Modelling composting complexity: the use of emergent, information rich, computational units as a solution to the over parameterization problem.

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1 Introduction

The point where the fundamental laws and processes of science meet our technologies is a point of considerable computational complexity, as evidenced by the compromises needed to achieve a solution for several particle sizes at constant temperature (that is excluding environmental conditions) in the mathematical approach of Hamelers (2001).

If a pure mathematical approach suffers from over parameterisation without incorporating changing temperatures then a pragmatic model using this approach will need even more parameters and be even more problematic. In contrast, the high regression coefficient with experimental data that was obtained by Chapman (2009a) despite using demonstrably incorrect assumptions (the oxic/anoxic transition is not as 'sharp' as the zero-order oxygen consumption kinetic makes the boundary) indicates that some detail can be left out without compromising the model precision. This raises many questions with implications for developing models that are intended to be used practically.

This paper explores the composting landscape using the concepts of seamlessness (a thinking tool for preserving the underlying causation) and constraint resolution when seamlessness is compromised, as a means of focussing attention on the most important information (Chapman, 2010). Attention can then focus on mechanisms by which this important information can be carried through these constraints and be incorporated into our models.

There are three components of a compost model's structure that can be shown to help resolve the constraints that limit seamlessness:

- *Analytical boundary* based on a geometrical form. This enables all sizes and types of particle to be accommodated in the mathematics by using a particular geometry (sphere in the case of composting). The inconsistencies between the 'perfect' geometry and the 'imperfect' particle can then be dealt with separately.
- Formation of *computational units*: these combine sub-particle scale volumes of compost (micro-environments) with a known set of data that includes – start time, substrate concentration etc. As these are determined from the analytical boundary they capture all the electron acceptor spatial variability within composting – with the added advantage of enabling a predictor of odour production.
- *Finite element method*. Enables incorporation of environmental effects (particularly changing temperature) and the moving oxygen boundary into the set of parameters needed for the mathematics. The modelling non-space between the end of one time interval and the beginning of the next is used to change the value of temperature affected model parameters.

Arranging the *model structure* in this way enables the simplest version of the necessary models (first-order microbial kinetic and zero-order oxygen consumption solution of the second law of diffusion) to be used. This model structure means the dominant 'pattern' (oxygen as an electron acceptor) is faithfully preserved albeit the 'actual' location of the oxic/anoxic transition may not be captured by this strategy.

The resulting model is very practical as any combination of type and size of particle can be used in any container (technology) and the effect on the 'system' performance in any climate can be determined.

2 Overview

Composting is complex. At the physical level, substantial variability exists within the 3 phases particularly as the air phase is unevenly intertwined with the solid phase. Superimposed on this physical variability is the variability arising from the interaction of two disciplines: microbiology and physics. The complexity is such that over-parameterization emerges as a significant issue for composting (Hamelers, 2001).

In Chapman (2008) a number of compromises were made to achieve his simple solution. Many compromises arose from the need to use the second law of diffusion to explain oxygen distribution. In a subsequent paper (Chapman, 2009a), determination of the microbial kinetic parameters was put on a firm theoretical footing and a very high regression coefficient was obtained ($r^2 = 0.99$ for the high quality data set). It seemed as if the precision of the model was not compromised despite some of the detail being knowingly excluded. This seemed to beg for an explanation.

It was later shown that substrate diffusion and solubilisation (Chapman, 2009b) and the imperfect particle surface (Chapman, 2009c) were internalised into other parameters. Indeed, it is implied that *excluding* these known details made the model more precise, as it enabled accurate determination of the remaining parameters.

If we can exclude some 'knowledge' such as substrate diffusion, yet retain (or even enhance) our model precision, then there must be something of more significance than knowledge to the modelling question. Increasing knowledge does not necessarily result in increased understanding.

A composting model fills an organisational role in that it contains and manages the contributing elements to achieve the goals of the researcher. For example, composting could be seen as two separate models (a microbial kinetics model and a substrate model) with an overlay of the fundamental laws and processes that are not incorporated in the two models; a three component model. With these components, a major point for consideration is the interaction between the different models, and their interaction with the fundamental laws.

If we cannot know everything about composting then a question arises as to whether there is some sort of optimum we could aim for with our models. The theme explored in this paper is the notion that the **model structure is an important contributor to optimum knowing**, and that there is likely to be an optimum structure for any model of composting.

3 Constraints needing to be resolved by the model structure

The notion of a constraint on our understanding can be applied to the composting model's organisational role; these being areas where the various models do not fit well together or the models

do not fit well with the overlay of fundamental laws and processes. Putting additional thought into these areas is likely to be highly beneficial to the model structure. It is further suggested that there are organisational units (called computational units) which can be formed around these constraints and that if identified these units provide a useful and powerful tool within the model structure.

3.1 The emergence of the need for an *analytical boundary*

Consider that the fundamental laws and processes occur according to the conditions existing at that point in space and time. Hence a molecule will move if it is in a concentration gradient, a microbe will grow according to the conditions it finds itself in. If we could understand everything at the atomic scale then composting could be described by the sum of all these effects, thus:

Equation 1

$$Observed\ composting\ rate = \sum_{space} (fundamental\ laws, fundamental\ processes)$$

At this level, microbiology is also constrained by these fundamental effects (Battley, 1987).

If a finite element method (using a fine 3 dimensional grid) were used to solve Equation 1 for a compost pile, then some of those points in composting space would be air while others would be solid. The solid is the composting 'factory' and therefore only those points that fall in solid need to be summed in Equation 1.The air is primarily a transport system. From the modelling perspective, separating the air from the pile is difficult because it is so intertwined. Consequently, determining whether a point in composting space is air or solid is also difficult, yet necessary if Equation 1 were to be used. By contrast, measuring the quantity of air is a comparatively easy task.

In addition, the solid/air boundary is a special location in composting for several reasons:

- The gas transport system meets the gas consumption (oxygen) & generation system (CO_2 & odours).
- The boundary is datum for determining oxygen distribution in the solid.
- Diffusion processes begin from this boundary datum.
- Henry's law applies only at the boundary.

