The effects of diffusion and viscosity on ruminant faecal excretion of markers in a simple compartmental model

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Using equations obtained in a previous analysis, results are computed numerically which illustrate the effects of diffusion and viscosity on faecal excretion patterns of markers in ruminants. Results are first given for plug flow, a velocity gradient produced by viscosity, and diffusion, each mechanism operating alone. Plug flow gives a period during which no marker appears in the faeces, then a sharp increase in faeces marker concentration, followed by rapid washout. A velocity gradient gives a more gradual appearance of marker in the faeces followed by a slower washout. Diffusion alone (although not realistic for ruminant marker kinetics) can give early appearance of marker followed by slow washout. Combining diffusion with a velocity gradient produced by viscosity can give a range of behaviour, depending on the effective diffusion coefficient, D'; an approximate method is used to compute these solutions. Because plug flow with no velocity gradient plus diffusion gives results similar to convective flow with a velocity gradient plus diffusion, we believe it will not be possible to determine the main mechanisms defining marker outflow patterns from observations of marker kinetics alone, and more detailed investigations will be needed. Although estimates of quantities such as mean transit time are unaffected by detailed mechanism, the interpretations of measures such as sigmoidicity, sharpness of the faecal marker concentration $v.$ time curve, and length and nature of the washout tail are highly dependent on mechanism.

Ruminants: Digesta markers: Compartmental model: Diffusion: Viscosity

The use of digesta markers in ruminants provides a well-established methodology for investigating the dynamics of the ruminant digestive tract (e.g. Faichney, 1975; France *et al.* 1988). The technique involves oral or direct application of an indigestible, non-absorbable marker to the rumen, with the subsequent measurement of the time course of marker concentration in the faeces and often that of the accumulated marker excretion. Compartmental analysis is then usually used to interpret these data, and a number of compartmental models have been proposed and characterized for this purpose. The models are of the sequential irreversible type (reviewed by France *et al.* 1985, 1988), and they permit the estimation of biological measures such as the rate of passage out of the rumen, the transit time in the gastrointestinal (GI) tract, and the rate of faecal production.

The GI tract is usually represented by a series of well-mixed pools connected by simple plug flows with first-order kinetics applying throughout. Diffusion and viscosity are neglected and their importance has not been assessed quantitatively. Recently, France *et al.* (1993) introduced diffusion and viscosity into the traditional formalism and, while they derived integral equations for the solutions, they were unable to make further progress analytically. Our objective here is to compute numerical solutions for the scheme incorporating diffusion and viscosity proposed by France *et al.* (1993), and to illustrate the qualitative and quantitative effects of these processes. This enables us to compare and contrast model predictions with results obtained from experiment, leading to an improved understanding of how these physical mechanisms, which seem certain to impinge on nutrition, may affect faecal marker curves.

Blaxter *et al.* (1956) suggested that the ruminant gut is essentially composed of two mixing compartments and a tubular compartment, and that digesta flow can be described by a model consisting of two exponential components and a discrete time delay. Subsequently, Grovum & Williams (1973) used this model to describe the change in marker concentration in sheep faeces following an intraruminal dose of marker and showed that the longer mean residence time was associated with the rumen. Other workers, however, have encountered difficulties in fitting this model to faecal marker excretion curves, particularly in cases where a slow initial increase in faecal marker concentration was evident. Milne *et al.* (1978) and Faichney & Boston (1983) both increased the number of mixing pools in Blaxter's scheme to three in order to describe their data satisfactorily.

This slow initial increase in marker concentration prompted Ellis *et al.* (1979) to suggest the inclusion of a γ time dependency of two in the faster rate constant of Blaxter's model. The introduction of a time dependency of two into the model is in essence representing the GI tract by three mixing pools and a discrete delay with two contiguous pools having the same rate constant (France *et al.* 1985). Whilst this 'time-dependent, time-independent' model was found to be superior to the original Blaxter model and its refinement by Milne *et al.* (1978) and Faichney & Boston (1983), Dhanoa *et al.* (1985) found it sensitive to initial data points and not always able to give good agreement between the predicted and observed concentrations in the ascending phase of the curve. This prompted these workers to propose and examine an alternative model (Dhanoa *et al.* 1985, 1989).

The scheme of Dhanoa *et al.* (1985) for describing faecal marker concentration curves is based on the premise that the ruminant GI tract can be represented by an unspecified number of exponential compartments with the pattern of marker excretion being largely defined by events occurring in the two compartments having the smallest rate constants (i.e. k_1 and k_2). In order to reduce the number of parameters so as to facilitate parameter estimation, the assumption was made that the rate constants of all other compartments increase successively by a small constant amount (i.e. $k_2 - k_1$). To facilitate estimation further, a mathematical approximation was introduced which resulted in a double exponential form of the model. A logarithmic transformation of this form was fitted to eighty-two excretion curves and was found to be superior to the other models (Dhanoa *et al.* 1985).

All models are compromises between the prevailing state of knowledge and mathematical feasibility given the constraints and quality of observed data. The modelling process may lead to data-analysis models, whether empirical or mechanistic, which can play an important role in nutritional research. However, it is necessary to show that these models represent mechanisms which for example control the postruminal flow of digesta through the GI tract. Diffusion and viscosity are processes which seem likely to affect nutrient absorption and utilization in ruminants, and are thus worth investigating to see if they contribute to the observed patterns of marker concentration in faecal samples.

Unfortunately the incorporation of these concepts into models leads to intractable mathematics as outlined by France *et al.* (1993). A way round these difficulties requires the use of numerical methods so that we can study the effects of these mechanisms on what might be observed. Such an investigation may provide corroboration and define the scope of data-analysis models which may be more realistic in other respects.

