Modelling of soil fragmentation dynamics

R.K. Misra^{a,*} and P.J. Sands^b

^aFaculty of Engineering and Surveying, University of Southern Queensland, Toowoomba, Queensland 4350, Australia

^b39 Oakleigh Avenue, Taroona, Tasmania 7053, Australia

Abstract

An understanding of soil fragmentation during aggregate breakdown is useful in studies of erosion, tillage and traffic. Modelling efforts in soil fragmentation has largely focussed on characterisation of the size and mass distribution of aggregates using fractal approach and less on the nature and magnitude of the applied energy that produces fragmentation. In this paper, we report a model of soil fragmentation that assumes soil to comprise two fractions: a strongly bound fraction (primary particles) and a weakly bound fraction (aggregates). As the energy input on the soil increases, fragmentation of some of the weakly bound fraction produces an increase in the amount of primary particles. For simplicity, only three size classes of primary particles (sand, silt and clay) are considered. Results show that the model can be applied to soils of a wide range of structures and is capable of producing improved description of aggregate hierarchy. Application of the model to studies of tillage and erosion is discussed.

Keywords: Aggregate hierarchy; Aggregate stability; Fragmentation; Model; Soil structure

1. Introduction

A soil is often subjected to external stresses from rain, runoff, tillage and traffic, or to internal stresses (e.g. during swelling, heat generated during wetting) that may cause failure of soil material producing a change in size distribution of the original soil. We refer to this failure as soil fragmentation which is a form of structural failure similar to multiple fracture of dry, brittle earth material (Perfect, 1997). When a soil is moist, it is difficult to conceive brittle fracture or fragmentation as the soil tends to deform that changes its size but no change in number. However, when a soil is wet beyond saturation, fragmentation can occur if energy is applied externally as during the measurements of aggregate stability with wet sieving (Kemper and Koch, 1966; Le Bissonnais, 1996) or sonification (Raine and So, 1993) or during soil erosion by the impact of rain or runoff (Teixeira and Misra, 1997). Thus, soil fragmentation occurs when soils are very dry or very wet and only if there is a source of energy available to cause fragmentation.

During fragmentation the applied stresses or energy must overcome the strength of cohesive bonds between particles and/or aggregates, but independent measurement of size and applied energy is often difficult because size measurement involves an additional input during sieving (Nimmo and Perkins, 2002). Despite these difficulties, standard duration of sieving combined with sonification of soil water suspensions can improve estimation of applied energy.

^{*} Corresponding author: Fax: +61 7 46312526.

E-mail address: misrar@usq.edu.au (R.K. Misra)

Aggregate hierarchy is an aspect of soil structure that assumes fragmentation occurs along planes of weaknesses and large aggregates tend to be weak and unstable as they include pores between smaller aggregates (Dexter, 1988). Oades and Waters (1991) extended this approach to propose that the existence of aggregate hierarchy must indicate a stepwise breakdown of aggregates when the disruptive energy applied to soil is increased. If the aggregates of a soil breakdown to release silt and clay directly, then aggregate hierarchy does not exist. They used a graphical approach of particle and aggregate size analysis to distinguish soils with and without aggregate hierarchy. Tipkötter (1994) focussed on the breakdown of mesoaggregates ($60-2000 \mu m$) into smaller particles to determine the optimum energy required to disrupt aggregates and recognised two forms of mesoaggregates: fragile and stable. More recently, Field and Minasny (1999) applied an empirical approach using the kinetics of first order reaction to describe breakdown and dispersion of soil aggregates into silt and clay size.

This paper describes a fragmentation model based on the mass balance in various size fractions including a strongly bound fraction which is stable and similar to primary particles (sand, silt or clay) and aggregates of these sizes that are weakly bound and thus prone to fragmentation with accumulated input energy.

2. Theory

In the fragmentation model described here we consider soil to be composed of only three size classes of soil particles and aggregates, and breakdown of large aggregates occurs into smaller aggregates and particles with unidirectional transport of material at any given level of applied energy (Fig. 1). Thus, we ignore possible simultaneous aggregation and fragmentation.



Fig. 1. Schematic diagram of classes $(C_1...C_3)$ of soil particles and aggregates of decreasing size. Arrows indicate the direction of aggregate breakdown and transfer of particles and aggregates from higher to lower size class. k_{ij} are rates of mass transfer of soil from the weakly bound fraction (W_i) in each class. The strongly bound fraction (S_i) represents stable particles in each size class.