The solid/air boundary is therefore a crucial element for expression of the fundamental laws and processes in the composting landscape, yet does not emerge as a parameter in a finite element method using Equation 1. Some points may land on the boundary and consequently there may be some statistical representation of its influence in a finite element method, but this would bear little correlation to its actual significance in the observed composting time course. For the influence of the solid/air boundary to be fully expressed in any model then this boundary needs to be incorporated as a separate factor.

Composting is a 3-phase system with a surface.

3.2 The particle as an analytical boundary

In composting, the solid can be usefully taken as a collection of particles of various sizes and types. The points in space contributing to the observed composting rate in Equation 1 will all occur within these particles. Consequently all the contributing space elements will be captured if we sum all the

particles. The concept of a particle is also consistent with the fundamental need for a surface to incorporate the solid/air boundary. Some difficulties emerge when we attempt to describe these particles within the constraint of a limited set of geometrical forms; these issues being resolved by use of the *analytical boundary* concept and discussed in detail in Chapman (2008); Chapman (2009c).

The influence of the solid/gas boundary becomes the boundary conditions of the particle and the finite element method can be used within the analytical boundary. The state of the air-space surrounding the particle becomes a separate computational problem, but this computation retains links to the boundary conditions of the particle.

If Q is used to denote the composting rate, then Equation 1 can be reformulated for particles as:

Equation 2

$$Q_{pile}(t) = \sum (Q_{particle}(t))$$

Where the space elements in each particle act according to the fundamental laws and processes:

Equation 3

$$Q_{particle}(t) = \lim_{analytical\ boundary} \sum_{space} (fundamental\ laws, fundamental\ processes)$$

The analytical boundary in Equation 3 is the geometrical representation of a composting particle, (Chapman, 2009c).

Indeed, if we experimentally determined the composting time course of each particle (using the same air conditions as would be found at its location in the composting pile), then a description of the composting time course of the pile will be a sum of each particle's contribution. Any difference could be attributed to variation in oxygen concentration surrounding the particle or interactions between particles within the pile. This is not mathematically complex.

It follows that if we could easily model the time course of each composting particle, then the time course of the pile would be a simple procedure of summation. Indeed, if there were only one electron acceptor and understanding its distribution did not require diffusion laws, then using microbial kinetics with several fractions would no doubt give a sufficient description of a particle's composting time course, within limits. This was the approach used by Chapman (2009a) to simplify the data set to determine the basic microbial kinetic parameters.

The formation of an analytical boundary based on a geometrical representation of a particle would therefore be a useful one as it provides:

- Separation of the air based transport system from the composting 'factory'.
- An anchor point (a surface) for the use of diffusion laws.
- Linkage between a mathematical representation of a particle (e.g. smooth surfaced sphere) and a composting particle.

However, considerable complexity is involved in modelling the composting behaviour of each particle. Tools for making sense of this complexity are discussed in Chapman (2010) and these tools (rootedness, seamlessness and constraint resolution) are used here to examine a particle in more detail.

Within the analytical boundary, maintaining seamlessness requires resolution of several constraints.

- Accounting for the difference between the smooth surface implied in any geometrical description of a particle and the surface roughness of an actual particle.
- Meshing diffusion laws with microbial kinetics – particularly the spatial elements in the distribution of the various electron acceptors.
- Emerging variation in substrate concentrations at sub-particle scales and its implications for any microbial kinetic description.
- Mathematical considerations such as non-steady state conditions.
- The effect of environmental factors (particularly changing temperature).

3.2.1 Surface roughness constraint

The analytical boundary formed above is a geometrical form chosen to 'represent' the typical composting particle. The actual particle will differ in both shape and surface roughness from this geometrical perfection. This difference is a mismatch between the model surface and the actual particle surface; it is another example of a constraint on our understanding.

Various tools could be used to adjust for this difference (e.g. a shape factor). However, Chapman (2010 c) showed that with experimentally determined parameters, the effect of surface roughness is incorporated into other parameters and hence accounted for without needing an additional parameter. For a system suffering over-parameterization problems this is a useful insight. It does however require acceptance of the notion of a 'combined' parameter, one a little less than scientific perfection.

3.2.2 Oxygen distribution constraint

In addition to the effect of surface roughness raised above, a number of considerations arise from the application of diffusion laws to oxygen distribution in a composting particle. Complete seamlessness would require mathematical space in the model for each electron acceptor as the electron acceptor provides the connection to the fundamental chemical equations of microbial kinetics and is the vehicle by which seamlessness is extended to particle scale.

Determining the electron acceptor for any point in a composting particle becomes a separate computation involving the application of diffusion laws to oxygen, within the limits that at low oxygen levels other electron acceptors will be favoured by the microbes. It adds a spatial dimension to microbial kinetics functioning within the analytical boundary of the 3-phase system, composting.

Chapman (2008) chose to use a zero-order oxygen consumption rate in the second law of diffusion as this formulation returns an oxygen penetration distance. This enabled a clear separation of aerobic from anoxic/anaerobic degradation. An oxygen based electron acceptor is used within the aerobic zone and anoxic/anaerobic electron acceptors in the remaining parts of a particle. Chapman (2008) chose to assume the anoxic/anaerobic contribution was negligible and hence could be ignored; however a subsequent paper using the same data indicated that an anoxic contribution was detectable (Chapman, 2009a).

Substantial debate could occur over this method for determining the location of the aerobic/anoxic transition. Chapman used a Monod microbial kinetic to argue the validity of using a zero-order oxygen consumption rate for use in the second law of diffusion. However, this same kinetic shows that both zero and first order should be used, zero-order at high oxygen concentrations and first-order at low oxygen concentrations. The zero-order oxygen consumption rate that was used is only valid for a part of the aerobic distance. However, this formulation enabled determination of an oxygen penetration distance and the use of finite volume methods (Chapman 2008). The value of returning an

oxygen penetration distance was very high in this case, as Chapman was more interested in knowing the odour production potential from the anaerobic/anoxic core of the particle. The compromise was easy to make at the time.