COMPARTMENTAL MODEL AND GENERAL THEORY

The scheme used is shown in Fig. 1. Compartment 1 is assumed to be well-mixed and represents the proximal tract including the rumen. It is well known that both particle size and density affect rumen outflow (e.g. Kaske *et al.* 1992), and this simplification is justified here by the impossibility of studying all possible complexities at once. Compartment 2 represents the distal tract including the intestines; it is approximated by a cylinder of length L and radius R through which transport of marker may occur by convective flow with mean velocity $\bar{U}$ (see Table 1 for definition of symbols, units and standard or initial values). It is assumed that the fluid in the system is incompressible and the compartment volumes do not change. The mean transit time of compartment 2 is $\bar{\tau}$, with

$$\bar{\tau} = \frac{L}{\bar{U}}. \tag{1a}$$

There may be a velocity gradient within the cylinder (velocity U is a function of radius r); also diffusion can occur, and the diffusion coefficients may be enhanced by turbulent mixing. Compartment 1 has volume V_1; it contains mass of marker X_1 which has concentration C_1. Concentration and mass are related by

$$C_1 = \frac{X_1}{V_1}. \tag{1b}$$

It is assumed that the volume V_1 is constant (the fluid input flux to compartment 1 is therefore equal to the flux from compartment 1 which is $\pi R^2 \bar{U}$), so that

$$\frac{dC_1}{dt} = \frac{1}{V_1} \frac{dX_1}{dt}. \tag{1c}$$

A single dose of marker, Δ, is administered to the rumen at time $t = 0$, so that the initial value of C_1 is

$$C_1(t = 0) = \frac{\Delta}{V_1}. \tag{1d}$$

A system of cylindrical polar axes with radius r and distance along the axis x is assigned to compartment 2. Assuming that the tranverse and longitudinal diffusivities (D_t, D_l) are constant (do not vary with position or time), and denoting the flow velocity at radius r as $U(r)$, the equation governing the concentration $C_2(x, r, t)$ in compartment 2 at position (x, r) and time t is

$$\frac{\partial C_2}{\partial t} = D_l \frac{\partial^2 C_2}{\partial x^2} + D_t \left(\frac{\partial^2 C_2}{\partial r^2} + \frac{1}{r} \frac{\partial C_2}{\partial r} \right) - U(r) \frac{\partial C_2}{\partial x}. \tag{1e}$$

Essentially this is the continuity equation in the absence of chemical reactions that might produce or remove marker. The first two terms on the right represent the diffusive movement of marker and the last term the convective movement.

The boundary conditions are assumed to be

$$C_2(0 < x < L, r, t = 0) = 0, \quad C_2(x = 0, r, t) = C_1(t), \quad C_2(x = L+, r, t) = 0. \tag{1f}$$
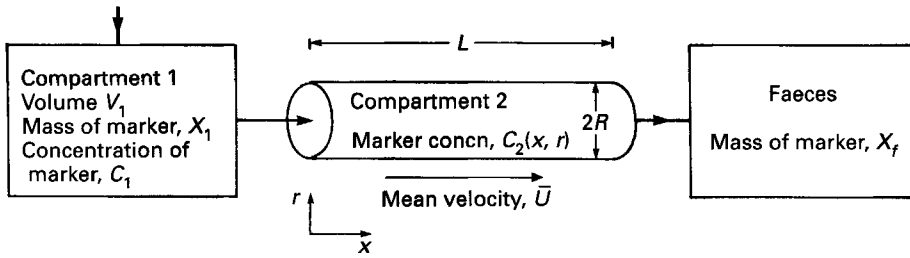
Fig. 1. Two-compartment representation of the ruminant gastrointestinal tract. Compartment 1 is a well-mixed pool described by the quantities shown. Compartment 2 is a cylinder of length L and radius R whose contents move at a mean velocity of $\bar{U}$. The faeces are external to the tract.

Table 1. *Definitions of principal symbols and numerical values*

(The number(s) of the equation(s) where the symbol is introduced is given in parentheses)

Symbol	Definition	Initial value, Standard value and units
	Independent variables	
r	Radial (transverse) coordinate in compartment 2	cm
t	Time variable	h
x	Axial (longitudinal) coordinate in compartment 2	cm
	State variables	
$C_2(x, r, t)$	Marker concentration at position (x, r) in compartment 2 $(1e)$	0 mg/cm³
$C_{2,J}(t)$	Marker concentration in Jth element of compartment 2 $(4b)$	0 mg/cm³
$X_f(t)$	Mass of marker in faeces (Fig. 1)	0 mg
$X_1(t)$	Mass of marker in compartment 1 (Fig. 1, $1n$)	Δ mg
	Other variables	
$C_1(t)$	Marker concentration in compartment 1 $(1b)$	mg/cm³
$C_{2\rightarrow f}(t)$	Mean concentration of marker flowing to faeces $(1l)$	mg/cm³
$\hat{c}_{2\rightarrow f}(t)$	Mean faecal concentration of marker flowing to faeces $(1m)$	mg/g faeces dry matter
F_J	Marker flux per unit area into Jth element of compartment 2 $(4b, 4d, 4e)$	mg/cm² per h
$O_{1\rightarrow 2}, O_{2\rightarrow f}$	Output marker fluxes from compartment 1 into 2, and from compartment 2 to faeces $(1g, 1h)$	mg/h
$r_{max}(t)$	Maximum radius of material reaching faeces $(3g)$	cm
$U(r)$	Velocity of fluid at radius r in direction x (Fig. 1)	cm/h
$\tau(r)$	Transit time at radius r $(3b)$	h
	Parameters and derived parameters	
A	Cross-sectional area of compartment 2 $(5d)$	3·142 cm²
D_l, D_t	Longitudinal and transverse diffusivities $(1e)$	10000 cm²/h
D'	Effective diffusion coefficient $(5c)$	10000 cm²/h
k	Passage rate from compartment 1 $(2b)$	0·2 h
L	Length of compartment 2 (Fig. 1)	1000 cm
P_f	Rate of faeces production $(1k)$	157·1 g faeces/h
R	Radius of compartment 2 (Fig. 1)	1 cm
$\bar{U}$	Mean flow velocity through compartment 2 (Fig. 1, $1j$)	100 cm/h
V_1	Volume of compartment 2 (Fig. 1)	1571 cm³
$V_{1\rightarrow 2}, V_{2\rightarrow f}$	Volume flux from compartment 1 into compartment 2, and from compartment 2 to faeces $(1j)$	314·2 cm³/h
Δ	Marker dose applied to compartment 1 at $t = 0$	100 mg
ρ_f	Faecal density $(1k)$	0·5 g faeces DM/cm³
$\bar{\tau}$	Mean transit time of compartment 2 $(1a)$	10 h

The first states that at time zero compartment 2 is empty. The second states that the concentration on the input surface is constant and equal to that in compartment 1. The third states that the concentration on the output surface (at $x = L +$ a small increment) is zero: the faeces are quickly removed from the end of the GI tract, and there is no possibility of movement of marker from the faeces pool back into the tract.

