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A new approach for large scale simulation of complex spatial processes: the 3D soil evolution model mARM

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Modelling complex spatially distributed processes over large areas is a challenge facing many environmental disciplines. In some cases even when the physics and relationships are known they are too complex for large scale simulations. In the field of pedogenesis researchers have a good understanding of the physical processes affecting soil evolution but struggle with predicting their spatial and temporal variability. Spatial and temporal relationships in soil properties are known to be a significant factor in many hydrological and geomorphological processes. Modelling detailed distribution of soil properties is therefore important but yet to be fully achieved over large scales.

In order to predict the spatial distribution of soil properties a new approach is needed in the form of detailed large spatial and temporal scale simulation of soil evolution. These simulations could not be done using conventional physically-based model due to their computational complexity and limited dimensionality. A more comprehensive and computationally efficient algorithm is needed. Our solution is a new pedogenesis model called mARM. mARM (matrices-ARMOUR) uses transition matrices in conjunction with physically-based equations to achieve a highly modular and computationally efficient modelling platform. This new approach and the modularity of the mARM platform allow us to simulate a variety of soil processes over long periods and large areas (millions of years and 1000's pixels).

In its latest version (presented here) mARM has been extended to three spatial dimensions (mARM3D) by adding a soil profile component. This 3D model is a major breakthrough in pedogenesis modeling since this is the first time profile as well as surface processes are simulated over large scales. The modularity of mARM3D allows us to use it as a virtual laboratory to examine a variety of soil processes and relationships such as:

- Depth-dependent weathering rate equations (presented here)
- Runoff fluctuations (as a result of climate or environmental changes)
- Weathering geometry (proportion of particle split)
- Weathering-Erosion relationships and rates

In addition to the above capabilities, mARM is intended to be integrated as a component in a landform evolution model (i.e. TelluSim) which will allow such a model, for the first time, to account for time and space variation in soil properties. In this paper we describe the mARM3D model framework which can potentially be used in other complex spatial models. We also present selected results from the mARM3D simulations at hillslope and landscape scale which show the effect of profile weathering physics on surface soil distribution.

Keywords: *Soil, pedogenesis, catchment scale, landform evolution*

1. INTRODUCTION

Many hydrological and geomorphological processes have strong links to soil properties. Soil erosion and runoff, for example, may vary in response to different soil types and conditions. However, many large scale hydrological and geomorphological models do not account for varying soil properties for two main reasons. (1) The spatial distribution of these properties is unknown and (2) the soil related relationships in the model are uncertain. Therefore many modelers tend to assume homogeneity of soil in their modeled domain despite its potential significance.

Soil properties not only vary in space but in time. Soil constantly evolves as a function of sediment transport and weathering processes. It may reach a state of dynamic equilibrium in which the rate of soil production is matched by soil removal and tectonics. But when simulating long-term processes such as landform evolution the changes in soil properties may be significant (Minasny and McBratney, 2006) and therefore can affect the accuracy of the simulation.

In order to address the above issues a soil evolution (pedogenesis) model is required. The importance of soil evolution modelling, for geomorphology and soil studies, has been well documented in the literature (e.g. Minasny and McBratney, 1999). Most qualitative pedogenesis models are based on empirical relationships between soil properties and landform (Minasny et al. 2008). There is an increasing recognition that a more mechanistic approach is required for simulating such a complex system (Minasny and McBratney, 2006). Minasny and McBratney (2006) have used a mass-balance model to classify pedogenesis units on a landscape and Salvador-Blanes et al. (2007) have presented a process-based profile evolution model. Minasny et al. 2008 have recognized the need for linking landscape and profile processes as the main challenge of pedogenesis modelling.

Here we present the mARM soil evolution modeling framework. It is based on a novel approach which coupled transition matrices numerics with physically based equations. This approach is extremely computationally efficient which allows large scale simulation (spatial and temporal) of complex systems. mARM simulates surface and profile processes over large areas (catchment) and long time span (millennia). Its process physics are based on the one-dimensional ARMOUR model (Willgoose and Shermaan, 2006). We also present selected results from hillslope and catchment scale simulations.