However, compromises seem to be unavoidable with any oxygen consumption kinetic. Consider that if the second law of diffusion was solved using a Monod type kinetic describing oxygen consumption rate then two things emerge:

- There would be no oxygen penetration distance. At low oxygen concentrations the Monod kinetic becomes first-order; oxygen concentrations may get very low, but never zero.
- Consequently, an extra computation would be required to determine the aerobic/ anoxic transition (necessary for the seamless application of microbial kinetics to a composting pile). For which the consequences of adding additional parameters to an already over parameterized system would need to be assessed.

In addition, the aerobic/anoxic transition is a fuzzy boundary, raising the question as to whether a precise definition of its location is possible or desirable. Or at least raises the question as to whether any increase in precision in determining its location will result in a net increase in our understanding. The emergence of 'combined' parameters argued in Chapman (2009b) would suggest there is no net advantage, and possibly some disadvantages if the necessary mathematical manipulations remove environmental effects from the model.

3.2.3 Steady state v's non-steady state

The second law of diffusion needs to be solved for the boundary conditions that apply to the researcher's model. The simplest solutions are for steady state conditions, consequently these are most commonly used (Danckwerts, 1950).

However, true steady-state conditions in composting would be extremely rare. Deviations from steady state occur in a range of areas such as:

- Changing environmental conditions:
  - Temperature
  - pH
- Changing substrate concentrations as composting proceeds.
- Fluctuating oxygen concentrations in the interstitial air.

In addition, the decreasing substrate concentrations over time lead inevitably to increasing oxygen penetration distances. A moving boundary solution of diffusion laws is required (this same conclusion arises with a Monod solution as the trigger point for the aerobic/anoxic transition would move inwards as oxygen concentrations rose).

Preserving seamlessness with the available mathematical solutions when interfacing diffusion laws with microbial kinetics is a constraint requiring consideration. Particularly with several electron acceptors that have distributional elements arising from a degree of interdependence between them. However, in a highly complex system the benefit of using a high precision non-steady state, moving boundary, mathematical solution of the second law to determine oxygen distribution may be lost by the additional computational complexity. In addition, this would most likely only apply to a data set at constant temperature – limiting the application of the model.

The limit to our understanding of composting by use of models would seem to be occurring at the sub-particle scale. Specifically, the additional complexity arising from the need to use diffusion laws to explain the distribution of oxygen. Within the context of the fundamental laws and processes it would be the point in the modelling landscape where microbial kinetics meets diffusion laws within the 3-phase system of composting – a level of complexity not apparently amenable to an easy solution while retaining seamlessness.

In some ways this is analogous to the mathematician's problem with approaching zero and the associated infinity. This was solved in Newton's case by basing the analysis on one, rather than zero. Similar transformations are perhaps needed for the composting context. In which case, composting could be seen as a 3-phase system with a surface plus *something else*. In this case, *something else* is a method for coping with the constraint on seamlessness arising from the added complexity of introducing diffusion laws to explain oxygen distribution.

3.3 Using the model structure to extend seamlessness

Consider an oxygen penetration distance (z) determined with a zero-order oxygen consumption solution of the second law:

Equation 4

$$z = \sqrt{\frac{2 \times D \times C_0}{VOR}}$$

By way of example of the usefulness of using z to extend seamlessness, consider that temperature affects: the diffusion coefficient (D), the solubility of oxygen in water (C_0), and the rate constant (a necessary parameter for VOR). It follows that z will contain the **net** effect of all these impacts.

The net effect of the three temperature affected parameters of Equation 4 are reduced to one (i.e. z).

Oxygen penetration distance (z) then is a useful parameter by which seamlessness can be maintained between diffusion laws and microbial kinetics at the particle scale. In the above example, the effect of temperature on all parameters at the fundamental level is incorporated into subsequent calculations that may use z. Indeed, the assumptions necessary to be able to use a zero-order solution of the second law of diffusion (and consequently derive Equation 4), may well incorporate an absolute error in the sense that the 'actual' aerobic transition may differ slightly from the computed one. However, the relative effects, that is the net effect of a *change* in a fundamental parameter (such as temperature), is unaffected by this absolute error.

Considering that many parameters in composting have no absolute value and are determined experimentally (e.g. k), and combining this with the notion of the emergence of 'combined' parameters Chapman (2009b), would suggest that any absolute error arising from the zero-order assumption would have negligible effect on the model precision. Indeed the regression coefficients obtained by Chapman (2009a) would suggest that this is true. Yet because seamlessness to the fundamental parameters is preserved, then the effect of a change in any fundamental can be quantified in the model output.

For example, using Equation 4 Chapman (2008) was able to show that a rate constant with a Q_{10} of 2 would appear experimentally as a Q_{10} of 1.47. If there were no effect of temperature on C_0 and D then the observed Q_{10} would be explained only by the change in aerobic proportion and would be 1.414 (i.e. $2 * \sqrt{(1/2)}$ where $\sqrt{(1/2)}$ is Equation 4 with the effect due to the change in aerobic proportion

arising from the change in the rate constant only). The difference between 1.414 and 1.47 arises from the net effect of temperature on the solubility of oxygen in water and the change in the diffusion coefficient. Of these the solubility of oxygen in water would have the most impact as its value is 2 orders of magnitude higher than the diffusion coefficient. Indeed it is the net effect of the changes in C_0 and D which accounts for the observed Q_{10} dropping from 1.47 at 6 ^{o}C to 1.36 at 37 ^{o}C (see Appendix 1 for details and Appendix 2 for results supporting this).

For composting, oxygen penetration distance (z) could be considered an *emergent property*. It results from the interaction of diffusion laws with microbial kinetics, specifically oxygen as an electron acceptor. The value of z is net of all the fundamental laws and processes at the base of each discipline. Its value is not only specific to a certain microbial kinetic in a certain substrate at a point in time, but also specific to the surrounding oxygen concentration (such as location in the pile, aeration regimes etc).

