

PARAMETER DETERMINATION IN COMPOSTING – Part III

Analytical boundary

P.D. Chapman

INTRODUCTION

Composting is a microbiologically driven process and this necessitates consideration at the microbe scale as this is the scale at which both microbial kinetics and the basic laws of nature operate.

As a contribution to modelling at sub-particle scales, Chapman (2008) proposed a finite volume approach, called micro-environment analysis (MEA), to extend our instrumentation precision to sub-particle scales. MEA however, is still a very ‘course’ tool as it used a spherical geometry which implies that a particle is spherical, has a smooth surface and is not affected by its neighbour (specifically the particle is assumed to be surrounded by air at the same oxygen concentration). Composting particles will clearly differ from this geometrical ideal.

We cannot deny the involvement of these aspects in composting. The question for this paper is how our models accommodate (or not) these aspects. Surface roughness and the consequences of ignoring its effect on parameter determination is considered in detail.

Analytical boundary

The concept of an *analytical boundary* was used by Chapman (2008) to denote the boundary location in modelling space that *represents* a composting particle. This arose from the need to apply diffusion laws to explain the distribution of oxygen at micro-environment scales (sub-particle scale). This analytical boundary exists in modelling space (in the sense that a particle will be described by a *representative geometrical form* e.g. a sphere, cylinder or planar). Our parameters are therefore determined within the context of this geometrical form; consequently it is only if the geometrical form *exactly* describes an actual particle that the value of the parameters could be said to be true. All other situations will generate parameters which reflect in some way the differences between the geometry and the actual particle.

These differences are likely to be:

- Irregular particle shape.
- The surface of the geometry would differ from the real particle surface, impacting surface area dependent calculations.
- Some of the air-space will exist within the analytical boundary and affect parameter determination, such as:
 - Micro-pores effect on the diffusion coefficient.
 - FAS determinations which measure total air volume, rather than the volume outside the analytical boundary.

- Micro-environment #1 volume calculations – MEA assumes that all the micro-environment is composed of contributing substrate. The outer micro-environment is likely to have a different proportion of air-space than those formed deeper in the particle. Consequently it is likely to behave differently to the others as it will have a lower energy density.

One could model each of these effects and in theory adjust for them; and then solve the over parameterization problem that would be compounded by these additional parameters. However, a simpler solution may be to accept the imperfection and allow the effects to be incorporated into other parameters; particularly if these other parameters fit more easily into the proposed model. For example, micro-porosity is a potentially important component of a composting particle's time course but it may be adequately represented by incorporating it into the diffusion coefficient that applies on the particle side of the analytical boundary. Similarly, a shape factor could be used in conjunction with particle size to determine an 'effective particle diameter'. That is, two parameters can be merged into one. The effective particle diameter being the net effect of both particle size and its shape characteristics i.e. how the particle behaves relative to its geometrical size (it includes the imperfections but is not inherently capable of predicting them).

If there is no allowance for these micro-scale effects in our models and these models require parameters to be determined from experimental data, then a question arises as to what happens to the consequences of these micro-scale effects. This paper explores this question for the surface roughness effect.

METHOD

Meshing a model's perfect Geometry with an imperfect particle surface

An analytical boundary based on a geometrical form is very useful as it accesses the rigour of mathematics; however the real world is not so perfect. How this chosen geometrical form relates to a real particle is therefore relevant to the modelling question.

For the case of a composting particle, a diffusing substance responds to concentration differences in its immediate vicinity. However, when considering oxygen diffusion from the surrounding pores into a composting particle, the oxygen must first transfer from the air to the particle surface and this is governed by Henry's law rather than diffusion laws (Sole-Mauri, Illa, Magri, & Prenafeta-Boldu, 2007). Both Henry's law and diffusion laws apply to the particle surface - they are surface area phenomenon. Indeed, surface flux (the quantity of oxygen which crosses a unit surface in unit time) derivations of diffusion laws are commonly used in composting (Bouldin, 1968); (Hamelers, 2001).

Consider a part of a particle surface (A in Figure 1) and its relationship with:

- the interstitial air,
- the actual oxygen penetration distance (B), and
- the geometry chosen to represent the particle (C).