The output flux of marker from compartment 1 into compartment 2 at time t, $O_{1\to2}(t)$, is obtained by integrating the convective and diffusion fluxes over an annular element of the input surface to compartment 2 of area $2\pi r dr$, to give (using Fick's first law of diffusion)

$$O_{1\to2}(t) = 2\pi \int_0^R \left[U(r)\, C_1(t) - D_i \frac{\partial C_2}{\partial x}(x = 0, r, t) \right] r\, dr. \tag{1g}$$

Similarly, the output flux of marker from compartment 2 to faeces is

$$O_{2\to f}(t) = 2\pi \int_0^R \left[U(r)\, C_2(x = L, r, t) - D_i \frac{\partial C_2}{\partial x}(x = L, r, t) \right] r\, dr. \tag{1h}$$

The differential equation for the mass of marker in compartment 1 is

$$\frac{dX_1(t)}{dt} = -O_{1\to2}(t). \tag{1i}$$

The volume flow rates from compartment 1 to 2, and from compartment 2 to faeces, $V_{2\to f}$, are equal and independent of time, with

$$V_{1\to2} = V_{2\to f} = 2\pi \int_0^R U(r)\, r\, dr = \bar{U}\pi R^2, \tag{1j}$$

where the mean fluid velocity, $\bar{U}$ is defined. The rate of faeces production, P_f, is

$$P_f = \bar{U}\pi R^2 \rho_f = V_{2\to f}\rho_f, \tag{1k}$$

where ρ_f is the faecal density.

The mean concentration of marker in the fluid flowing to faeces, $C_{2\to f}(t)$, is

$$C_{2\to f}(t) = \frac{O_{2\to f}(t)}{V_{2\to f}}. \tag{1l}$$

The mean faecal concentration of marker in units of mg marker/g DM of faeces in the output from compartment 2, $\hat{c}_{2\to f}(t)$, is

$$\hat{c}_{2\to f}(t) = \frac{C_{2\to f}(t)}{\rho_f} = \frac{O_{2\to f}(t)}{P_f}. \tag{1m}$$

The rate of change of marker accumulated in the faeces is

$$\frac{dX_f}{dt} = O_{2\to f}(t) = \hat{c}_{2\to f}(t)\, P_f. \tag{1n}$$

PLUG FLOW

It is assumed that the wall of compartment 2 (Fig. 1) is perfectly smooth; there is no velocity gradient across the tube; diffusion is ignored. Equation 1g with $U(r) = \bar{U}$ and $D_i = 0$ gives

$$O_{1\to2}(t) = \pi R^2 \bar{U} C_1(t). \tag{2a}$$

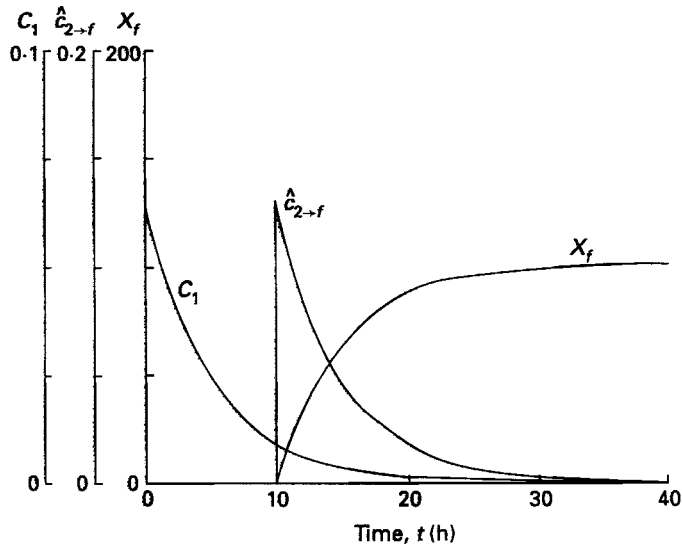Fig. 2. Plug flow, C_1 (mg cm³) is the marker concentration in compartment 1 (Fig. 1, equation 2c). Also shown are: the faecal concentration of marker in the output from compartment 2 to faeces, $\hat{c}_{2 \to f}$ (mg/g faeces dry matter, equation 2f); and total marker accumulated in faeces, X_f (mg, equation 2g). Parameters are as in Table 1, but with the diffusion constants set to zero and for perfectly smooth walls.

Combining equations 1i, 2a and 1c, therefore,

$$\frac{dC_1}{dt} = -kC_1, \quad \text{where} \quad k = \frac{\pi R^2 \bar{U}}{V_1}. \tag{2b}$$

This gives a decay or passage rate of $k = 0.2/h$ (inserting parameter values from Table 1; the parameter values in Table 1 are rounded values, and have not been adjusted for any particular situation or animal). The concentration in compartment 1 is

$$C_1(t) = \frac{\Delta}{V_1} e^{-kt}. \tag{2c}$$

For plug flow with transit time τ, the output from compartment 2 at time t is simply what entered compartment 2 at time $t - \tau$, giving

$$C_2(x = L, r, t) = C_2(x = 0, r, t - \tau). \tag{2d}$$

With equation 1h, the flux of marker to faeces is

$$O_{2 \to f}(t) = \pi R^2 \bar{U} C_2(x = L, r, t) = \pi R^2 \bar{U} C_2(x = 0, r, t - \tau) \quad \text{for} \quad t \geqslant \tau. \tag{2e}$$

With equations 1m, 1f, 2c and 2b, the faecal marker concentration is

$$\hat{c}_{2 \to f}(t) = \frac{k\Delta}{P_f} e^{-k(t - \tau)}, \quad t \geqslant \tau. \tag{2f}$$

The total marker mass accumulated in faeces is obtained by equation 1n, to give

$$X_f(t) = \Delta(1 - e^{-k(t - \tau)}), \quad t \geqslant \tau. \tag{2g}$$

This is illustrated in Fig. 2. The temporal distribution of marker concentration in compartment 1 (C_1) is reproduced in the output to faeces with a time delay of τ. In the

Discussion section, Table 2 and Fig. 7 comparisons are made between the plug flow mechanism and other mechanisms, and with observed responses.

VELOCITY GRADIENT

It is assumed that the walls of compartment 2 are rough so that the fluid in contact with the wall is stationary; diffusion is ignored. The velocity at radius r, $U(r)$, is assumed to be given by (e.g. Newman & Searle, 1948)

$$U(r) = 2\bar{U}\left(1 - \frac{r^2}{R^2}\right). \tag{3a}$$

Thus with equation $3a$ the velocity at the centre ($r = 0$) is twice the mean velocity $\bar{U}$ and decreases parabolically to zero at the walls ($r = R$). Transit time τ is a function of radius r:

$$\tau(r) = \frac{L}{U(r)} = \frac{L}{2\bar{U}(1 - r^2/R^2)}. \tag{3b}$$

The output from compartment 1 (equation $1g$) gives the same result as for plug flow ($2a$) (as it must), with (substituting $3a$ into $1g$ and putting $D_t = 0$)

$$O_{1\to2}(t) = 2\pi \int_0^R \left[2\bar{U}\left(1 - \frac{r^2}{R^2}\right)C_1(t)\right] r\, dr = \pi R^2 \bar{U} C_1(t). \tag{3c}$$

Therefore equations $2b$ and $2c$ still apply.