3.4   Using seamless parameters to form computational units

Given that substantial information can be given a physical form in the value of z, then any subsequent use of z will incorporate this information.

Knowing z, it becomes possible to calculate a volume of compost by the difference in volume between two spheres with radii that differ by z. This volume of compost is a micro-environment of Chapman (2008).This mathematical procedure therefore links a particle size and shape with microbial kinetics and diffusion laws and, as z is determined using seamless parameters, then any subsequent use of these micro-environments will also incorporate the seamlessness inherent in z. The formation of sub-particle scale computational units (of which micro-environments are a part) is proposed as a vehicle for resolving many of the constraints and preserving seamlessness in composting.

By way of example, micro-environments form at a particular point in time and this becomes datum for substrate degradation. They also have a location in space (both within a particle and this particle's location within a pile). Because of this 'other' embedded information, many modelling questions can be resolved by using micro-environments in subsequent calculations. The particle may change its location in the pile or the electron acceptor may change from oxygen to nitrate but the micro-environment retains its location in the particle. The change in electron acceptor results in a different substrate degradation rate. Much of the complexity that arises when microbial kinetics meets diffusion laws in the context of a composting particle becomes embedded in defining the boundaries of the micro-environment; while the history of the composting particle becomes embedded in the substrate concentration. The spatial complexity within a composting pile reduces to a mathematical sum of a large number of micro-environments; where the state of each micro-environment at the next time interval is determined by use of the relevant electron acceptor.

Micro-environments are the physical manifestation of the complexity of the microbe/diffusion law/substrate interface. A computational unit takes this physical manifestation and attaches to it all the other information that is relevant to the model requirements (time of formation and substrate concentration in the case of composting). This simplifies the model as the only information needing to be computed for the next time interval is the type of electron acceptor to use; all the other necessary information is held by the computational unit.

Forming a computational unit when seamlessness becomes constrained enables the seamlessness *up to that point* to be incorporated into the computational unit – the time (and location) that aerobic composting begins. This would only occur if z were determined by the kinetic itself. Had Chapman

used some arbitrary thickness (i.e. human imposed z rather than have the *interaction* of microbial kinetics and diffusion law determine the value of z) in his onion ring type volumes of compost, then these effects would not have been carried through to subsequent calculations.

Some constraints may not need the formation of a formal computational unit as existing parameters can fill this need. For example, the diffusion law/microbial kinetic interface described above uses VOR to carry the net result of microbial activity across to diffusion laws. The aerobic subset of microbial complexity (i.e. NB(t), several fractions and the associated substrate concentration) reduces to a single parameter. Indeed diffusion laws are entirely outside microbial complexity as the same equations would apply if oxygen were removed chemically.

4   Extending seamlessness into the social interface

Consider identifying a socially important value (such as odour in a composting toilet), then show that most odour is produced in the *absence* of oxygen. Then if one can show a strong correlation (albeit negative in this case) between odour production potential and the seamless parameter z we have a means of extending seamlessness into human use of our technologies.

In relating the odour production potential (1- aerobic proportion) to z, the information inherent in the value of z is carried into the determination of aerobic proportion (Φ_{aer}) - and consequently odour production potential. Aerobic proportion ($\Phi_{aer}(t)$) then becomes another information rich parameter describing the net effect of the interaction of microbial kinetics with all of: the substrate, diffusion laws, Henry's law, *within the context of the particle* (particularly, particle size and surrounding oxygen concentration – and these are affected by technology design). We have a mechanism by which seamlessness can be extended into the social interface by influencing technology design. In this case Φ_{aer} is negatively correlated to odour production and smell is an important social determinant of a technology's success.

With this social interface extension, a first-order microbial kinetic equation which is consistent with the fundamental laws and processes, for which oxygen distribution is from the particle surface and hence described by the second law of diffusion is:[1]

Equation 5

$$Q_{aer\,(S)}(t) = k_{aer\,(S)} \times E_S(t) \times NB_{aer\,(S)}(t) \times \Phi_{aer}(t)$$

For which aerobic proportion (Φ_{aer}) is a significant information carrier serving the task of extending seamlessness from micro-environment scale up to particle scale and into the pile which is contained in a technology.

5   Incorporating environmental effects into the model structure

A typical composting particle exists as part of a composting system in changing environmental conditions, in particular changing temperature. Changing environmental conditions however affects composting at the fundamental level (i.e. rate constant, diffusion laws, Heny's law) and needs computational space in any model to enable seamlessness between the fundamental laws and

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[1] Note that the micro-environment variability in substrate concentration is not captured in Equation 5. At the micro-environment scale there is no need to use Φ. No proportion is required, as only one electron acceptor is used, which may or may not be oxygen.

processes and an operating compost pile. Seasonal, diurnal and climatic changes would be difficult to ignore in a model intended to be used practically.

Given the advantages in using the simpler steady-state solution discussed in Section 3.2.3, then in order to use these simpler formulations the constraint arising from many of these constants needing to change their value needs to be resolved. A constant in a scientific model needs to become a variable, albeit a deterministic variable, in the real world application.

If temperature were constant then Equation 5 is comparatively simple to solve. Temperature however acts globally, it affects many elements at the fundamental level. The question for the model is how to incorporate the effects of temperature, considering that with its global influence it does not lend itself to forming a computational unit. In essence Equation 5 should be written with a second subscript (T) designating the specificity to temperature:

$$Q_{aer\,(S)(T)}(t) = k_{aer\,(S)(T)} \times E_{S(T)}(t) \times NB_{aer\,(S)(T)}(t) \times \Phi_{aer\,(T)}(t)$$

Where k is directly affected by temperature; while the remainder (E_S, NB_S and Φ_{aer}) are a mix of direct and emergent influences of temperature.

The modelling task is to enable environmental effects to manifest by changing the value of affected constants at their fundamental point of influence without losing precision. This is an optimisation issue.