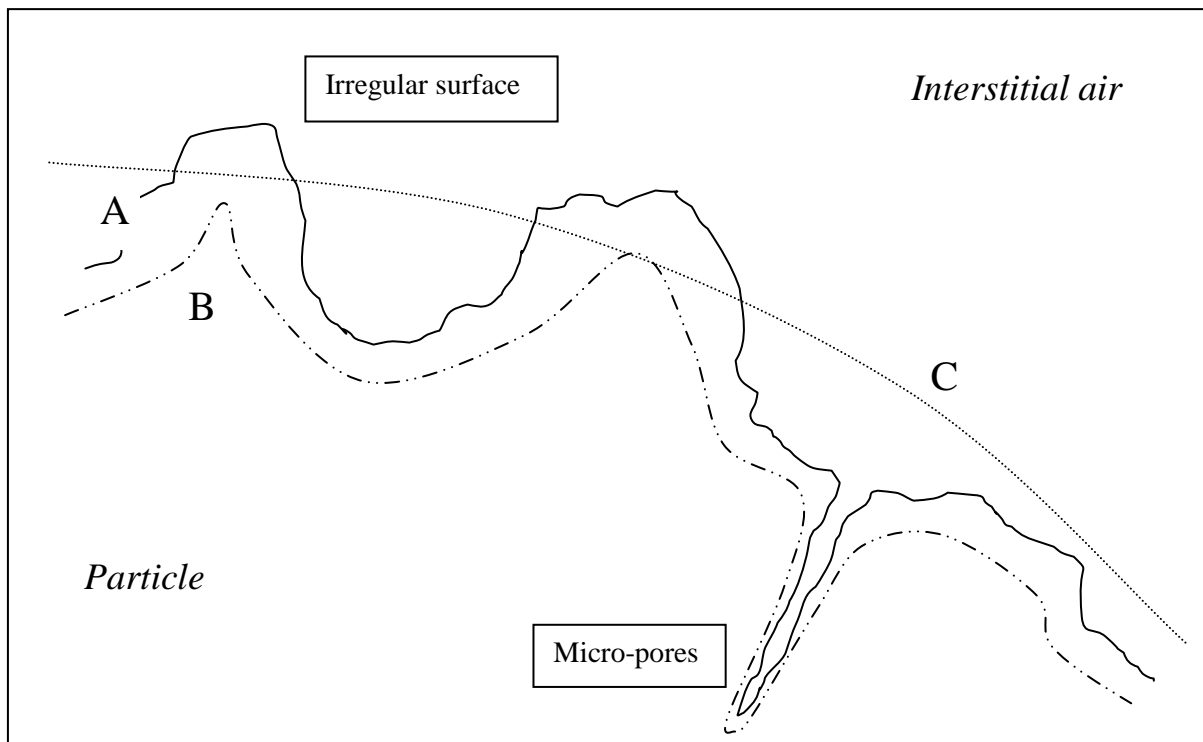


Figure 1 – The nature of the relationship between a particle surface (A) the geometry attempting to describe the composting time course (C) the actual oxygen penetration depth (B).

The actual oxygen penetration distance will be reasonably consistent for all surfaces. Although variation from the average would occur in the base of ‘trenches’ where penetration distance would be less than average (the surface flux of oxygen must supply a larger volume of compost); and the ‘peaks’ where the penetration distance would be expected to be greater than average (the surface flux has less volume of compost to supply). This variation could be modelled by using the appropriate geometry at each characteristic surface feature, such as:

- a hemispherical or cone geometry for describing the distribution in specific humps on the surface, and
- a cylindrical geometry to model the trenches and micro-pores (micro-pores would differ from trenches in having a steadily decreasing oxygen concentration with distance into the pore).

However, using an ‘average’ oxygen penetration distance has some appeal as the greater than average parts will tend to balance with the less than average parts. Spending time and computing power on this detail is not likely to greatly increase our understanding of composting. This variation in oxygen penetration distance is likely to be far less important than the oxygenated surface area available. In contrast, any surface irregularities which increase the surface area will increase the total amount of oxygen entering the particle, and increase the particle’s composting rate.

