conduction. The thickness of the stagnant layer decreases as the flow velocity of the bulk fluid increases; this decreases the resistance to heat transfer and therefore increases the coefficient;
- the area of contact between the surface and the fluid  $(A, m^2)$ ;
- the difference in temperature between the surface and the bulk fluid  $({}^{\circ}C)$ .

That is, for the case where heat is transferred from the outer surface of the bioreactor wall to cooling water in a cooling jacket, we would write:

$$
Q_{conv} = h A \left( T_{wall\ outer\ surface} - T_{water} \right). \tag{18.10}
$$

This equation applies if we can assume that the fluid is well mixed and can therefore be represented by a single temperature. The equation will be more complicated if we want to describe how the temperature of a fluid increases as it flows in a unidirectional manner past the surface.

To increase heat removal from the bioreactor wall, it is necessary to increase one or more of the three terms. The heat transfer coefficient can often be increased by increasing the velocity of fluid flow, while the area of contact can be increased by using projections on the wall or a bioreactor geometry that increases the overall wall surface area (for a given bioreactor volume). The driving force for heat transfer (i.e., the temperature difference) can be increased by cooling the water before it is passed through the water jacket.



**Fig. 18.3.** Convective heat transfer from a surface to a well-mixed flowing phase. **(a)** The example shown here is for heat transfer from the bioreactor wall to surrounding air or the water in a water jacket. **(b)** Similar considerations apply for the transfer of heat from the surface of a bed to a passing gas phase

### **18.4.2 Convective Heat Removal from Solids to Air**

The rate of heat removal from the solid phase to the gas phase by convection  $(Q_{conv}, J h^{-1})$  depends on (Fig. 18.4):

- $\bullet$  the coefficient for heat transfer between the solid particles and the air phase  $(h, h)$ J m<sup>-2</sup> h<sup>-1</sup> °C<sup>-1</sup>), the value of which depends on the velocity of the air flow;
- the superficial area of contact between the solids and the air phase  $(A, m^2)$ ;
- $\bullet$  the difference in temperature between the solids and the air phase ( $\degree$ C).



**Fig. 18.4.** Heat and mass transfer between the solid and gas phases in the case where the solid and gas phases are treated as separate phases

To describe solid-to-gas heat transfer we therefore write:

$$
Q_{conv} = h A (T_{solid} - T_{air}). \qquad (18.11)
$$

Note that the area of contact between the solid and gas phases can be difficult to measure and therefore the product "*h A"* is often expressed and determined as a global heat transfer coefficient that combines the two quantities (" $hA$ ", J h<sup>-1</sup> °C<sup>-1</sup>). It may even be expressed as the overall coefficient per  $m<sup>3</sup>$  of bed volume (i.e., with units of J h<sup>-1</sup>  $\degree$ C<sup>-1</sup> m<sup>-3</sup>-bed).

The amount of heat removed from the solids by convective cooling can be increased by increasing the air flow rate or decreasing the air temperature at the air inlet. Either of these strategies should increase the average temperature difference between the air and solid phases. Also, the higher air flow rate will increase the value of the heat transfer coefficient.

At times the solids and air are assumed to be in thermal equilibrium (this is the assumption of a pseudo-homogeneous bed). Note that this does not necessarily mean that the bed has the same temperature at all positions. It means that the solid particles at any particular position within the bed are at the same temperature as the gas phase at that position. Therefore a single temperature variable can be used to represent the temperature at a given position in the bed. In this case it is not necessary to write an equation describing solids-to-air heat transfer, as this is subsumed in the term that describes the heat removal associated with the flow of gas through the bed.

#### **18.4.3 Convective Heat Removal Due to Air Flow Through the Bed**

The rate of heat removal by flow of the air through the bed  $(Q_{conv}, J h^{-1})$  depends on (Fig. 18.5):

- the mass flux of dry air  $(G, \text{kg-dry-air m}^{-2} \text{h}^{-1})$ , which is given by the superficial velocity of the air  $(V_z, m h^{-1})$  multiplied by the density of the air  $(\rho_{air}, kg-dry$ air  $m<sup>3</sup>$ . Of course, the superficial velocity itself is simply equal to the volumetric flow rate  $(m^3$ -dry-air  $h^{-1}$ ) divided by the total cross sectional area of the bed (note that this is the total area, not the area occupied by the void spaces);
- the cross-sectional area of the bed  $(A_b, m^2)$ ;
- the heat capacity of the air  $(C_{Pair}, J \text{ kg-dry-air}^{-1} \text{°C}^{-1});$
- $\bullet$  the difference between the air temperatures at two different locations ( $\degree$ C).