We know that Equation 6 reduces to Equation 5 if temperature is constant and that Equation 5 is solvable. This occurs as the temperature affected parameters are input as a constant. It follows that if the deterministic variables (arising from changing environmental conditions) can be converted into constants, then Equation 5 can be used. The modelling task narrows to achieving this conversion. Equation 5 though has a time course so there is no space in this time course in which this conversion could occur (otherwise they would be a variable). The modelling task narrows further to finding a place *outside* the modelling time course to achieve this conversion. From a modelling perspective, this could be achieved by 'stopping' the model time course, changing the value of the relevant constants then 're-starting' the model time course using the new constants. The modelling equivalent of a movie; that is, a series of constants each slightly different from the previous creating the illusion of movement i.e. a variable which *appears* to be a constant. This would suit a finite element method where the measured temperature is assumed to be constant until the next reading occurs.

In this manner, environmental impacts can be input into a model at the fundamental level and Equation 5 can be used as the temperature affected parameters are input as a constant, albeit for only a finite period of time. In a sense, temperature impacts are incorporated as a separate calculation *outside* the main modelling procedure. That is, the change occurs in that modelling non-space between the end of one interval and the beginning of the next.

This could also be viewed as a form of segmentation where environmental effects are incorporated by forming a separate set of calculations specifically designed to convert a deterministic variable into a constant. They are carried out independently of the model but are intimately connected with the model. It is the model structure, the finite steps, which produces the net effect of environmental changes over time, rather than having them input as a separate parameter.

5.1 The moving oxygen front

Calculating oxygen penetration distance with a single computation (as implied above) has limits in time. As composting proceeds the available substrate is consumed and the composting rate declines. Lower the oxygen consumption rate (VOR in Equation 4) and z will increase. In effect an increasing z will mean that the substrate at the moving oxygen front will experience a change in the rate constant. In addition to the changing rate constant, the substrate concentration in this newly oxygenated compost is likely to differ from its neighbour. Spatial variability in substrate concentration will arise and a single VOR will not be able to be used in Equation 4. The variability becomes too great to be supported by a single calculation. Emerging variation in substrate concentration combined with some volumes of compost changing their electron acceptor could be seen as a constraint on seamlessness requiring further consideration.

Considering also that incorporating environmental effects (especially temperature) is likely to move the computation method to a finite element method, then there is value in incorporating the substrate variability into the same method.

5.1.1 Including the moving oxygen front in the finite element method

The time course of substrate concentration is a component of Equation 5 – driven by the rate constant. It can be shown that for any substrate concentration/k combination a time will exist (t_0) when the substrate concentration equals the starting substrate concentration (C_0). For an aerobic rate constant, this time coincides with the rate constant transition from anoxic/anaerobic to aerobic; the time when the oxygen front moves into new substrate. This transition therefore has a time and a position in the particle which is determined by diffusion laws. We already know how to incorporate the fundamentals into z (and consequently aerobic proportion), and the anoxic/anaerobic to aerobic transition is a sub-set of z as it occurs at the moving boundary. It follows that a computational element which utilises z and accommodates the time of transition to aerobic degradation will also accommodate: the fundamental laws and processes, the emerging substrate variability and the moving boundary.

This can be achieved by considering that a time based finite element approach will utilise two times t_1 at the start of the finite element and t_2 at the end of the element. With a moving oxygen boundary then two z's will exist, one at each time interval ($z(t_1)$ and $z(t_2)$). These two z's define a volume of compost at a known place in the composting particle; a finite volume of compost defined by the finite time interval which is a component of absolute time. These are the micro-environments in Chapman (2008).

Emerging substrate variability, the moving boundary, and environmental effects can all be incorporated seamlessly into a finite volume method.

6 Discussion

Seamlessness is a thinking tool that prompts the need to ensure the mathematical descriptions of the processes happening at the base of a complex system have an expression in the model output.

If the parameters in each of the mathematical descriptions forms a thread of seamlessness, and the thread can be traced from the fundamentals to the model output, then the resulting model will be closest to some notion of optimum. These threads are information linkages and information can be carried in many forms. The particular emphasis of this paper is on finding structural elements in the model formulation that carry seamlessness through derivational constraints.

Maintaining seamlessness between the microbiological fundamentals (taken as being a specific electron acceptor/substrate combination in a microbial kinetics model) and the particle, within the context of changing environmental factors, required three organisational considerations to cope with the ensuing constraints:

1. Where a physical manifestation occurred:
    a. the particle based, *analytical boundary* separating the air phase from the composting phase and
    b. the notion of a sub-particle scale *micro-environment* arising from using a finite element method. In this case, a finite time element generated a finite volume when diffusion laws determined that oxygen first reached a new volume of compost.
2. Where new or existing parameters adequately served the information carrying tasks. For example:
    a. VOR as a single parameter encapsulating all the complexity of microbial kinetics and carrying the result seamlessly across to diffusion laws.
    b. Z encapsulating the net effect of environmental, microbial, and diffusion law interactions. This enabled all these effects to be incorporated into the physically manifest micro-environment.
    c. Aerobic proportion (Φ) which links particle size and z with microbial kinetics and therefore links all the fundamentals to the observed composting rate of a particle.
    d. The notion of a 'combined' parameter, being one whose value encapsulates other fundamental parameters. The influence of these other aspects (which can include the model structure), is reflected in the value that is experimentally determined. For example, the effect of a diffusible substrate is incorporated into the rate constant if a non-diffusible substrate solution of diffusion law is used (Chapman, 2009b). Surface roughness is incorporated into the diffusion coefficient and E(0) (Chapman, 2009c), when not entered as a separate parameter.
3. Where mathematical procedures proved useful:
    a. Modelling constants that become variables when environmental conditions change could be retained as constants when using a finite element method.
    b. The use of overlaying, interdependent sets of equations and iteration as a way of solving the mathematical problem of over-parameterization. Only those parameters necessary for a particular set of equations need to be *computationally* visible.
    c. Boundary conditions providing mechanisms by which interactions between the computational units could be managed (e.g. Henry's law managing the boundary conditions between the air phase and the particle analytical unit).