Let C_i be the size classes of aggregates and particles with $C_1 > C_2 > C_3$. These sizes closely correspond with the size of sand (20-2000 µm), silt (2-20 µm) and clay (<2 µm). Let M_i be the total mass of aggregates in the size class i (i = 1, 2, 3). In each class except the smallest, there are two types of aggregates: strongly bound aggregates that can not be fragmented easily, and weakly bound aggregates that can be fragmented into aggregates and particles of smaller size. The pattern of aggregate breakdown and transport of aggregates into various size classes is as shown in Fig. 1. The rate constants k_{ij} apply to the breakdown of the weakly bound aggregates. Also, when aggregates break down to class C_i , it is assumed that a fraction γ_j of the fragments produced in class C_j will be in the strongly bound form, and the remainder in the weakly bound form and hence can not be further fragmented. In the case of the terminal size class (C_3 or clay) there is no need to differentiate between strongly and weakly bound aggregates, as these are particles with no scope of further breakdown.

Let S_i and W_i be the mass of soil as strongly and weakly bound soil materials of size class *i*. Then at any given input of energy *E* applied to soil,

$$M_i(E) = W_i(E) + S_i(E) \tag{1}$$

From the assumptions of the model described in Fig. 1, the differential equations for the masses of the weakly bound materials in each size class (for three size classes) are:

$$\frac{dW_1}{dE} = -(k_{12} + k_{13})W_1, \tag{2a}$$

$$\frac{dW_2}{dE} = k_{12} (1 - \gamma_2) W_1 - k_{23} W_2 \text{ and}$$
(2b)

$$\frac{dW_3}{dE} = k_{13} (1 - \gamma_3) W_1 + k_{23} (1 - \gamma_3) W_2$$
(2c)

and for the strongly bound components

$$\frac{dS_1}{dE} = 0, \ \frac{dS_2}{dE} = k_{12}\gamma_2 W_1 \text{ and } \frac{dS_3}{dE} = k_{13}\gamma_3 W_1 + k_{23}\gamma_3 W_2$$
(3)

The rate of breakdown is dependent on the initial amount of material present and the negative sign indicates a decrease in the initial amount. Eqs. (1-3) also ensure that the system conserves mass across the size classes. The initial conditions are the mass of aggregates S_{i0} and W_{i0} in each size class at the initial energy, E = 0. If only the total masses M_{i0} are known, these are distributed between the strongly and weakly bound fractions in the ratio γ_i to $(1-\gamma_i)$: $S_{i0} = \gamma_i M_{i0}$ and $W_{i0} = (1-\gamma_i)M_{i0}$.

Equations (2-3) are a system of simple linear differential equations with constant coefficients and can be solved using the standard matrix method for such equations. The general solutions for $W_i(E)$ are

$$W_{1}(E) = a_{11}e^{-(k_{12}+k_{13})E}$$

$$W_{2}(E) = a_{21}e^{-(k_{12}+k_{13})E} + a_{22}e^{-k_{23}E}$$

$$W_{3}(E) = a_{31}e^{-(k_{12}+k_{13})E} + a_{32}e^{-k_{23}E} + a_{33}$$
(4)

where

 $a_{11} = W_{10}$,

$$a_{21} = (1 - \gamma_2) \frac{k_{12}}{k_{23} - (k_{12} + k_{13})} a_{11} \qquad a_{22} = W_{20} - a_{21}, \ a_{31} = -(1 - \gamma_3) \frac{k_{13}a_{11} + k_{23}a_{21}}{k_{12} + k_{13}}, a_{32} = -(1 - \gamma_3)a_{22} \qquad a_{33} = W_{30} - a_{31} - a_{32}.$$
(5)

Integration of Eqs (3) gives the $S_i(E)$:

$$S_{1}(E) = S_{10}$$

$$S_{2}(E) = S_{20} + \gamma_{2} \frac{k_{12}a_{11}}{k_{12} + k_{13}} \left(1 - e^{-(k_{12} + k_{13})E}\right)$$

$$S_{3}(E) = S_{30} + \gamma_{3} \frac{k_{13}a_{11} + k_{23}a_{21}}{k_{12} + k_{13}} \left(1 - e^{-(k_{12} + k_{13})E}\right) + \gamma_{3}a_{22} \left(1 - e^{-k_{23}E}\right)$$
(6)

Eqs. (4-6) provide the variation in strong and weakly bound components of soil aggregates in three size classes at various levels of applied energy. They are characterised by the three rates of fragmentation k_{12} , k_{13} and k_{23} , the fractions γ_i of newly formed aggregates in each size class that are strongly bound, and the initial mass of aggregates in each size class. It should be noted that for the class C₃, $\gamma_3 = 1$ because this represents the clay size particles which are strongly bound and stable.