2. MODELLING APPROACH

The surface simulation in mARM is based on the one-dimensional ARMOUR model (Willgoose and Shermaan, 2006). It simulates two main processes: surface armouring and physical weathering of surface particles. The armouring process encompasses selective removal (erosion) of particles by overland flow and weathering is modeled by splitting the particles at a pre-defined rate and geometry. In ARMOUR these processes are simulated by detailed tracking and manipulating of sediment and grading mass and using real runoff datasets. This detailed physically-based approach is computationally demanding and therefore limited in terms of spatial and temporal domains. We used transition matrices numerics to express these physical processes and significantly reduce computational run-time (by a factor of approximately 10^5). The mARM modelling concept, physics and math are described in details in Cohen et al. (2009a,b). Below is a conceptual description of the model.

2.1. Surface armouring (erosion)

Soil grading is represented by a vector ($\underline{G_k}$) whose entries are the proportion of a grading size class (k) in the simulated domain (a thin surface layer in this case) sediment budget. The size range and number of grading classes is defined by the user. Erosion rate (E) represent the proportion of the surface layer volume (or mass) removed in one time step t. The erodability of each size class (Er_k) is represented by the armouring transition matrix.

$$\begin{bmatrix} G_1 \\ G_2 \\ \vdots \\ G_k \end{bmatrix}_{t+1} = \begin{bmatrix} G_1 \\ G_2 \\ \vdots \\ G_k \end{bmatrix}_t + E \begin{bmatrix} Er_1 & 0 & 0 & 0 \\ 0 & Er_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & Er_k \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \\ \vdots \\ G_k \end{bmatrix}_t$$

The transition from state t to $t+1$ represents the proportion of material removed from each size class. This allows us to calculate and track detailed changes in soil grading as a function of erosion.

Erosion rate is calculated by the commonly used equation

$$E = e\frac{q^{\alpha_1} S^{\alpha_2}}{{d_{50a}}^{\beta}}$$

where e is the erodibility factor, q is discharge per unit width ($m^3/s/m$), S is slope, d_{50a} is the median diameter of the material in the armour layer and α_1, α_2 and β are exponents which need to be calibrated. The transition matrix values (erodibility of each size class) is calculated by

$$Er_k = \begin{cases} \dfrac{a}{{d_k}^m}\underline{G}_k & for \quad k < M \\ b\dfrac{a}{{d_k}^m}\underline{G}_k & for \quad k = M \\ 0 & for \quad k > M \end{cases}$$

where d_k is the mean diameter of size class k (k=1 is the smallest diameter grading class), the power m needs to be calibrated (normally positive with a value about 0.75; see, for example, Henderson, 1966), a and b are scaling factors, and M is a size threshold that determines the largest particle diameter that can be entrained in the flow (Shield stress threshold). The parameters of these equations were calibrated by matching mARM 1D simulations to ARMOUR (described in Cohen et al., 2009a).

In both ARMOUR and mARM the processes are simulated in layers with constant volume. Therefore when material is removed from the surface (by erosion) it needs to be re-supplied with material from a subsurface layer. In ARMOUR (and mARM1D) this sub-surface layer has a constant pre-defined grading while in mARM3D it is the top layer of the simulated profile. Deposition of sediment on the surface is algorithmically similar to the erosion mechanism in mARM. But in order to realistically simulate time varying deposition the model needs to track sediment transition through the system which is not done in mARM. This will be achieved in the future when mARM will be integrated in a landform evolution model (i.e. TelluSim).

2.2. Surface and profile weathering

The weathering process is simulated similarly on the surface and profile layers. The profile model we used in mARM3D is similar in concept to the model presented by Salvador-Blanes et al. (2007) where the profile is divided into a finite number of layers with a predefined and spatially and temporally constant depth. In this paper we used only physical breakdown of soil particles to model the weathering process. Although chemical weathering (dissolution) is algorithmically possible (as suggested in Cohen et al., 2009a) and may be of great significance over long simulations it is not used here for simplicity. We also chose not to include translocation processes (i.e. Bioturbation and Eluviation and illuviation) in this version of the model, again for simplicity. Soil production processes (from bedrock to regolith) are simplified by being considered as part of the general physical weathering of soil particles. This means that bedrock is expressed by the largest grading class and its physical breakdown is treated similarly as any other size class.