From the modelling perspective, MEA requires determining the volume of each micro-environment and this is most conveniently done using oxygen penetration distance. This enables the volume to be determined by difference between the inner and outer spheres (see case II below for the details of this). The ‘actual’ oxygen penetration distance however is a particle surface phenomenon and diffusion laws apply to the particle surface rather than our model surface. The greater surface area of the particle relative to our model geometry will mean that the observed composting rate will be

greater than our models would predict if the same diffusion coefficient were applied to our geometry surface. It is how this difference in the surface area is accommodated in models which include surface area based processes which is the issue addressed here.

Specifically, it is the *apparent* increase in the composting rate from geometrical perfection which is of interest here. Note that strictly speaking it is our model which is incorrect, not the observed composting rate, but please allow a small degree of anthropocentrism here.

Two cases can be argued. The first case is from the particle perspective while the second case is from the model perspective.

Case 1 – Oxygen flux at the particle surface

To simplify the maths, consider a special case of surface roughness where ridges and troughs exist with an angle of 90° (one may also find it convenient to consider the particle to be represented by a flat surface of the same area so the ridges can occupy the entire area).

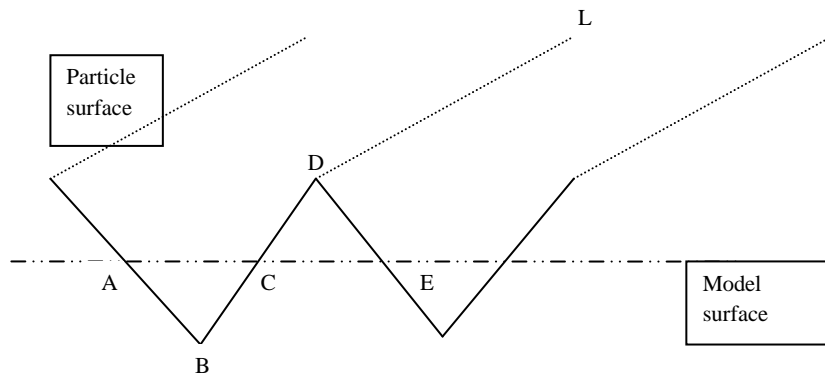


Figure 2 – A hypothetical surface roughness composed of ridges and troughs at a 90° angle.

In Figure 2 at any intersection of the model surface with the actual surface AE, the particle surface area is $(AB + BC + CD + DE) * DL$ while the model surface area is $AE * DL$. For this special case if $AB = BC = CD = DE = 1$, then $AC = CE = \sqrt{2} = 1.414$ and $AE = 2.828$. The ratio of the two surface areas is:

Equation 1

$$\frac{SA_{particle}}{SA_{model}} = \frac{4 \times DL}{2.828 \times DL} = 1.414$$

If the surface flux of oxygen is determined by diffusion laws and each gram of oxygen generates 15.94 KJ of energy, then the observed composting rate will be determined by the particle surface area and the flux of oxygen:

Equation 2

$$Q_{particle} = SA_{particle} \times oxygen\ flux \times 0.0627$$

Where the oxygen flux can be determined using Bouldin's (1968) – model II (the model used by Chapman 2008):

Equation 3

$$\text{oxygen flux} = \sqrt{2 \times C_0 \times D \times VOR} \quad \text{mg O}_2 \text{ cm}^{-2} \text{ s}^{-1}$$

Where C_0 = oxygen concentration in the surface of the particle.

$$VOR = \text{volumetric oxygen consumption rate} \quad \text{mg O}_2 \text{ cm}^{-3}$$

The composting rate (Q_{particle} in Equation 2) is determined experimentally, yet our models are attempting to explain this observed value using a particular geometry. In terms of the model, our calculations are based on SA_{model} (see Chapman (2009) for determining parameters needed for this model), yet we are unable to ignore the fact that the observed composting rate is determined by the SA_{particle} . Hence rearrange Equation 1 and insert into Equation 2:

Equation 4

$$Q_{\text{particle}} = SA_{\text{model}} \times 1.414 \times \text{oxygen flux} \times 0.0627$$

Equation 2 and Equation 4 balance with the same value for oxygen flux if we adjust our model surface area for the actual surface area of the particle (1.414 in this case). Our model is consistent with the particle composting rate.