Applied over the whole bed (i.e., in a balance that considers the difference between the air inlet and the air outlet), the rate of heat removal by convection  $(J h^{-1})$ would be given by:

$$
Q_{conv} = G_{air} C_{Pair} A_b (T_{outlet} - T_{inlet}),
$$
\n(18.12)

where in this case  $A_b$  is the cross sectional area of the bioreactor.

However, in static beds, in which the temperature is a function of height within the bed, it is often of more interest to write an equation that allows the calculation of the temperature as a function of height. In this case, the balance equation is initially written over a thin layer of the bed. Within this equation the convection term will appear as:



**Fig. 18.5.** Illustration of the various parts of the expression for the removal of sensible energy in the air stream. **(a)** In an overall energy balance over a bioreactor; **(b)** In a balance written over thin layer of the bed

$$
Q_{conv} = G_{air} C_{Pair} A_b \frac{dT}{dz} \Delta z, \qquad (18.13)
$$

since the temperature difference  $({}^{\circ}C)$  between the inlet and outlet of this thin layer is simply the temperature gradient  $(dT/dz, {}^{\circ}C \text{ m}^{-1})$  multiplied by the thickness of the thin layer  $(\Delta z, m)$ .

Typically the energy balance equation will be divided through by the volume of the thin layer during later rearrangements, such that in the final equation this term will appear containing neither  $A_b$  nor  $\Delta z$ . Note also that if the temperature at the outlet of the thin layer is higher than the temperature at the inlet of the thin layer, then convection will be reducing the sensible energy of the thin layer, and therefore this term will be preceded by a negative sign if it appears on the right hand side of an equation such as Eq. (18.1). In fact, it is often put on the left hand side of the balance equation.

Note also that it is often convenient to use the same term to express the contribution of the water vapor to the removal of sensible energy. Given the humidity  $(H, \text{kg-water kg-dry-air}^{-1})$  and the heat capacity of the vapor  $(C_{Pvapor}$ , J kg-vapor<sup>-1</sup>  $^{\circ}C^{-1}$ ), the term would simply become:

$$
Q_{conv} = G(C_{Pair} + HC_{Pvapor})A_b \frac{dT}{dz} \Delta z. \qquad (18.14)
$$

Again,  $A_b$  and  $\Delta z$  may be cancelled out in the manipulations that are made to arrive at the final equation in the bioreactor model.

Note that convective cooling by the forced aeration of a static bed in which there is continual heat liberation by the growth process will cause temperature gradients in the bed. This phenomenon was explained in Fig. 4.3.

### **18.5 Evaporation**

Evaporation can be important in various instances within SSF bioreactors:

- $\bullet$  at the surface of a bed exposed to the air (for example, the surface of a tray);
- between the air and solid phases in a forcefully-aerated bed.

The equations used to describe evaporation in the various circumstances will have many similarities with the equations used to describe heat transfer, as will become apparent in the subsections below. Note that the diffusion of liquid water or water vapor is not described here, since bioreactor models typically assume that it is negligible. If it were to be included in a model, the diffusion term would have a mathematical form similar to Eq. (18.9).

### **18.5.1 Evaporation from the Solids to the Air Phase**

The rate of evaporation from the solids to the gas phase within the bed depends on (Fig. 18.6):

- the difference between the water activity that the solid actually has  $(a_{wsolid}$ , dimensionless) and the water activity that it would have if it were in equilibrium with the gas phase  $(a_{\text{wsolid}}^*)$ ;
- the area of contact between the solid and gas phases  $(A, m^2)$ ;
- the mass transfer coefficient  $(k_w)$ , which is the mass of water transferred per unit of time per unit of area per unit of driving force. Since the driving force is expressed in terms of water activity, which is dimensionless, the units of  $k_w$  are simply kg-H<sub>2</sub>O m<sup>-2</sup> h<sup>-1</sup>.



**Fig. 18.6.** Illustration of the various ways of expressing evaporative loss of water and evaporative heat removal (convective heat removal is not considered here). **(a)** In the case in which the solid and gas phases are treated as separate phases; **(b)** In the case in which the solid and gas phases are treated as a single pseudo-homogeneous phase

We can therefore write the local rate of evaporation  $R_{evap}$  (kg-H<sub>2</sub>O h<sup>-1</sup>) as:

$$
R_{evap} = k_w A (a_{wsolid} - a_{wsolid}^*)
$$
 (18.15)

As in the case of convective heat removal, it is common to combine the mass transfer coefficient and the area to obtain an overall transfer coefficient ("*kA*").

