

## MODELS OF PARTICLE AGGREGATION AND THEIR USEFULNESS

*M.F. De Boodt*

State University of Ghent, Coupure Links 653, B-9000 Ghent, Belgium

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**A b s t r a c t.** Two major approaches of modelling aggregation of soil particles (morphological and virtual) have been discussed. Both approaches were found to be complementary and necessary to gain insight in the agglomeration processes involved.

**K e y w o r d s:** particle aggregation, models, soil structure

### INTRODUCTION

Particle aggregation is a major concept in the assessment of soil structure. The latter word is often used in soil science. It is derived from the Latin word 'struere', meaning the way a number of stones or particles are building up a unity of stony or particle entities. In this respect the bonds between the particles are very important because they determine for a major part the stability of the aggregation, i.e., the way they are put together. The bonds can be a water meniscus as well as any more permanent, often colloidal substance such as organic matter and/or metallic hydroxides or complexes of both. Besides, more solid material can also act as a cementing agent like calcium salts or clay particles or consolidated iron-organic matter complexes, sometimes enriched with manganese.

It is obvious that there exists a large number of possibilities to put soil particles together. With suitable cementing agents an optimal substratum for plant growth can be obtained. The major questions are often about the mechanisms behind it and which arrangements are

the best? It is understood that there is not a single and simple answer to it. It depends on the soil texture, the climatological conditions, the aerobic or anaerobic situation, the depth of the soil layer and the genetical development of the soil profile and its use. So many factors have to be taken into account in order to appreciate a given way of particle aggregation.

To simplify the questions, models can be very useful as they can serve as a guidance. Therefore an appropriate model should meet the following requirements:

a) providing a visual picture of particle arrangements which are considered to be appropriate for the texture, the site and the use one wants from the structured soil;

b) providing an idea of what is possible or optimal in terms of the spatial distribution of the solid material allowing the existence of voids and pores which have well defined functions in a substratum for plant growth or for any other aim [7];

c) providing an insight why a given aggregation will resist better than another one the stresses and strains due to climatological conditions or mechanical impacts. They can be biological as a consequence of plant growth or man-made as a consequence of sowing, harvesting and other cultural activities.

When putting a great number of different items together ending up in a large number of

possible configurations, one can use models to bring clarification in the interactions and role of the particles involved. The approaches can be quite different. Two major ways of endeavour can be recognized for modelling the aggregation of the soil particles.

The first one (Fig. 1) is the direct consequence of the observation of thin slides most often made of horizontal cuts through aggregates. Depending of the scale of observation using a petrographical microscope, the aggregation will be assessed as homogeneous massive, bulky or heterogeneous. In this case the matrix, the particles and pores can be clearly recognized (Fig. 1a and 1b). The more sandy the assembled particles are the more transparent the picture will be. The matrix, the coatings, the mottles, the nodules and also the porosity are easily recognized. This will be a very valuable approach in studying the genesis of a soil profile. Taking more observation points in the profile the structural development and the processes of soil development can be studied in depth. Also the role of biological activities can be assessed illustrating how they follow or not the eluviating and illuviating processes in the subsequent soil horizons.

These kind of models, known as the analytical approach, has been used both by soil physicists [8], as well as by soil pedologists [5].

The second type of model has been developed with a completely different approach. It does not show a real picture but a virtual one based on physical, chemical and physico-chemical laws. It helps us to understand the aggregating behaviour of the different substances in the soil, be they solid and crystalline or colloid and amorphous or interstratified in nature.

These types of models are represented in drawings completely conceived in the human mind reflecting the picture of aggregation as it can be deduced from basic sciences and the deductions it stands for (see Fig. 2). These representations of particles in structural units are often seen as vertical cuts through aggregates in which the mutual positions and the size of the soil particles and their clusters as well as the sizes of the voids and pores are of major