However, if this ratio is unknown or not used, then in order for Equation 2 and Equation 4 to equate via their common value Q_{particle} (knowing the two surface areas are different), there must a difference in oxygen flux in inverse proportion to the surface area ratio i.e.:

Equation 5

$$\frac{\text{oxygen flux}_{\text{particle}}}{\text{oxygen flux}_{\text{model}}} = \frac{SA_{\text{model}}}{SA_{\text{particle}}}$$

However the parameters used to determine the flux in Equation 3 need to apply to the particle, yet we are describing the composting time course using a model. Consequently, for Equation 3 to be valid as a descriptor of oxygen flux when in the perfect geometry of the model, then the difference in the oxygen flux identified in Equation 5 must arise from either or both:

- VOR (i.e microbial kinetic (k) and/or substrate parameters (E(0)) and/or
- Diffusion coefficient (D).

If the model has a high r^2 then it follows that the parameters determined for a particle which is less than perfectly smooth and not perfectly spherical will accommodate this imperfection in its parameters. Consequently, they will differ slightly from 'real' parameters (those determined for a particle which is perfectly spherical and perfectly smooth). There is a question as to which parameter(s) accommodates this imperfection, but not a question as to the imperfections being accommodated.

Indeed Chapman (2008) used the diffusion law flux approach (Equation 3) in conjunction with the flux determined from the observed composting rate and actual particle surface area to attempt to detect the effect of substrate diffusion¹ and needed to adjust the diffusion coefficient to get the two graphs to align (see footnote to Figure 6-8; P.118). Note the same effect would have arisen had he

¹ Note that Chapman now attributes the effect to anoxic degradation rather than substrate diffusion, as substrate diffusion was shown to be accommodated in the fraction's parameters (see Part II of this series).

changed $E(0)$. This is possible experimental evidence of the surface roughness effect, although making the particles with finer size tolerances and counting the actual number would be needed to confirm this.

Case II – Model perspective

Chapman (2008) determined micro-environment volume proportion by subtracting the volume of the inner sphere from the volume of the outer sphere and divided the result by the particle volume. Thus, if z_{model} is the oxygen penetration distance (from the model geometry perspective) and r is particle radius then the aerobic proportion (Φ) can be determined by:

Equation 6

$$\Phi = \frac{\text{Volume}(r) - \text{Volume}(r - z_{\text{model}})}{\text{Volume}(r)}$$

Z can be determined for a zero-order oxygen consumption rate solution of diffusion law. This is relative to the particle surface rather than the model surface so an appropriate subscript is required:

Equation 7

$$z_{\text{particle}} = \sqrt{\frac{2 \times D \times C}{VOR(t)}}$$

The volumetric oxygen consumption rate (VOR) required in Equation 7 is determined from the observed volumetric composting rate (Q) (Chapman 2008) by:

Equation 8

$$VOR(t) = Q(t) \times 0.0627$$

To relate z_{particle} to z_{model} consider that the ‘actual’ aerobic volume can be determined to a close approximation by assuming z_{particle} applies equally across all surfaces. Then the aerobic volume (V_{aer}) can be determined using a planar geometry:

Equation 9

$$V_{\text{aer}} = SA_{\text{particle}} \times z_{\text{particle}}$$

If the surface area ratio of particle and geometry is defined as γ , then $SA_{\text{particle}} = SA_{\text{model}} * \gamma$.