Combining equations $1h$, $2d$ and $3a$, in the absence of diffusion, the output marker flux to faeces is

$$O_{2\to f}(t) = 2\pi \int_0^R \left[2\bar{U}\left(1 - \frac{r^2}{R^2}\right)C_2(x = 0, r, t - \tau)\right] r\, dr. \tag{3d}$$

Since (with equations $1f$ and $2c$)

$$C_2(x = 0, r, t - \tau) = C_1(t - \tau) = \frac{\Delta}{V_1} e^{-k(t-\tau)}, \quad t \geqslant \tau, \tag{3e}$$

therefore using equations $1m$, $3d$, $3e$ and $3b$ the mean faecal concentration of marker in the output from compartment 2 (mg marker/g faeces DM) is

$$\hat{c}_{2\to f}(t) = \frac{4\pi \bar{U} \Delta e^{-kt}}{V_1 P_f} \int_0^{r_{max}(t)} \exp\left(\frac{kL}{2\bar{U}(1 - r^2/R^2)}\right)(1 - r^2/R^2)\, r\, dr. \tag{3f}$$

$r_{max}(t)$ is the radius of the annulus of material which just reaches the faeces compartment at time t, that is, when the transit time τ is equal to the actual time t. From equation $3b$, $t = L/[2\bar{U}(1 - r_{max}^2/R^2)]$, giving

$$r_{max} = R\sqrt{\left(1 - \frac{L}{2\bar{U}t}\right)}. \tag{3g}$$

The last two equations can only be used for times $t \geqslant t_v$, where t_v is the time at which the fastest moving axial ($r = 0$) component of the distribution exits from compartment 2, where
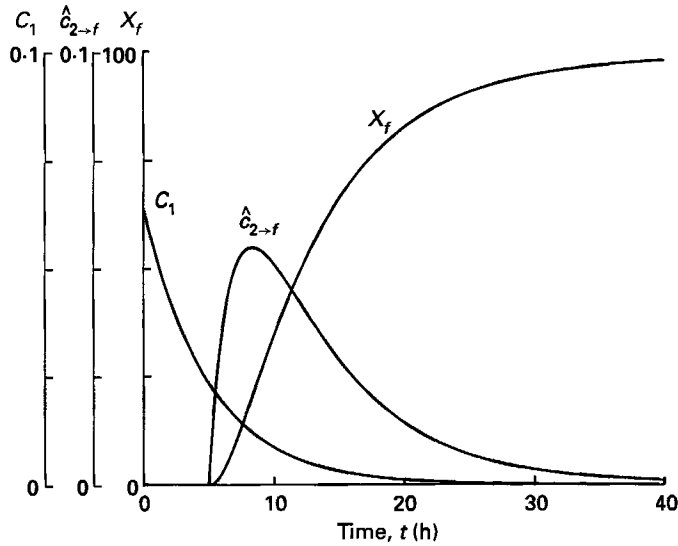
$$t_v = \frac{L}{2\bar{U}}. \tag{3h}$$

Fig. 3. Viscous flow with a velocity gradient. C_1 (mg cm³) is the marker concentration in compartment 1 (Fig. 1, equation 2c). Also shown are: the faecal concentration of marker in the output from compartment 2 to faeces, $\hat{c}_{2\to f}$ (mg/g faeces dry matter; equation 3f); and total marker accumulated in faeces, X_f (mg, equation 1n with 3f). Parameters are as in Table 1, but with the diffusion constants set to zero and for rough walls in compartment 2. n 100 (equation 3k). Integration interval 0·2 h.

To evaluate the mean faecal concentration of marker flowing to the faeces, $\hat{c}_{2\to f}(t)$, we write

$$\hat{c}_{2\to f}(t) = g(t) \int_0^{r_{\max}(t)} h(r)\,dr, \qquad (3i)$$

which defines

$$g(t) = \frac{4\pi \bar{U} \Delta e^{-kt}}{V_1 P_f}, \quad h(r) = \exp\left(\frac{kL}{2\bar{U}(1-r^2/R^2)}\right)(1-r^2/R^2)\,r. \qquad (3j)$$

$r_{\max}$ is divided into n segments each of length $\Delta r_{\max}$, so that

$$r_j = j\Delta r_{\max}, \quad j = 0, 1, 2, \dots, n; \quad r_{\max} = n\Delta r_{\max}. \qquad (3k)$$

For numerical integration we use the trapezium rule approximation to evaluate the mean faecal marker concentration:

$$\hat{c}_{2\to f}(t) = g(t)\,\Delta r_{\max}[\tfrac{1}{2}h(r_0) + h(r_1) + \dots + h(r_{n-1}) + \tfrac{1}{2}h(r_n)]. \qquad (3l)$$

Equation 1n is applied to give the rate of change in mass of faecal marker, $X_f(t)$, by substituting $\hat{c}_{2\to f}(t)$ from equation 3l and the value of the parameter P_f (Table 1). Numerical integration of this rate of change from an initial value of zero provides the accumulated mass of faecal marker.

Fig. 3 illustrates the time course of marker concentration in compartment 1 (C_1), the mean faecal marker concentration leaving compartment 2 ($\hat{c}_{2\to f}(t)$) and the accumulated faecal marker mass ($X_f(t)$). Comparing Fig. 3 for purely viscous flow with Fig. 2 for plug flow, it is seen that the maximum in the faecal marker concentration occurs at 8·4 h for a mean fluid transit time of 10 h, and that the accumulated marker mass in faeces now shows a slight sigmoid increase. Other comparisons are made in the Discussion section, Table 2 and Fig. 7.