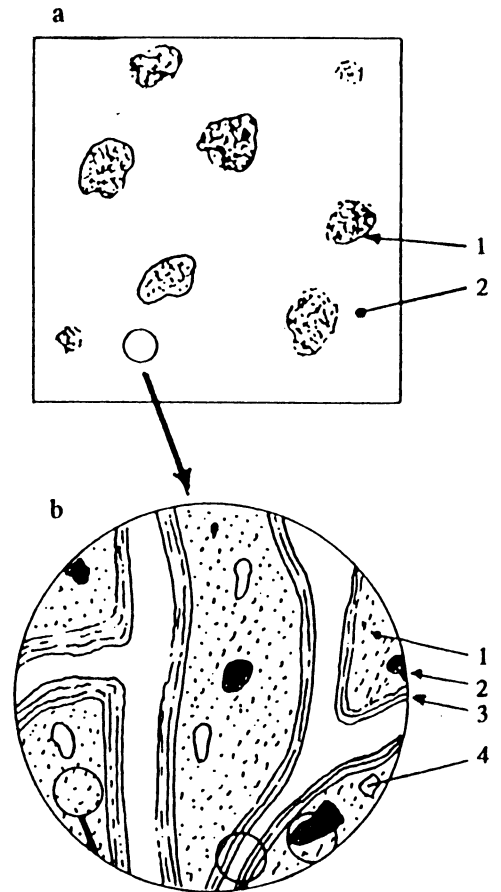
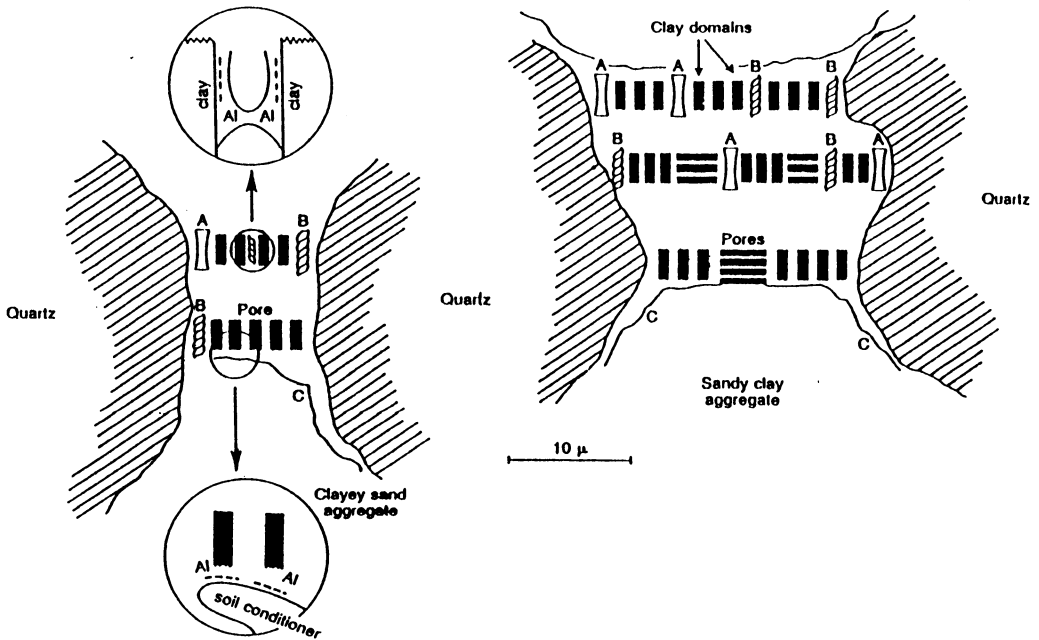


Fig. 1. Homogeneity-heterogeneity at different scales of observation as shown by thin sections. a) Mottled clay (field sample): two homogeneous zones can be distinguished: with the naked eye: 1 - reddish mottles in a 2 - yellowish matrix. b) At low magnification the homogeneous matrix is seen to be composed of four homogeneous units: 1 - matrix, 2 - iron oxyhydrate nodules, 3 - clay coatings and 4 - pores (after Bullock *et al.*, [2]).

importance. In such models the micro-aggregates are clearly distinct from the sandy particles together with the structural units when building up macro-aggregates. To make the relative position of the particles versus one another clear and distinct, it has been imperative to enlarge the size of the clay particles versus the sandy grains. It is indeed understandable, when one wants to show dispersed or flocculated clay particles, coatings or bonds between