The local rate of heat removal from the solid phase by evaporation ( $Q_{evap}$ , J h<sup>-1</sup>) is given by:

$$
Q_{evap} = \lambda k_w A (a_{wsolid} - a_{wsolid}^*)
$$
\n(18.16)

where  $\lambda$  is the enthalpy of vaporization of water (J kg-H<sub>2</sub>O<sup>-1</sup>).

Note that an isotherm can be used to order to write the driving force in terms of the water content. In this case the driving force for evaporation is the difference between the water content that the solid actually has  $(W, kg$ -water kg-dry solid<sup>-1</sup>) and the water content that it would have it were in equilibrium with the gas phase  $(W_{\text{sat}})$ , kg-water kg-dry solid<sup>-1</sup>). This affects the units used in the mass transfer coefficient. Chapter 22 will describe how the equation is written in this case.

At times the solids and air are assumed to be in moisture equilibrium, or, in other words, the air phase is assumed to be saturated with water at the temperature of the solids (this is the assumption of a pseudo-homogeneous bed). This has the consequence that the humidity at a particular position can be expressed as a function of the temperature at that position. In this case, it is not necessary to write equations describing solids-to-air water transfer and evaporative heat transfer, as these are subsumed within the terms that describe the water and heat removal associated with the flow of gas through the bed, as explained in the next section.

#### **18.5.2 Water Removal Due to Air Flow Through the Bed**

The flow of moist air through the bed typically leads to the removal of water from the bed (see Fig. 4.3). The overall rate of water removal (kg-water  $h^{-1}$ ) from the bed is:

$$
R_{conv} = G A_b (H_{outlet} - H_{inlet}), \qquad (18.17)
$$

where  $H_{\text{inlet}}$  and  $H_{\text{outlet}}$  are the humidities (kg-water kg-dry-air<sup>-1</sup>) at the air inlet and outlet, respectively. *G* (kg-dry-air  $m^2$  h<sup>-1</sup>) and  $A_b$  (m<sup>2</sup>) are as described in Sect. 18.4.3.

For an overall energy balance on a bioreactor, the rate of heat removal due to evaporation will then be:

$$
Q_{conv} = \lambda G A_b (H_{outlet} - H_{inlet}).
$$
\n(18.18)

However, as before, for beds that are not well mixed, it is often of more interest to write balances that allow the calculation of the temperature and humidity as functions of the position within the bed. In this case, a balance equation is written over a thin layer of the bed. The approach is different depending on whether the

solids and gas phases are treated as different phases or are lumped together and treated as a pseudo-homogenous phase.

#### *18.5.2.1 Solids and Gas Treated as Separate Phases*

If the solids and gas are treated as separate phases, then the convective flow term within the mass balance equation for water will appear as:

$$
R_{conv} = G A_b \frac{dH}{dz} \Delta z \,,\tag{18.19}
$$

since the humidity difference (kg-water kg-dry-air<sup>-1</sup>) between the inlet and outlet of this thin layer is simply the humidity gradient  $(dH/dz, kg$ -water kg-dry-air<sup>-1</sup> m<sup>-1</sup>) multiplied by the thickness of the thin layer  $(\Delta z, m)$ .

Typically during the manipulations of the water balance equation, it will be divided through by the volume of the thin layer, such that the term will appear without containing  $A_b$  and  $\Delta z$ . Note also that if the humidity at the outlet of the thin layer is higher than the humidity at the inlet of the thin layer, then the flow of air will be reducing the humidity of the thin layer, and therefore this term will be preceded by a negative sign if it appears on the right hand side of an equation such as Eq. (18.3). In fact, it is often put on the left hand side of the balance equation.

Note that evaporation removes energy from the solids and not from the air phase. Energy removal from the solids phase, which does not flow, has already been taken into account by Eq. (18.16). Therefore the energy balance on the air phase will not contain a term of the form of Eq. (18.19) multiplied by the enthalpy of evaporation.