DIFFUSION

With no bulk flow through compartment 2, velocity $U(r) = 0$, and there is no radial dependence of marker concentration. Equation $1e$ becomes

$$\frac{\partial C_2}{\partial t} = D_i \frac{\partial^2 C_2}{\partial x^2}. \tag{4a}$$

Compartment 2 is divided into n_L elements, each of length $\Delta L = L/n_L$, volume $\Delta V = \pi R^2 \Delta L$, and where the marker concentration at time t is $C_{2,J}(t)$, $J = 1, \ldots, n_L$. The flux per unit area of marker out of compartment 1 and into the first element of compartment 2 is assumed to be

$$F_1 = \frac{D}{\Delta L/2}(C_1 - C_{2,1}). \tag{4b}$$

This is a statement of Fick's first law of diffusion; the factor of 2 arises because the distance from compartment 1 to the midpoint of the first element in compartment 2 is $\Delta L/2$. Thus the rate of change of marker concentration in compartment 1 is

$$\frac{\mathrm{d}C_1}{\mathrm{d}t} = -\pi R^2 \frac{F_1}{V_1}. \tag{4c}$$

For elements $J = 2, 3, \ldots, n_L$, the flux of marker per unit area from the $J-1$th compartment into the Jth compartment is

$$F_J = \frac{D}{\Delta L}(C_{J-1} - C_J). \tag{4d}$$

Here, the distance between the midpoints of two adjacent elements in compartment 2 is ΔL (cf. equation $4b$). The flux per unit area out of the last (n_Lth) element of compartment 2 to faeces is assumed to be

$$F_{n_L+1} = \frac{D}{\Delta L/2}C_{n_L}. \tag{4e}$$

A factor of 2 arises again as in $4b$. It is assumed that the faeces are rapidly removed from the end of the GI tract, with an effective faecal marker concentration just outside the GI tract of zero (see $1f$), so that there is no movement of marker from the faeces pool back into the tract. The rates of change of concentrations in the $J = 1, 2, \ldots, n_L$ elements of compartment 2 which each have volumes of $\pi R^2 \Delta L$ are

$$\frac{\mathrm{d}C_{2,J}}{\mathrm{d}t} = \frac{1}{\Delta L}(F_J - F_{J+1}). \tag{4f}$$

With the assumption of zero bulk flow, the concentration of marker entering the faeces compartment is not a meaningful quantity, since there is no movement of faeces from GI tract into the faeces compartment accompanying the diffusive outflow of marker into the faeces compartment. The rate of change of marker mass in the faeces compartment is

$$\frac{\mathrm{d}X_f}{\mathrm{d}t} = \pi R^2 F_{n_L+1}. \tag{4g}$$

In Fig. 4 the marker concentration in compartment 1 (C_1), that in the last element of compartment 2 ($C_{2,J}, J = n_L$), and the accumulated mass of marker in the faeces (X_f) are shown. In Fig. 4(a), where diffusion constant $D = 100000$ cm^2/h, there is a delay of 1–2 h
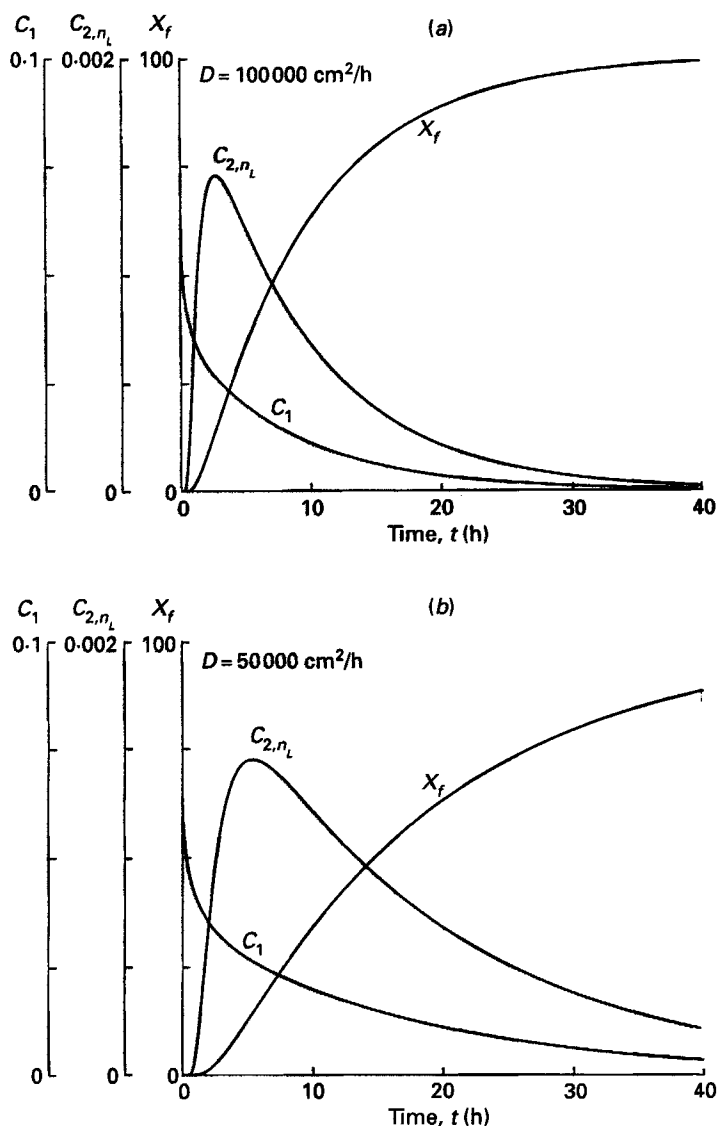
Fig. 4. Diffusion without convective flow. C_1 (mg/cm^3) is the marker concentration in compartment 1 (Fig. 1, equation 4c). Also shown are: the concentration of marker in the output from compartment 2 to faeces (C_{2,n_L}, mg/cm^3, equation 4f); and total marker accumulated in the faeces, X_f (mg, equation 4g). Parameters are as in Table 1, but with the convective velocity $U(r)$ set to zero. (a) Diffusion constant, $D = 100000$ cm^2/h; number of elements in compartment 2, $n_L = 10$; integration interval, $\Delta t = 0.02$ h. (b) Diffusion constant, $D = 50000$ cm^2/h.

before marker appears at the end of compartment 2, and the total amount of marker in the faeces reaches half its asymptotic value of 100 mg in about 7·5 h. In Fig. 4(b), D is reduced to 50000 cm^2/h; this doubles the time lag before marker begins to appear at the end of compartment 2, and also the time taken for the total faeces marker to reach half its asymptotic value. The results are not materially changed by taking twice the number of elements in compartment 2 and one quarter of the integration interval. The emptying of compartment 1 is rather different with pure diffusion than for plug flow or convective flow with a velocity gradient (Figs. 2 and 3); it is faster initially but slower in the later stages.