3. Experimental data

Testing and evaluation of the model was based on unpublished data from aggregate fragmentation experiments of Teixiera (1998). These data were obtained for soils at three commercial eucalypt plantation sites in Tasmania, namely Dover (D), Ridgley (R) and Maydena (M). All were from the upper 0.2 m at each site and their properties were given in Teixeira and Misra (2005). Soil D was poorly aggregated loamy sand, soil R strongly aggregated clay, and soil M a clay loam with low aggregate stability when wet.

3.1 Experimental conditions

Soils were dried and processed to reduce aggregates to ≤ 8 mm. An ultrasonic probe (Dawe Soniprobe model 1130A) at a frequency of 23 kHz was used for sonification of soil (8.3 g air-dry) water (50 g) suspensions. The temperature of suspension was measured continuously with a thermistor probe attached to a datalogger. The power output readings of the ultrasonic probe was measured using the energy balance approach of Raine and So (1993) and Roscoe et al. (2000). Each soil (D, R and M) was replicated three times and soils were chosen randomly for sonification. For each soil, eight different durations of sonification were used: 15, 60, 100, 180, 360, 540, 720 and 900 s, which corresponded to an ultrasonic energy input of 57, 229, 381, 686, 1372, 2057, 2743 and 3429 J g⁻¹ for all soils. During sonification temperature of the suspension was kept below 45 °C to avoid any possible influence of high temperature on aggregate stability. After sonification, the suspension was transferred to a 1 L measuring cylinder by passing it through a sieve of 53µm aperture via a funnel. Excess deionised water was used to wash the soil through the sieve, and to fill the cylinder up to the 1 L mark. The soil retained on the sieve (fraction \geq 53 µm) was dried at 105 °C for 24 hours and its weight determined. Particle size analysis (PSA) of $<53 \,\mu\text{m}$ was measured with the pipette method of Gee and Bauder (1986) to obtain the proportion of silt and clay. PSA was also made for soil samples simply immersed in water but without sonification to determine the effect of immersion wetting on initial aggregate size distribution of the soil samples at zero energy input. At each

energy input, the collected data represented both aggregates and particles in a given size range for 3 size classes, 20-2000, 2-20 and $<2 \mu m$.

3.2 Data analysis

The model was implemented in Excel and fitted to the experimental data for the soils D, R and M using SOLVER to adjust the value of all coefficients by minimising the residual variance between the observed and fitted data. Standard error of estimates and other statistics were obtained using SOLVERSTAT (Comuzzi et al., 2003).



Fig. 2. The relationship between the mass of fragmented aggregates in three size classes (sand, silt and clay) and applied energy. Observed data are shown as symbols and fitted data as lines.

4. Results and Discussion

Fig. 2 shows the dynamics of fragmented aggregates with increased energy input from sonification. The fragmentation model described the data well for soils D and R, but to a lesser extent for soil M (Table 1). As mentioned before, soil M has very low stability and required a small amount of energy for breakdown. For all soils, the proportion of material in silt (2-20 μ m) and clay (< 2 μ m) sizes increased initially with increasing amount of energy and reached steady-state or stable proportion afterwards. Similar trends have been reported for several vertisols with ultrasonic dispersion (Raine and So, 1993, Field and Minasny, 1999). From the values of parameters of the model for the three soils shown in Table 1, some aggregate hierarchy existed with an indication of stepwise breakdown of aggregates in all the three soils with rate constants (k_{12} , k_{13} and k_{23}) > 0. A zero value for γ_2 for soil R suggests low aggregation of this soil in the silt size fraction.

Table 1. Coefficient of determination (r^2) and parameters of the fragmentation model fitted to the data in Figure 1. Number in parenthesis denotes standard error of estimate.

Parameters	Soil D	Soil R	Soil M
r^2	0.999	0.996	0.0.982
k_{12}	0.0043 (0.0009)	0.00027 (0.00006)	0.0119 (0.0013)
<i>k</i> ₁₃	0.0004 (0.0009)	0.00010 (0.00004)	0.0093 (0.0012)
<i>k</i> ₂₃	0.0027 (0.0050)	0.00002 (0.00006)	0.0033 (0.0015)
γ_1	0.8495 (0.0054)	0.40000 (0.0824)	0.4729 (0.0085)
γ_2	0.8159 (0.1546)	0.00000 (0.0000)	0.7669 (0.0395)

A large body of evidence in the literature shows that when soils are exposed to disruptive forces (due to weathering, erosion and tillage) they experience less equivalent energy than the maximum energy (\sim 3000 J g⁻¹) used in sonification studies to break down

aggregates. The energy dissipated by various tillage equipment is within a range of 0.1-0.3 J g⁻¹ (Russell, 1973; Watts et al., 1996). Similar estimates are also available in erosion studies. For example, an estimate by North (1976) showed that a rainstorm of 75 mm h⁻¹ during one hour could dissipate 12 J g⁻¹ of energy into the soil surface. In most natural rainstorms, energy of rain would be < 0.05 J g⁻¹ (Wischmeier and Smith, 1978).