**Fig. 2.** Model of a soil aggregate stabilized by organic matter or by soil conditioners showing clay domains, organic matter, polymers and quartz. The size of clay domains is strongly exaggerated: A - weak linkage due to water meniscus, B - linkage due to humus or sesquioxides, C - linkage due to micelles or polymers (soil conditioners). Dotted lines indicate H-bonding. Notice also the role of aluminium ions. Magnified inserts: organic matter-clay interaction or polymer-clay interaction (after Emerson [6] and De Boodt [3,4]).

sandy particles the space needed for each differs considerably as their sizes are so different. The clay domains or flocculates are of the order of microns while sandy grains are 50 to 100 times larger. These types of models are not true pictures but virtual ones which are subjected to changes as the insights in aggregation mechanisms progress. This approach has been used by a number of researchers, e.g., Emerson [6], De Boodt [3,4], Russell [10], and others.

**MORPHOLOGICAL CHANGES**

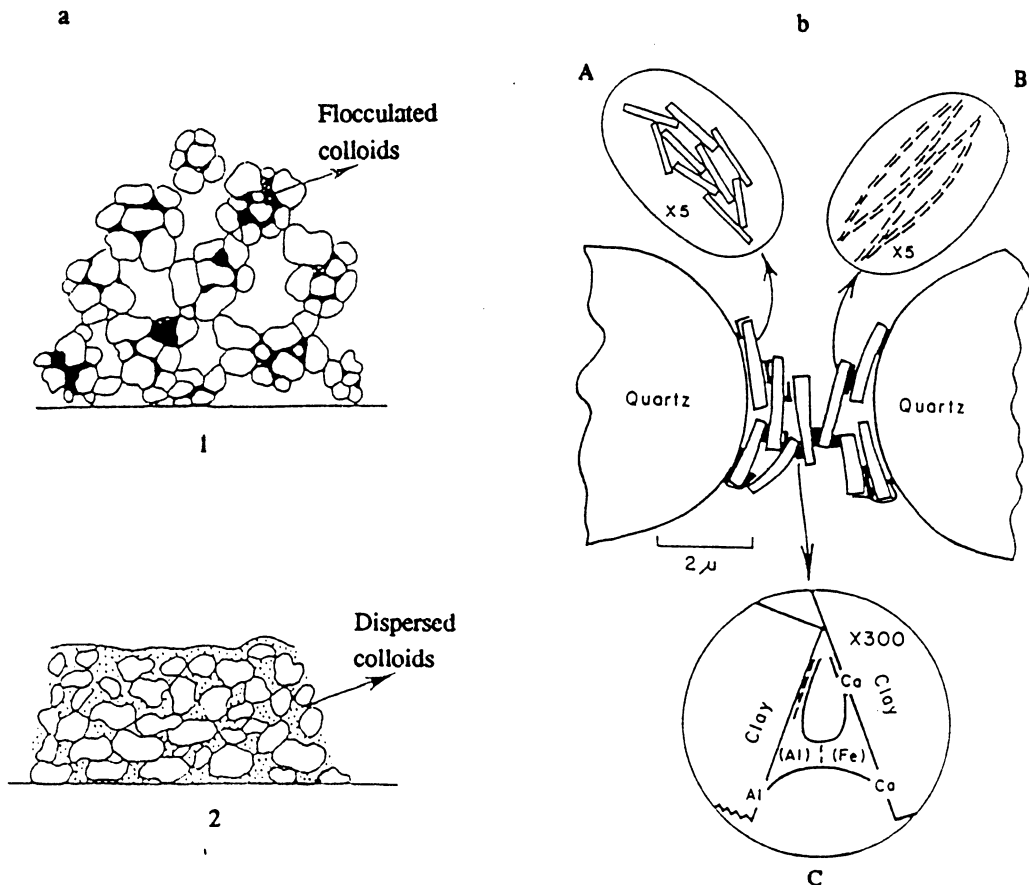
In agriculture, a number of cultural practices are known to favour good tilth. They can be mechanical, physical, chemical or biological [10]. This subdivision is purely theoretical as in practice it is mostly a combination of all these which will promote the good structuration and hence the particle aggregation. The best lasting effect is obtained when physico-

chemical processes are involved followed by the biological ones. Mechanical effects are the most rapid and often the most spectacular to be obtained but also the least resistant against destructive forces [9].