Note that, for stable integration, the integration interval, Δt, must be of the order of, or less than, $\Delta L^2/4D$. This result is equivalent to requiring that the amount of substance moving out of an element during time Δt to an adjacent element where the concentration is zero is less than 25% of the amount of substance in the first element: that is, area × concentration gradient × $\Delta t < \frac{1}{4}$ volume × concentration, or $AD(C/\Delta L)\Delta t < \frac{1}{4}A(\Delta L)C$, giving the result above. If Δt is greater than this value, there are damped oscillations, sustained oscillations, or exponentially growing oscillations.

DIFFUSION AND VISCOSITY: AN APPROXIMATE TREATMENT

Assuming a parabolic velocity profile as in equation $3a$, the general equation for the concentration in compartment 2 ($1e$), $C_2(x, r, t)$, becomes

$$\frac{\partial C_2}{\partial t} = D_l \frac{\partial^2 C_2}{\partial x^2} + D_t\left(\frac{\partial^2 C_2}{\partial r^2} + \frac{1}{r}\frac{\partial C_2}{\partial r}\right) - 2\bar{U}\left(1 - \frac{r^2}{R^2}\right)\frac{\partial C_2}{\partial x}. \qquad (5a)$$

Taylor (1953) showed that if compartment 2 is sufficiently long that mixing occurs across the flow then the mean concentration across a transverse section at position x, $C_{2,tm}(x, t)$, obeys the equation

$$\frac{\partial C_{2,tm}}{\partial t} = D'\frac{\partial^2 C_{2,tm}}{\partial x^2} - \bar{U}\frac{\partial C_{2,tm}}{\partial x}. \qquad (5b)$$

The effective longitudinal diffusion coefficient D', is given by

$$D' = D_l + D_\infty, \quad D_\infty = \frac{\bar{U}^2 R^2}{48D_t}. \qquad (5c)$$

This equation describes an additional term in the effective longitudinal diffusion coefficient of D_∞, arising from the longitudinal dispersion caused by the velocity gradient. We use this approximation to estimate the combined effects of longitudinal and transverse diffusion with a velocity gradient (see also Smith, 1990).

It is assumed that the marker concentration in compartment 1, $C_1(t)$, falls as a simple negative exponential as in $2c$ (but see Fig. 4 where the initial decline in C_1 is faster than a negative exponential), and this defines the marker concentration at $x = 0$ in compartment 2. Using equations 4.1 and 4.2 of France et al. (1993), the mean marker concentration (mg marker/cm³) flowing to faeces is equal to that at the distal end of compartment 2 ($x = L$) which is

$$C_{2\to f}(t) = C_{2,tm}(x = L, t) = \int_0^t \frac{k\Delta}{A}e^{-kt'}\frac{\exp\{-[L - \bar{U}(t - t')]^2/4D'(t - t')\}}{[4\pi D'(t - t')]^{\frac{1}{2}}}\,dt'. \qquad (5d)$$

Cf. France et al. (1993), equation 4.9. Here cross-sectional area $A = \pi R^2$ and $k = A\bar{U}/V_1$; t' is a dummy variable of integration. The faecal marker concentration is (dividing by faecal density)

$$\hat{c}_{2\to f}(t) = \frac{C_{2\to f}(t)}{\rho_f}. \qquad (5e)$$

To calculate numerical solutions for faecal marker concentration, we use the trapezium rule approximation

$$f(t) = \int_0^t y(t')\,dt', \qquad (5f)$$

$$f(t) = \Delta t(\tfrac{1}{2}y_0 + y_1 + y_2 + \ldots + y_j + \ldots + y_{i-2} + y_{i-1} + \tfrac{1}{2}y_i), \qquad (5g)$$

where $i\Delta t = t$, $j\Delta t = t'$ and $y_j = y(t') = y(j\Delta l)$, $j = 0, 1, 2, \ldots, i-1, i$. The faecal marker concentration is written as (combining equations $5d$ and $5e$)

$$\hat{c}_{2 \to f}(t) = \int_0^t y(t') \, dt' = \int_0^t g(t') h(t-t') \, dt', \qquad (5h)$$

where

$$g(t') = \frac{k\Delta}{\rho_f A} e^{-kt'}, \quad h(t-t') = \frac{\exp\{-[L - \bar{U}(t-t')]^2/4D'(t-t')\}}{[4\pi D'(t-t')]^{\frac{1}{2}}}. \qquad (5i)$$

To compute the y_j of equation $5g$, we write $y_j = y(t') = g(t') h(t-t') = g_j h_{ij}$, where

$$g_j = \frac{k\Delta}{\rho_f A} e^{-kj\Delta t}, \quad h_{ij} = \frac{\exp\{-[L - \bar{U}\Delta t(i-j)]^2/4D'\Delta t(i-j)\}}{[4\pi D'\Delta t(i-j)]^{\frac{1}{2}}}. \qquad (5j)$$

Denoting the (constant) rate of faeces production by $P_f(1k)$, the total mass of marker accumulated in the faeces, X_f, is

$$X_f(t) = P_f \int_0^f \hat{c}_{2 \to f}(t) \, dt. \qquad (5k)$$

Noting Taylor's expression (1953, equation 16), for the present approximation to apply requires that the transverse diffusion coefficient D_t satisfies

$$D_t \gg \frac{2R^2 \bar{U}}{3 \cdot 8^2 L} = 0 \cdot 014 \text{ cm}^2/\text{h}, \qquad (5l)$$

where the values $R = 1$ cm, $\bar{U} = 100$ cm/h and $L = 1000$ cm have been inserted. In water at 20°, sucrose and albumin have molecular diffusion constants of $0 \cdot 019$ and $0 \cdot 0021$ cm^2/h. These molecular diffusion coefficients are negligible in the present context and do not satisfy $5l$. We therefore assume that diffusion arising from turbulent mixing is dominant and sufficiently large as to satisfy $5l$. A transverse diffusion coefficient of only 1 cm^2/h satisfies $5l$, and this implies that a particle would move 1 cm in an hour which does not seem unreasonable as a minimum value. With the parameter values above, equation $5c$ becomes