These estimates suggest that the disruptive forces experienced by soils and the associated energy during 10-15 min of sonification or with a standard method of particle size analysis are too extreme when compared with the natural forces from rain, runoff and tillage. Despite such wide disparity in the energy required for fragmentation in dispersion studies and erosion, the structural behaviour of soils from mechanical stresses and applied energy from various sources remains fairly similar. For example, studies by Teixeira and Misra (1997) indicated the susceptibility of the soils to wetting to be in the order M (very susceptible) > D > R (least susceptible). This is consistent with the data presented in Fig. 2. Thus, the model presented here could be useful to indicate erosion behaviour of soils and possibly the characteristic of sediment generated during erosion.

References

- Comuzzi, C., Polese, P., Melchior, A., Portanova, R., Tolazzi, M., 2003. SOLVERSTAT: a new utility for multipurpose analysis. An application to the investigation of dioxygenated Co(II) complex formation in dimethylsulfoxide solution. Talanta 59, 67-80.
- Dexter, A.R., 1988. Advances in characterization of soil structure. Soil Tillage Res. 11, 199-238.
- Field, D.J., Minasny, B., 1999. A description of aggregate liberation and dispersion in A horizons of Australian vertisols by ultrasonic agitation. Geoderma 91, 11-26.
- Gee, G.W., Bauder, J.W., 1986. Particle-size Analysis. In: Klute, A. (Ed.) Methods of Soil Analysis. Part I. Physical and Mineralogical Methods, Agronomy Monograph no. 9, American Society of Agronomy and Soil Science Society of America, Madison, pp 383-411.
- Kemper, W.D., Koch, E.J., 1966. Aggregate Stability of Soils from Western United States and Canada. Agricultural Research Service, Technical Bulletin no. 1355, USDA, Washington.
- Le Bissonnais, Y., 1996. Aggregate stability and assessment of soil crustability and erodibility: I. Theory and methodology. European J. Soil Sci. 47, 425-437.
- Nimmo, J.R., Perkins, K.S., 2002. Aggregate stability and size distribution. In: Dane, J.H., Topp, G.C. (Eds.) Methods of Soil Analysis. Part 4. Physical Methods, Soil Science Society of America, Madison, pp 317-328.
- North, P.F., 1976. Towards an absolute measurement of soil structural stability using ultrasound. J. Soil Sci. 27, 451-459.
- Oades, J.M., Waters, A.G., 1991. Aggregate hierarchy in soils. Aust. J. Soil Res. 29, 815-828.
- Perfect, E., 1997. Fractal models for the fragmentation of rocks and soils: a review. Engineering Geol. 48, 185-198.
- Raine, S.R., So, H.B., 1993. An energy based parameter for the assessment of aggregate bond energy. J. Soil Sci. 44, 249-259.
- Roscoe, R., Buurman, P., Velthorst, E.J., 2000. Disruption of soil aggregates by varied amounts of ultrasonic energy in fractionation of organic matter of a clay Latosol: carbon, nitrogen and δ^{13} C distribution in particle-size fractions. European J. Soil Sci. 51, 445-454.
- Russell, E.W., 1973. Soil Conditions and Plant Growth. 10th edition. Longman Group Limited, London.
- Teixeira, P.C. 1998. Erosion and nitrogen loss from forest soils in relation to soil structure. PhD thesis, University of Tasmania, Australia.
- Teixeira, P.C., Misra, R.K., 1997. Erosion and sediment characteristics of cultivated forest soils as affected by the mechanical stability of aggregates. Catena 30, 119-134.
- Teixeira, P.C., Misra, R.K., 2005. Measurement and prediction of nitrogen loss by simulated erosion events on cultivated forest soils of contrasting structure. Soil Tillage Res. 83, 204-217.
- Tipkötter, R. 1994. The effect of ultrasound on the stability of mesoaggregates (60-2000 μm). Z. Pflanzenernähr. Bodenk. 157, 99-104.
- Watts, C.W., Dexter, A.R., Longstaff, D.J., 1996. An assessment of the vulnerability of soil structure to destabilisation during tillage. Part II. Field trials. Soil Tillage Res. 37, 175-190.
- Wischmeier, W.H., Smith, D.D., 1978. Predicting Rainfall Erosion Losses. A Guide to Conservation Planning, Agricultural Handbook no. 537, USDA, Washington.