The two physical manifestations of the model structure (analytical boundary and micro-environment) have computational advantages, particularly when finite element methods are used to find a solution by enabling environmentally affected variables to be entered as constants. Much of the composting complexity can be embedded in these structures which are easier for the human mind to envisage.

6.1 Other benefits of using model structure

If environmental effects can be incorporated in the modelling non-space formed between the end of one time element and the beginning of the next, similar manipulations could also occur to the physical manifestations in the same modelling non-space. For example:

- Moisture content and particle size are positively correlated and hence changes in moisture content can influence particle size and by its intimate association, the analytical boundary.

- Similarly, moisture content changes in a micro-environment could be reflected in z, with secondary impacts on substrate concentration and so on.
- Matric potential, capillary effect, surface tension, vapour pressure etc., could be used to determine the nature of water's association with the particle. And also the contact points between two particles.

The model task in a sense becomes one of managing the boundary conditions of the computational units. The notion of overlaying, interconnected levels of computation was used to determine high precision kinetic parameters in Chapman (2009a), and similar notions apply at the particle scale.

This approach is more aligned with segmentation techniques rather than parameter lumping techniques. Finite element methods enable separation of the computation elements (segmentation of the calculations resulting in segmentation of the parameters). For example, the temperature data set or the effects of changes in moisture content do not need to be embedded into the model. They can be an entirely separate computation. Consequently, the parameters that they would need are also removed; assisting the over-parameterization problem, yet their effect on the composting time course is retained.

All the mathematical descriptions and their parameters need analytical space in a high quality model. A useful test for model adequacy may be to test for a place for each of the most relevant parameters in a proposed model. For example, temperature affects the solubility of oxygen in water, the diffusion coefficient and the microbial rate constant. All three of these fundamental properties combine to produce an additional effect in Chapman's (2008) model, a change in the aerobic proportion. Any attempt to explain the temperature effect on the composting rate which does not allow all these fundamental properties to be expressed will contain a structural distortion (see Appendix 1 for a detailed discussion of this).

6.2 Parameter precision

The notion of seamlessness discussed above enables a logic path to be traced from a parameter to its fundamental roots, the rootedness of the parameter. Maintaining seamless however, is not the only element required for model adequacy.

A parameter may be well rooted but embedded in so much complexity that the value is unable to be determined accurately from experimental data, it may have low precision. The use of 'may' in the previous sentence alludes to the problem that arises; which is that we have no way of determining whether the calculated value is its 'true' value if r^2 is the only assessment applied.

The precision of the parameter value is inherent in the r^2, but is not exclusively explained by it. For example, the effect of the one-exponent constant in the NB parameter runs counter to the effect of the rate constant. With limited data sets a high r^2 may be obtained with a combination of $C_{1\text{-exp}}$ and k that bears little resemblance to their actual values. This author was getting a rate constant value 4 times the final value (with a high r^2) before the more rigorous structure of Chapman (2009a) was developed. Precise determination of the rate constant relies on a data set with sufficient points that the NB parameter gets close to 1. Only then can all of the observed effect be reliably attributed to the rate constant and a precise value determined. See Chapman (2009a) for the detail of this and other microbial kinetic parameters.

If the notions of rootedness and precision were normalised to 1 then total compost understanding could be seen as a function of many parameters, their rootedness and their precision.

Equation 7

$$Compost\ understanding = f_x(parameter_x \times rootedness_x \times precision_x)$$

With Equation 7, if precision is not compromised then compost understanding would be increased by incorporating more parameters in the model. However, if the over-parameterization problem were to compromise the precision of one or several parameters, then a point could exist where the benefit of incorporating an additional parameter is offset by the loss of precision.

6.3 The use of weightings

Sensitivity analysis enables identification of the parameter which has the greatest impact on the composting time course. If the total of the relative effects of all the parameters summed to 1, then each parameter will have an effect which is some proportion of 1.This is its relative weighting. For example, Chapman (2008) considered physics to be more important than biology as a descriptor of the composting time course. If there were only two parameters (physics and microbiology) then physics would have a relative weighting > 0.5 and microbiology a relative weighting < 0.5. Compromising the precision of a parameter with a low relative weighting will have less effect on the model precision than compromising the precision of a parameter with a high relative weighting.

$$Compost\ understanding = f_x(parameter_x \times rootedness_x \times precision_x \times weighting_x)$$

Any use of weightings will need to be guided by the mathematical/statistical ability to determine the precision of a particular parameter. Where precise determination of the value is difficult, then the parameter weighting can be a useful guide as to the best course of action. For example, full seamlessness would require a diffusible substrate solution for the second law of diffusion. However, the additional parameter (diffusion coefficient of substrate in the particle) and additional computational complexity invites the question as to whether to model this in its scientific form or find other ways for accounting for the known effect, such as Chapman's (2010 b) combined parameter approach. With the emergence of combined parameters, the weighting for the diffusible substrate solution would become very low, as its **effect** is included in the combined parameter. Consequently it can be ignored as a model consideration for most composting applications without affecting the model accuracy.

Similarly, the decision in Chapman (2009a) to limit the data set used to calculate the slow rate constant was a weighting exercise. Two courses of action were indicated by the difficulty in fitting the slow fraction model to the data: account for anoxic degradation in the core of the particle (this would be the preferred option to maintain seamlessness – but was programmatically more difficult) or alternatively, remove the part of the data set that contributed little to the observed time course (had a low weighting) so the calculated rate constant better explained the time course in the area where the fraction's contribution was significant (had a high weighting).

6.4 Extending the scale

A composting pile is composed of a number of particles, each at a specific location in a pile. Introducing a space element generates two considerations:

- Particles can be composed of different substrate. Different particle types require a separate computation for each type, but this is not a constraint on our understanding.
- One of the boundary conditions of each particle is the oxygen concentration C_0 and this will also exhibit spatial variability. It is related to pore-air oxygen concentrations by Henry's law.