**PHYSICO-CHEMICAL IMPACT**

The way different soil particles are aggregated is certainly an important aspect in modelling. However, in a drawing of a given model the structural stability is not so apparent although it is an essential part of particles aggregation. When models are well drawn they can suggest, to some extent, the degree of aggregate stability as can be seen in the pictures 3a and 3b, respectively due to Duchaufour [5] and Emerson [6]. With a few lines it becomes clear that the aggregate stability is present in Fig. 3a-1 and Fig. 3b but not in Fig. 3a-2.

In Fig. 3b the colloidal substances are shown in a more detailed way than in Fig. 3a.



**Fig. 3.** Two virtual models of soil aggregate (a and b) due to Duchaufour [5] and Emerson [6], respectively. a: 1 - crumble structure with bonds of flocculated colloids, 2 - compact structure with matrix of dispersed colloids, virtual model of a soil aggregate stabilized by organic matter showing clay domain, organic matter and quartz. Magnified inserts (b): A - kaolinite domain, B - illite domain, and C - organic matter-clay interaction. Dotted lines indicate H-bonding.

As one is dealing with virtual models, in the future still more attention will be paid to the very fine particles which are responsible for the bonds. They can be clays, oxyhydroxides from aluminium, iron, manganese, etc. Also carbonates of calcium and sodium can be present as well as sulphates besides organic matter and organo-mineral complexes. The degree of flocculation, in first instance, will depend on the salts and ions present like  $\text{Ca}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$  as well as on the pH. The colloidal material is dispersed when the mentioned ions are practically absent but replaced by  $\text{Na}^+$  and  $\text{HCO}_3^-$  having a pH around or above 8.

The role of the flocculated colloids, a cementing agent making up the bonds, can be photographed as shown in Fig. 4. This means that a virtual model can become a realistic one. Indeed, when sandy particles are treated with an emulsion of organic micels, adding  $\text{Ca}^{2+}$  can break the emulsion and the micels gather under the meniscus thus forming the bonds which can be seen in the 100x magnified picture. Aggregation of sandy particles is a special issue as the colloid content is often not more than a few percentages. In this case the role of organic matter and fungi metabolites become important as shown in Fig. 4.

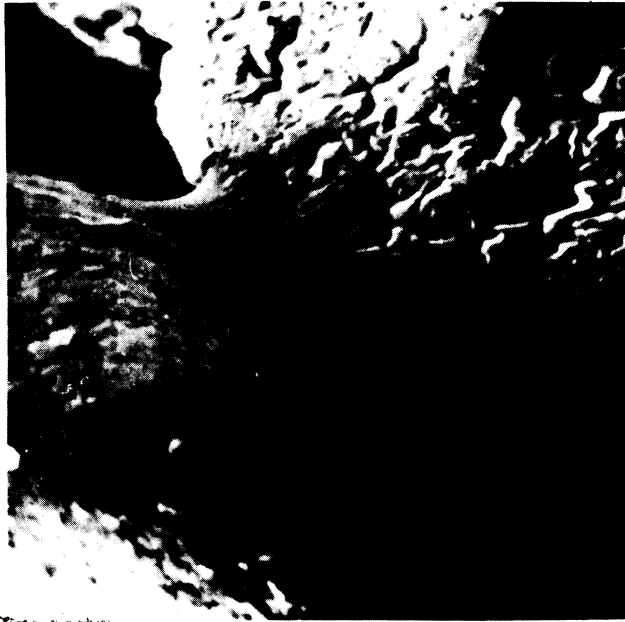


Fig. 4. Flocculated organic colloids are forming the bridge between sandy particles to form stable aggregates (Magnification 100x).

### Useful examples

From the above, it is obvious that the virtual models can be very useful. When crumbled, compact, blocky, platy or other types of structure have to be pictured and the morphology of the aggregation is known, the physico-chemical situation of the soil can be inferred as illustrated by the examples here after.

When a soil contains about 10-15 % of clay and the texture is evaluated to be loamy, dispersion of the colloids often occurs. The way the model has to reflect it is shown on Fig. 3a-2. Indeed, dispersion occurs when the pH is alkaline due to the presence of alkaline ions. If alkali earth ions have the major share in the ionic composition the pH might still be higher than seven but the colloids will be flocculated. In such circumstances the model will show a crumble structure.