$$D' = D_t + \frac{208}{D_t}. \qquad (5m)$$

With $D_t = D_t = D$, therefore,

$$D' = D + \frac{208}{D}. \qquad (5n)$$

In Fig. 5, D' is plotted against D. For low values of D (which also satisfy $5l$), the impact of the additional term on the effective longitudinal diffusion coefficient, D', can be considerable. Over part of the range, increase in D actually reduces effective longitudinal diffusion. While this might seem to be counter-intuitive, it is a result of increasing transverse diffusion reducing the ability of the transverse velocity gradient to produce longitudinal dispersion (which is now represented in the effective longitudinal diffusion coefficient, D'). For diffusion coefficients above 20 cm^2/h the additional term rapidly becomes unimportant. Fig. 6 illustrates solutions for the diffusion/velocity situation with a range of effective diffusion coefficients, D', assuming that Taylor's (1953) approximate method as outlined above is applicable. The marker concentration in compartment 1 (C_1) falls off as in Figs. 2 or 3. Fig. 6(a) gives the faecal marker concentration issuing from compartment 2 and Fig. 6(b) describes the total mass of marker accumulated in the faeces. It can be seen that,
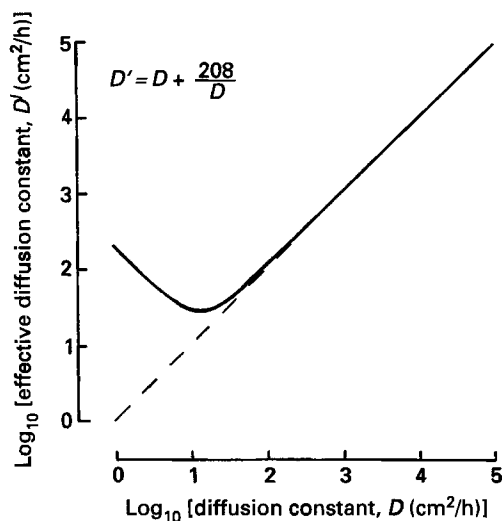
Fig. 5. Effect of a velocity gradient on the effective longitudinal diffusion coefficient, D', which is plotted against the diffusion coefficient, D, according to equation $5n$. It is assumed that the transverse and longitudinal diffusion coefficients are equal (see $5c$). The dashed line is for $D' = D$, in the absence of any contribution from the velocity gradient.

although high diffusion rates favour the early appearance of marker in the faeces, they delay the complete removal of marker from the GI tract. Further comparisons are made in the next section.

DISCUSSION

Some characteristics of the models are summarized in Table 2. Note that the case of plug flow + diffusion has not been explicitly treated: this case is formally identical to the velocity gradient + diffusion case using the Taylor (1953) approximation; to obtain the solutions for plug flow + diffusion, use the solutions of the Diffusion and Viscosity section, replacing the mean velocity $\bar{U}$ by the plug-flow velocity and the effective diffusion constant D' (in equation $5b$ and after) by the diffusion constant. In Table 2 the faecal marker concentration as a percentage of its maximum value which occurs at time $t = t_{max}$ is given for times $\frac{1}{2}t_{max}$ and $2t_{max}$. The $\frac{1}{2}t_{max}$ value is a measure of the sigmoidicity or sharpness of the leading edge of the faecal marker concentration curve. The $2t_{max}$ value is a measure of the rapidity of marker washout. The $\frac{1}{2}t_{max}$ and $2t_{max}$ values provide a two-parameter summary of the shape of the faecal marker concentration v. time curve.

In Table 2 the experimental responses shown in Fig. 7 are also included, with the purpose of seeing if considering the rumen as a mixing compartment and incorporating diffusion/viscosity concepts into movement along the small and large intestines can mimic experimental findings. It should be noted that the numbers given in Table 2 were obtained via the fitted curves of Fig. 7, where the errors are largest towards the edges of the distribution. In Table 2 and Fig. 7 data from both cattle and sheep are included. This gives a variety of observed responses with which to compare the results of the present theoretical investigation. However, for cattle in particular, to approximate the GI tract by the scheme in Fig. 1 may be a very poor approximation. Our sample in Fig. 7 and Table 2 of four faecal marker experiments is only illustrative of the many responses that have been observed.

First, we compare the models. It is clear that plug flow (row 1), a velocity gradient (row 2), and a low effective diffusion coefficient, D', in the velocity gradient + diffusion case (row
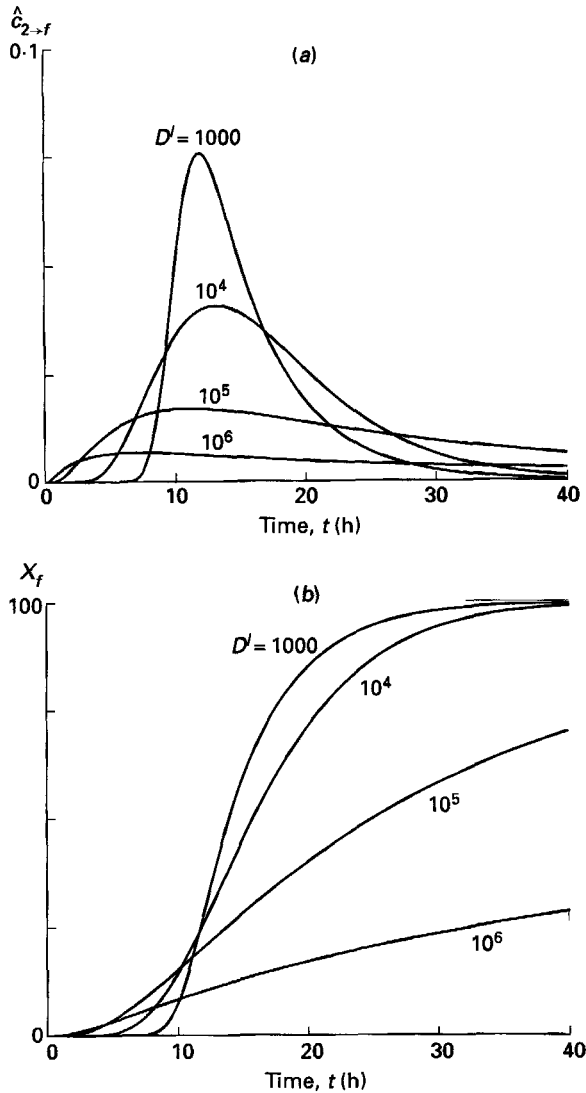
Fig. 6. Diffusion with convective flow and a velocity gradient using Taylor's (1953) approximation. (a) The concentration of marker in the output from compartment 2 to faeces, $\hat{c}_{2 \to f}$ (mg/g faeces dry matter, equation 5e). (b) Total marker accumulated in the faeces, X_f (mg, equation 5k). Parameters are as in Table 1, but with the effective diffusion coefficient, D' (cm^2/h, equation 5c) set to the values indicated. Integration interval, $\Delta t = 0.25$ h.