The aerobic volume of Equation 9 can be formulated relative to the *model* geometry by:

Equation 10

$$V_{\text{aer}} = SA_{\text{model}} \times \gamma \times z_{\text{particle}} = 4 \times \pi \times r^2 \times \gamma \times z_{\text{particle}}$$

Chapman’s model determines the model aerobic volume by the difference between two spheres thus:

Equation 11

$$V_{\text{aer}} = \frac{4}{3} \times \pi \times [r^3 - (r - z_{\text{model}})^3]$$

For the two volumes to equate, a ‘model equivalent z ’ (z_{model}) needs to be determined. To do this, equate Equation 10 with Equation 11 and rearrange:

Equation 12

$$z_{model} = r - \sqrt[3]{r^3 - 3 \times r^2 \times \gamma \times z_{particle}} \quad z_{model} \leq r$$

Note: z_{model} in Equation 12 can exceed particle radius. This arises from both the SA ratio and combining the essentially planar geometry of oxygen diffusion, used above, with the spherical geometry of the model.

Insert Equation 7 and Equation 8 into Equation 12 to enable the observed composting rate and diffusion laws to determine oxygen penetration distance within the model geometry framework.

Equation 13

$$z_{model} = r - \sqrt[3]{r^3 - 3 \times r^2 \times \gamma \times \sqrt{\frac{2 \times D \times C}{Q_S(t) \times 0.0627}}} \quad z_{model} \leq r$$

Using Equation 13 in Equation 6 could give a good approximation of diffusion laws' effect within the model geometry framework. However, the difficulty in determining the surface area ratio (γ), limits the application of Equation 13.

Consider what would happen if we did not adjust for particle surface roughness. That is $\gamma = 1$.

We have two ways of determining aerobic proportion: firstly, diffusion law determination (i.e. Equation 6 and Equation 13 above) and secondly from the microbial kinetics model. These should equate.

For any particular electron acceptor/fraction combination (S) the first-order kinetic composting model used by Chapman (2008) was:

Equation 14

$$Q_S(t) = k_S \times E_S(t) \times NB_S(t) \times \Phi(t)$$

Which can be rearranged to determine $\Phi(t)$ as the ratio of the observed composting rate: model composting rate using oxygen as an electron acceptor.

Combining all of the above into a single equation and using V to represent the volume of a sphere gives:

Equation 15

$$\frac{Q_S(t)}{k_S \times E_S(t) \times NB_S(t)} = \Phi(t) = \frac{V(r) - V\left\{r - \left[r - \sqrt[3]{r^3 - 3 \times r^2 \times \gamma \times \sqrt{\frac{2 \times D \times C}{Q_S(t) \times 0.0627}}}\right]}\right\}}{V(r)}$$

Note: The RHS of Equation 15 could be simplified further but in this form it is comparable to Equation 6 i.e. inner sphere radius = $r - z_{model}$.

If one could determine γ , then Equation 15 could be solved by iterative means, but the relevant point for this argument is that if $Q_S(t)$ changes then the effect on the LHS will differ from the effect on the RHS i.e. $Q_S(t)$ on the LHS versus $\sqrt[3]{1/Q_S(t)}$ on the RHS. That is, the difference in the composting rate arising from roughness on the particle surface would appear computationally as a 'change' in the

aerobic proportion that is determined. This is an inevitable consequence of changing γ in the RHS of Equation 15. This ‘change’ could include the implicit assumption that $\gamma = 1$ if there is no adjustment for surface roughness.

Because surface roughness is a pre-existing condition of a composting particle this ‘change’ in the composting rate would not occur in the composting time course. Rather, the higher composting rate would apply from the beginning and the value of the parameters would reflect this.

The question here, as in case I, is what parameter(s) would accommodate the surface roughness effect if it is not included as a separate parameter in the model? To investigate this question in more detail, consider two factors:

- The consequences of a change in $\Phi(t)$.
- The balance required in Equation 15 where microbial kinetic parameters only appear on the LHS.

Because the model parameters must describe the peak composting rate (the point used by Chapman to determine $E(0)$), then a change in aerobic proportion would also change the magnitude of $E(0)$ – assuming there is no direct impact on the value of k and $NB_{(t_{max})}$. A further constraint arises from the second point noted above, that is the need for Equation 15 to balance. In this constraint the aerobic proportion is determined on the RHS by particle geometry, diffusion law and the observed composting rate. There is thus a balance between biology on the LHS and physics on the RHS in Equation 15. Our models are describing the biology side of Equation 15. Yet changing the biology parameters in any iteration has no effect on the RHS (experimental data is used here); aerobic proportion will not change. It follows that all the effect of surface roughness is accommodated in the kinetic and substrate parameters. Initially in $E(0)$, however $E(0)$ will have a secondary effect on most other kinetic parameters via its effect on NB_{trans} (see Part I for the inter-relationships between all the kinetic parameters). It is possible that the value of the rate constant could be affected if these secondary effects extend to the one-exponent constant.