If the pH is lower, a more stable structure will appear when  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$  and  $\text{Al}(\text{OH})_n$  complexes are present. So the major information to be pictured is the role of the pH and also the

nature of the cations and anions together with the composition of the organic matter. In summary the information is as follows:

pH > 8, plus  $\text{Na}^+$ ,  $\text{OH}^-$ ,  $\text{HCO}_3^-$ :

dispersion, poor aggregation;

pH 6.5-8, plus  $\text{Ca}^{2+}$ :

flocculation, good aggregation;

pH 5-6.5, plus  $\text{Ca}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Al}(\text{OH})_n$ ,  $\text{Fe}^{3+}$ :

acid soils, good structure;

pH 4-5, plus moder or mor organic matter:

organo-alumino-ferric complexes will be fixed on the colloids and will disperse them, poor aggregation.

### PHYSICAL INTERACTIONS

The cementing agents in aggregates can be of very different nature:  $\text{CaCO}_3$ , oxyhydroxides, aluminium, iron oxyhydrates, silica, organic matter, etc. When flocculating agents are present they will promote precipitation. Alternation of humidity and drought will make the precipitates insoluble and hard. It is often

followed by the crystallization of the most abundant elements. They will form well defined massive concretions inside the aggregates (see Fig. 1).

Changes in moisture content of clayey soil favours changes in volume due to shrinking and swelling. This promotes voids isolating partially or completely structural units, characterized by well defined edges. The shape, the size and the quantity will depend on the pedoclimate, the clay type, the size of the particles and in particular on the presence or absence of organic matter.

When a soil is ploughed in relative dry circumstances, it will fractionate in clods as a consequence of physical forces. It can be recognized by the angular shaped clods, isolated by sharp clear cut voids. When such a soil aggregation is modelled these features must be apparent. This type of conglomerates is morphologically quite different from the aggregates obtained by physico-chemical interactions, known as flocculation or dispersion processes. These aggregations are characterized by flocculated cement-bridges between the structural units.

A third type of aggregation, i.e., namely the one of a biological origin shows yet other features which can be easily recognized and hence can be reproduced in the models.

#### BIOLOGICAL INTERACTIONS

Aggregates formed as a consequence of biological activities have their own morphology and a marked stability. They are abundant in the upper soil layers and dark colour marks the presence of organic matter. The activity of the microflora can be seen from the great number of very fine pores.

The meso- and macrofauna are mainly active through the transit of the soil particles in their intestines. This is more than just a mixing process as at that moment the digested particles are cemented by the internal secretions (Fig. 5). Other metabolites contribute also to the formation of spheric dark aggregates. So one can observe small spheres, beads and crumbs in the soil where an active biological life

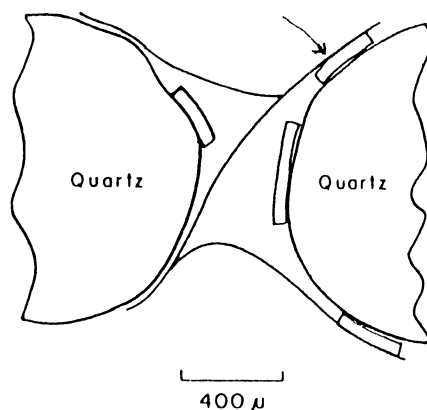


Fig. 5. Model for interaction of mineral particles and fungal hyphae. The smaller particles represent clay aggregates [6].

exists. These macro-aggregates are often due to the activities of enchytraeides, beetles and worms. These features are easily reproduced by the drawings supporting the modelling.

#### CONCLUSIONS

Like in so many scientific branches, modelling has been a very useful tool in:

- conveying concepts on how aggregation of soil particles is built up morphologically,
- putting forward the chemical, physical and biological laws which might govern the building up of the aggregation and hence how it might be improved.

Modelling aggregation of soil particles can be split-up in two major approaches. The morphological one is based on observation mainly due to thin slides observation and analysis. The other one does not reflect real pictures but can be classified as the virtual modelling. Both approaches are necessary to gain insight to the agglomeration processes involved as they are complementary. During the last decade most progress has been made by the virtual picture approach. Examples are given how the use of models can be helpful in picturing the different physical, chemical and biological interactions in particle aggregation processes offering possibilities for technical application of soil science.

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