4) give the sharpest leading edge to the faecal concentration v. time curve. Regarding diffusion alone (row 3) as perhaps being an unrealistic model, slow washout is given by a velocity gradient alone (row 2) or velocity gradient + diffusion with a high effective diffusion coefficient, D' (row 5).

Next when comparing the models with the experiments shown in Fig. 7 and Table 2, it should be remembered that the models apply strictly to soluble markers or cases where the particle markers behave homogenously. Soluble and particulate markers generally behave differently in the rumen but quite similarly in the small and large intestines. The complexities of particle behaviour may invalidate the model as a tool that can be applied

Table 2. *Characteristics of the different models: the faecal marker concentration as a percentage of its maximum value which occurs at time* t_{max} *is given for* $\frac{1}{2}t_{max}$ *and* $2t_{max}$

	Time, $t =$		
	$\frac{1}{2}t_{max}$	t_{max}	$2t_{max}$
Model			
Plug flow (Fig. 2)	0	100	13
Velocity gradient (Fig. 3)	0	100	39
Diffusion (Fig. 4*b*)	68	100	80
Velocity gradient + diffusion* (Fig. 6a):			
$D^{l} = 1000$	0	100	12
$D^{l} = 10000$	34	100	29
Experiment			
Holstein cows, silage†	3	100	3
Brangus steers, molasses + hay‡	20	100	44
Sheep, hay§	65	100	56
Steers, dried grass§	*c.* 2	100	57

* Equivalent to plug flow + diffusion (see p. 759).
† Beauchemin & Buchanan-Smith (1987) used a particulate marker.
‡ Ferreiro Gutierrez (1986) stained feed particles with magenta.
§ R. C. Siddons (unpublished results) used a particulate marker (Cr).

to faecal marker data in its present form. Moreover, the experiments apply to different species where different characteristics apply to the proximal and distal tracts. The Holstein cow data are not obviously compatible with any of the models although plug flow through the rumen itself could provide an explanation. Brangus steers are reasonably close to the velocity gradient + fast diffusion model. Sheep fed on hay appear similar to diffusion only. Steers on dried grass look most like a velocity gradient acting alone. The fact that the observed data cited here and model predictions do not concur suggests that the simple scheme and mechanisms assumed are unable to provide general solutions applicable across species, although this is perhaps not surprising. Nonetheless, the results are interesting and suggest that interpretations of marker data that ignore diffusion and viscosity may be hazardous.

Within its limitations our analysis shows that interpretation of marker data alone allows several possibilities. It may be concluded that the establishment of the important mechanisms depends on detailed observations of diffusion coefficients, velocities, turbulence and mixing within and possibly throughout the GI tract. For example, experiments with markers or tracers showing a degree of movement up the GI tract or revealing the marker distribution within the GI tract could be most valuable. The rate of heat loss from a small probe could give information about the fluid velocity at the end of the probe. The insertion and tracking of X-ray opaque materials might also yield interesting results.

This study illustrates the role and usefulness of numerical analysis in deriving solutions where analytical mathematical methods either break down or become too complex to handle. Such approaches will be more important where particle size distributions and their effects are also to be simulated. To build on current knowledge we need to understand the mechanisms which can effect the observed phenomenon. In basic or applied research simply to observe/measure and summarize is incomplete. Specialized investigation such as this work may challenge current beliefs and enhance understanding of ruminant nutritional principles.
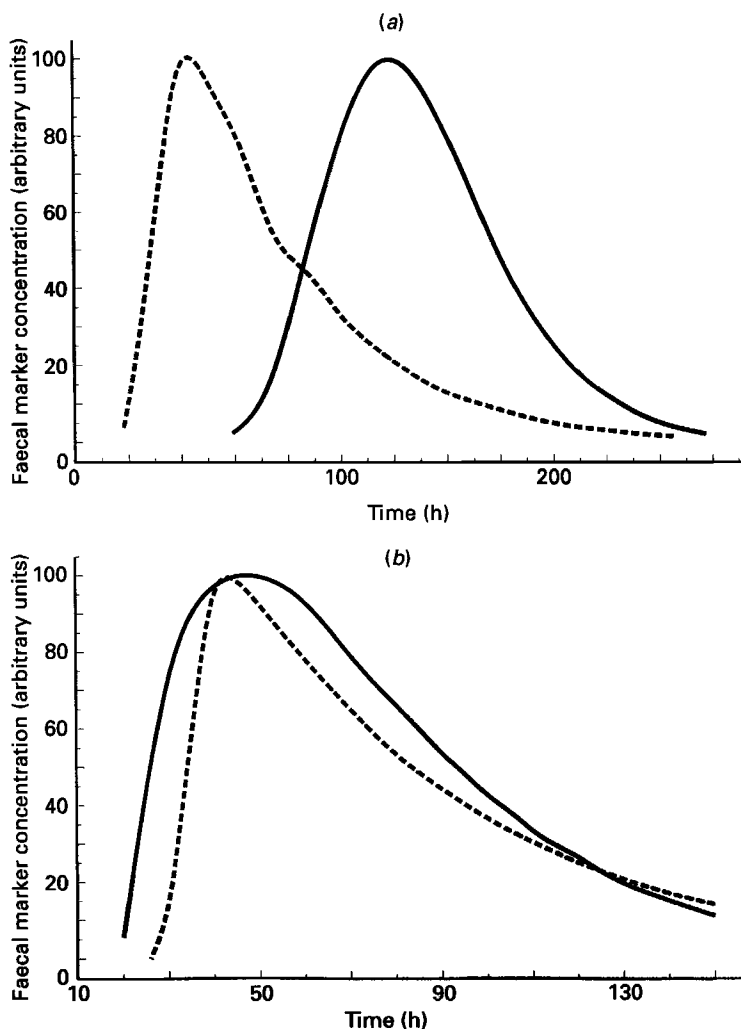
Fig. 7. Some observed faecal marker curves. The abscissas are faecal marker concentration in arbitrary units. (a) Holstein cows (———) on silage with particulate marker (Beauchemin & Buchanan-Smith, 1987) and Brangus steers (————) on molasses and hay with feed particles stained with magenta (Ferreiro Gutierrez, 1986). (b) Sheep (———) on hay and steers (————) on dried grass with a particulate Cr marker (R. C. Siddons, unpublished results).

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