#### *18.5.2.2 Solids and Gas Treated as a Pseudo-Homogeneous Phase*

When the assumption is made that the air is always saturated at the temperature of the solids (i.e., the assumption of a pseudo-homogeneous bed), the rate of evaporation  $(R_{evan}$ , kg-H<sub>2</sub>O h<sup>-1</sup>) is still written in the form of Eq. (18.19). In this case the rate of evaporative heat removal is given by

$$
Q_{evap} = \lambda G A_b \frac{dH_{sat}}{dz} \Delta z \,. \tag{18.20}
$$

This is not inconsistent with Sect. 18.5.2.1, since Eq. (18.16) is not used when the assumption of a pseudo-homogeneous bed is made. Further, even though evaporation removes the energy from the solids and not the gas, this makes no difference since the solids and gas are assumed to equilibrate immediately to the same temperature. The Antoine equation can be used to calculate the saturation humidity (*Hsat*) as a function of temperature, so it is useful to apply the chain rule of differentiation to cause the term " $dH_{sal}/dT$ " to appear explicitly in the equation:

$$
\frac{dH_{sat}}{dz} = \frac{dH_{sat}}{dT} \frac{dT}{dz}.
$$
\n(18.21)

Substituting Eq. (18.21) into Eq. (18.20) gives:

$$
Q_{evap} = \lambda G_{air} A_b \frac{dH_{sat}}{dT} \frac{dT}{dz} \Delta z \,. \tag{18.22}
$$

An equation relating  $dH_{\text{sat}}/dT$  to the temperature is developed in Sect. 19.4.1.

# **18.6 Conclusions**

This chapter has identified the forms of various terms that may appear within the balance/transport sub-model of a bioreactor model. Several of these will appear in energy and mass balances in the mathematical models of bioreactors presented in Chaps. 22 to 25. These equations contain various parameters that it will be necessary to determine before the model can be solved. Chapters 19 and 20 describe how these and other necessary parameters can be determined.

# **Further Reading**

*Selected examples from the SSF literature in which models are developed that describe the various heat and mass transfer phenomena described in this chapter. These models therefore contain terms similar to those shown in this chapter*

- Mitchell DA, von Meien OF (2000) Mathematical modeling as a tool to investigate the design and operation of the Zymotis packed-bed bioreactor for solid-state fermentation. Biotechnol Bioeng 68:127–135
- Mitchell DA, Tongta A, Stuart DM, Krieger N (2002) The potential for establishment of axial temperature profiles during solid-state fermentation in rotating drum bioreactors. Biotechnol Bioeng 80:114–122
- Oostra J, Tramper J, Rinzema A (2000) Model-based bioreactor selection for large-scale solid-state cultivation of *Coniothyrium minitans* spores on oats. Enz Microbial Technol 27:652–663
- Rajagopalan S, Modak JM (1994) Heat and mass transfer simulation studies for solid-state fermentation processes. Chem Eng Sci 49:2187–2193
- Saucedo-Castañeda G, Gutierrez-Rojas M, Bacquet G, Raimbault M, Viniegra-Gonzalez G (1990) Heat transfer simulation in solid substrate fermentation. Biotechnol Bioeng 35:802–808
- Stuart DM, Mitchell DA (2003) Mathematical model of heat transfer during solid-state fermentation in well-mixed rotating drum bioreactors. J Chem Technol Biotechnol 78:1180–1192
- Weber FJ, Oostra J, Tramper J, Rinzema A (2002) Validation of a model for process development and scale-up of packed-bed solid-state bioreactors. Biotechnol Bioeng 77:381– 393

*Basic and easy to read introductions to the modeling of heat and mass transfer in bioprocessing* 

- Van Den Akker HEA, Heijnen JJ, Leach CK, Mudde RF (1992) Bioprocess Technology, Modelling and Transport Phenomena. Butterworth Heinemann, Oxford.
- Johnson AT (1998) Biological process engineering: an analogical approach to fluid flow, heat transfer, and mass transfer applied to biological systems. John Wiley & Sons, New York.

*Introductions to heat and mass transfer phenomena (not in the context of bioprocesses)*

- Thomson WJ (2000) Introduction to transport phenomena. Prentice Hall, Upper Saddle River
- Brodkey RS, Hershey HC (2003) Transport Phenomena: A Unified Approach, vols. 1 and 2. Brodkey Publishing, Columbus, Ohio

*Overview of approaches to modeling heat and mass transfer in SSF bioreactors*

Mitchell DA, von Meien OF, Krieger N (2003) Recent developments in modeling of solidstate fermentation: heat and mass transfer in bioreactors. Biochem Eng J 13:137–147