It should be noted here that, as in case I, the difference due to surface roughness could also be accommodated in the diffusion coefficient. In this case aerobic proportion ($\Phi(t)$ in Equation 15) would also change, so the effect would be shared between D and the kinetic/substrate parameters. Note that D could change between the outer micro-environment (which would include micro-porosity and surface roughness), and subsequent micro-environments.

No attempt will be made here to determine precisely how the effect of surface roughness is taken up by each parameter, as the main aim of this paper is to show that the surface effect *is* incorporated into the parameters, the details may be of scientific interest but the consequences are of little practical significance. For anyone with an interest in this detail the potential linkages have been identified above.

RESULTS

Some possible evidence for the effects discussed above is visible in Chapman’s (2008) thesis results – reproduced in Figure 3. This data would suggest that both the diffusion coefficient and substrate concentration accommodate the difference between the model geometry and an actual particle.

Readers should note that these trials were not configured to specifically detect the effect of a perfect geometrical boundary with an imperfect particle surface. Interpret these conclusions with an appropriate level of caution.

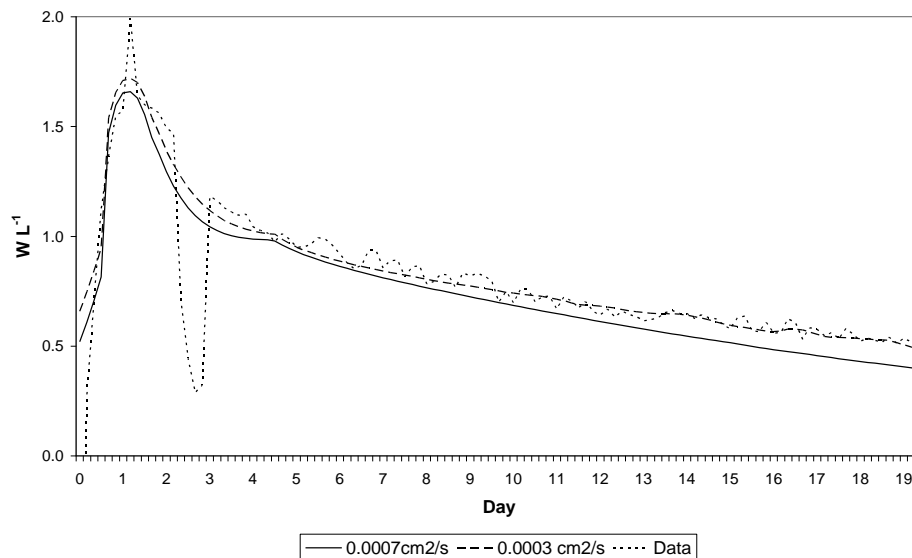


Figure 3– Modelled versus measured composting rate for the 1.33 cm pig faeces particles with 2 diffusion coefficients. Note the lower value diffusion coefficient required more substrate (0.015 v 0.01 MJ cm⁻³) for the model to fit the data curve. Data from Chapman (2008, p. 115).

CONCLUSION

If the intended use of a model is to understand the composting time course then there is no need to accommodate the detail that arises from the difference between our preferred model geometry and actual particle shape and surface characteristics.

This occurs because, with the need to determine many of the model parameters by experimentation, then fitting the model to the data incorporates these differences into other model parameters such as diffusion coefficient and substrate concentration.

This accommodation appears to include the particle surface characteristics (discussed in this paper) and substrate diffusion and solubilisation (in Chapman (2009)). The validity of simplified models as a means of avoiding the problems of over parameterisation that has been identified in composting can have a firmer theoretical footing.

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