It introduces an added level of complexity, a potential constraint on understanding as the pile oxygen concentrations need to be computed for each particle.

If the complexity of the diffusion laws/microbial kinetics/environment interaction at the particle scale is solved by the formation of computational units (micro-environments), then a natural question that arises is can a similar approach solve the emerging pile scale constraint?

The parameter which maintains seamless between the composting fundamentals and the particle's location in the pile is the oxygen concentration at the location. To accommodate the *pile* scale variability, a space element needs to be introduced into Equation 2:

Equation 8

$$Observed\ composting\ rate = \sum\nolimits_{space} (Q_{particle})$$

Where if pile oxygen diffuses from the pile surface then the second law of diffusion can be applied (Glinski & Stepniewski, 1985). A pile therefore reduces to diffusion with consumption, the same as a particle.

Due to the similarities between describing both a particle and a pile using diffusion laws, a possible useful tool for extending the scale is the notion of a *fractal analogy*. The analogy in this context being that much the same reasoning that was used at sub-particle scale also applies to the pile scale. Some of the detail may differ, a pile diffusion coefficient is diffusion in air while a particle is diffusion in water, and oxygen consumption in a particle needs to be determined iteratively as pile-air influences the particle and the particle in turn influences the pile-air. However, there is no breach of logic to extend the micro-environment concept to the pile scale.

7 Conclusion

Resolving constraints to seamlessness provides a useful mechanism that enables an overview of the underlying complexity of composting. From this perspective, the important 'bits' become apparent and can be given assistance to express in the model output. Seamlessness and constraint resolution in effect become tools to avoid being swamped by the mathematical complexity – a way of separating the trees from the forest. In part because each thread of seamlessness can be traced separately from the others, and if any compromise is needed, then the relative importance of the thread to the overall system can be considered. That is, how well the thread supports the model's purpose.

In addition, using the model structure to form computational units enables much of the underlying complexity to be embedded in a physical form that has a location in space. These physical forms (micro-environments) enable mathematics to occur either within or between them, further focussing the need on the output that is desired. The notion of an optimum structure for our models can be raised.

Within this structure there must be space for each of the contributing disciplines:

- Microbiology, first order kinetic used with consideration of electron acceptor and substrate.
- Physics, in particular diffusion of oxygen.
- Mathematics, in particular the use of the finite volume method as a tool for embracing all the contributing elements including the effect of environmental changes on model constants.

If all disciplines can fully express in the model structure for the conditions that the model is being applied to, then the model will be close to some notion of optimum.

This paper has identified methods that help locate the optimum structure for a composting model. Three techniques in particular have been identified and their usefulness shown:

- An analytical boundary based on a geometrical form.
- The formation of computational units.
- Finite element method.

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Appendix 1 – Q_10

Determining the effects of temperature on the observed Q_{10} in composting

A.1.   Derivation

The Arrhenius adjustment for temperature is in the form:

Equation 9

$$P_t = P_{t_{ref}} \times e^{C_{Ar} \times (t - t_{ref})}$$

Where: P can be any temperature adjusted parameter.

C_{Ar} = Arrhenius exponent constant ($0.069 \approx Q_{10} = 2$)

Microbial kinetics is modelled by first-order kinetics with the form:

Equation 10

$$Q(t) = k \times E(t) \times NB(t) \times \Phi(t)$$

For simplification, consider the effect of changing temperature over a very short time period, in which case the effect of a different k on the time course of E & NB can be ignored and Equation 10 reduces to:

Equation 11

$$Q(t) \propto k \times \Phi(t)$$

Where the temperature effect on aerobic proportion can be approximated by ignoring particle geometry effects, in which case the change in aerobic proportion due to temperature can be approximated by:

Equation 12

$$\Phi(t) \propto z = \sqrt{\frac{2 \times D \times C_0}{VOR}}$$

VOR is determined from the composting rate and hence is directly proportional to Equation 10, which can be further simplified by ignoring E and entering aerobic proportion as 1 (Equation 12 only applies to the aerobic portion of a composting particle). The temperature effect on k therefore explains the temperature effect on VOR.

Substitute Equation 12 into Equation 11. Let 'Arrhenius_ x' designate Equation 9 where the parameter letter is substituted for x. Then Equation 11 could be written in a temperature adjusted form as:

Equation 13

$$Arrhenius\_Q \propto Arrhenius\_k \times \sqrt{\frac{2 \times D \times C_0}{Arrhenius\_k}}$$

The observed Arrhenius exponent can then be determined for any two temperatures by rearranging Equation 9:

Equation 14

$$C_{Arr} = \left. \ln\left(\frac{Arrhenius\_Q(t_1)}{Arrhenius\_Q(t_2)}\right) \middle/ (t_1 - t_2) \right.$$

And the observed Q_{10} is the ratio of the composting rates $10^{o}C$ apart.

Equation 15

$$Q_{10} = exp^{C_{Arr} \times 10}$$

A.2. RESULTS

The temperature effects on D and C_o occur in countervailing directions and, as they occur in the same line in Equation 13, there is therefore a tendency for the change in the diffusion coefficient to cancel the change in oxygen solubility. However the value of the oxygen solubility is 2 orders of magnitude higher that the diffusion coefficient so the net effect is dominated by the drop in oxygen concentration with increasing temperature.
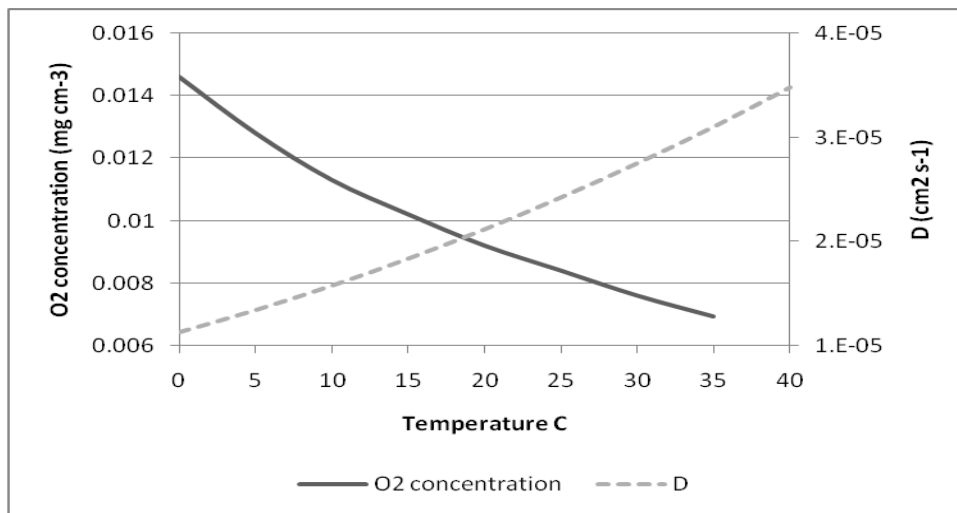
Figure 1 – The temperature effect on the diffusion coefficient and the solubility of oxygen in water. The Wilke-Chang equation was used for D and tables for solubility of oxygen in water (Polprasert, 1996).

The above equations were used to determine the observed Q_{10} that would arise from a rate constant with an actual Q_{10} of 2. The diffusion coefficient was determined using the Wilke-Chang equation (Haug, 1993) and the solubility of oxygen in water from Polprasert (1996). The solubility values were smoothed using a cubic polynomial to eliminate scatter and reveal the actual shape of the observed Q_{10}. The two values used in Equation 14 were $5^{o}C$ apart and the computed Q_{10} attached to the mean of the two values. Note this method differs slightly from the normalised approach used by Chapman (2008).

The decline in the observed Q_{10} arising from a microbial Q_{10} of 2 with increasing temperature arises from the net effect of the oxygen solubility in water and the increasing diffusion coefficient. The net

effect of this pairing is dominated by the decline in the solubility of oxygen in water, hence the decline in the observed Q_{10}.
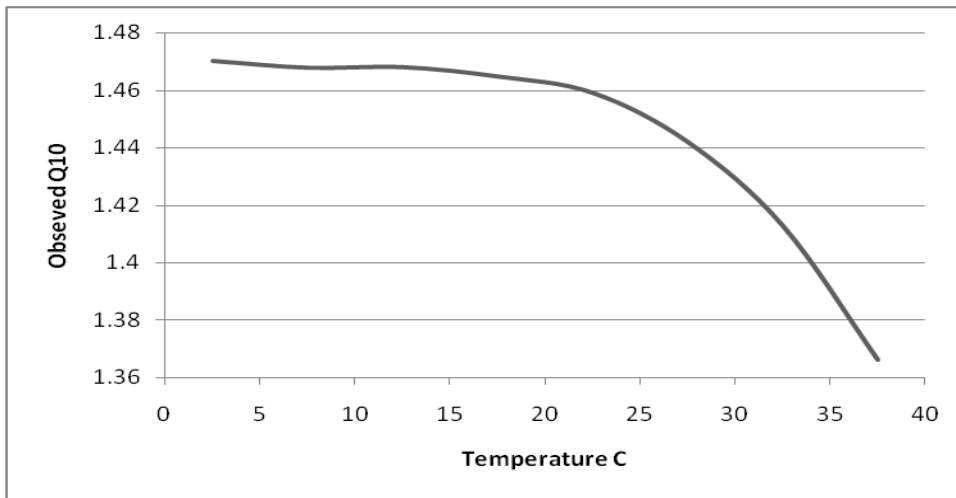

Figure 2 – The net effect on the observed Q_{10} of an *actual* Q_{10} = 2 using the above equations. The effect arises mostly from a change in aerobic proportion, with the decline due to the net effect of a declining value for the solubility of oxygen in water, and an increasing D.

Chapman's (2008) data support the theoretical arguments presented here (Figure 3).
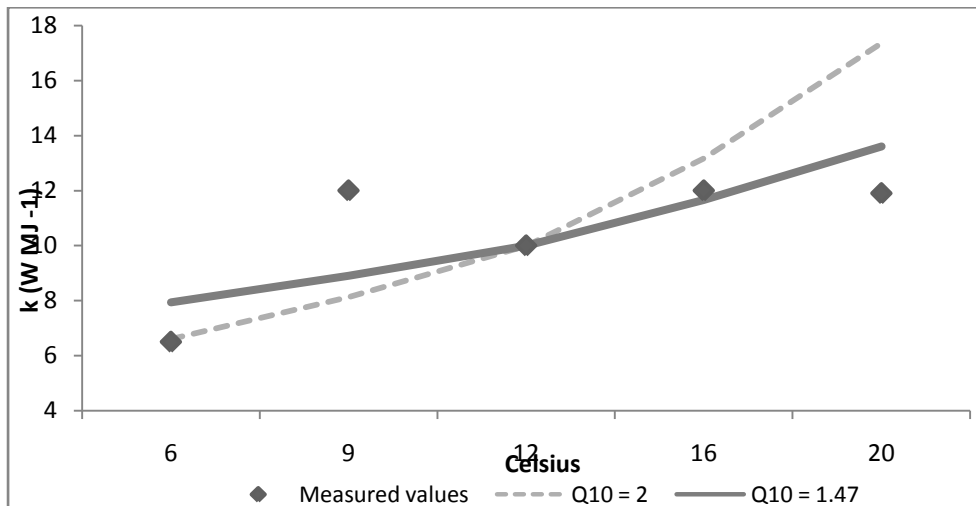

Figure 3 – Pig faeces data from Chapman (2008). The value of k in the 20°C trial was determined by the high precision method in Chapman (2009a), while the remainder of the values were determined by manually fitting the curve to the data. The method used to accommodate the temperature effect in this work differs slightly from the original; Chapman (2008) used a temperature adjusted Q of 1.49.