The weathering transition matrix (**B**) defines the relative change in each grading class (k) as a result of the fracturing of particles in the weathering mechanism. A single grading class will lose a proportion (W) of its volume to one or more smaller classes. If we assume that weathering is mass conservative then the weathering equation is

$$\underline{G} = \underline{G} + W\mathbf{B}\underline{G}$$

There are a number of complicating factors in the calculation. The first is that the grading range of the daughter particles will not necessarily fall on the grading ranges of the discretisation of the soil grading used in the calculations. Legros and Pedro (1985) and Salvador-Blanes et al. (2007) used a 1000 1μm 'boxes' to represent soil distribution in their profile weathering models enabling high-resolution transition between grading classes. Their approach is computationally inefficient and is therefore not suitable here. Interpolation, rather, is required to allocate the mass of daughter products to the requisite size ranges in the discretisation of the grading. In ARMOUR to avoid this problem weathering is calculated from an average particle size for each class. This means that a class will only contribute to only one smaller grading class. This can result in simulations from ARMOUR having spiky grading artifacts over time, something that the interpolation algorithm avoids. In the mARM weathering algorithm above we create a more flexible way of distributing material which is more realistic.

We examine two depth dependent weathering rate functions in mARM3D: exponential decline (Gilbert, 1877) where weathering rate decrease as a function of depth and the 'humped' (Ahnert, 1977), where weathering rate is highest close to the surface ('non-zero' depth) and then decreases exponentially with depth (Figure 1). These functions are used to assign a normalized value (*WRr*; between 0 and 1) to each profile layer. The humped equation we use is a modification of a function proposed by Minasny and McBratney (2006) for the humped bedrock weathering model

$$\frac{\partial e}{\partial t} = P_0[\exp(-k_1 h + P_a) - \exp(-k_2 h)]$$

where *de/dt* is the physical weathering rate, P_0 and P_a (m/year) are the potential (or maximum) and steady-state weathering rates respectively, h (m) is the soil depth and k_1 and k_2 are constants. We used Minasny and McBratney (2006) values of P_0=0.25 m/year, k_1=4 m^{-1}, k_2=6 m^{-1} and slightly modified P_a=0.02 m/year (their value was 0.05).

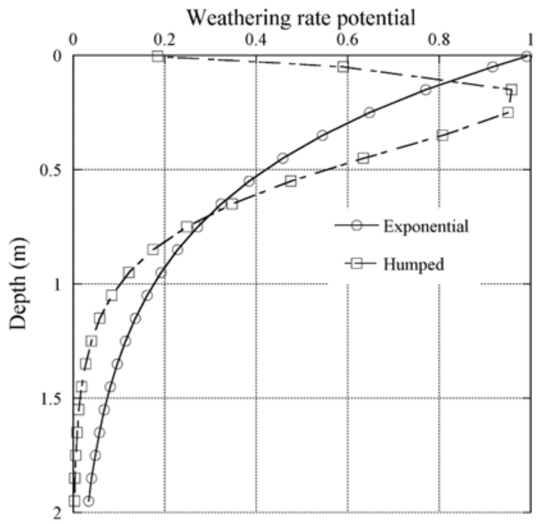

Figure 1. The two depth-dependent functions used in this study (exponential and humped).

The equation for calculating exponential decline with depth is

$$WRr = \beta Exp(-k_3 h)$$

where β is constant (maximum value; β =1 in this case) and k_3 is the amplitude. We found a good match between the two functions when k_3=1.738. This match refers to minimum differences in total weathering rates at the profile (area under the curve). The above values resulted with a difference of less then 0.1%.

The weathering process is calculated separately in each profile layer as a function of weathering rate and soil grading. However, vertical distribution of soil grading is affected not only by the weathering process but also by erosion from the surface. Since the profile is described by a finite number of layers with uniform and constant depth the calculated profile domain is finite and therefore its total mass or volume must be kept constant. This means that once material has been removed from the surface the profile is balanced by added bedrock in the lower layers. This is equivalent to lowering the soil profile although in mARM the size of the simulated profile domain does not change. This process changes the distribution of soil grading between the profile layers and is calculated by transferring a portion of each layer (equal to the volume of surface erosion) to the one directly above it.

This process will result in general coarsening of the soil profile. In a state of dynamic equilibrium this coarsening effect is balanced by the weathering process.

3. APPLICATION

We used mARM to examine a wide array of soil physics and relationships in a variety of landforms. Below we present selected cases as demonstrative tool rather than fully analyzed case studies. A fuller description and analysis of the results will be presented in Cohen et al. (2009b) and future publications.

3.1. Hillslope scale simulations

Small scale simulations are an effective way of examining new modelling concepts and hypotheses because they are simpler to interpret and manipulate. We simulated soil evolution over an approximated

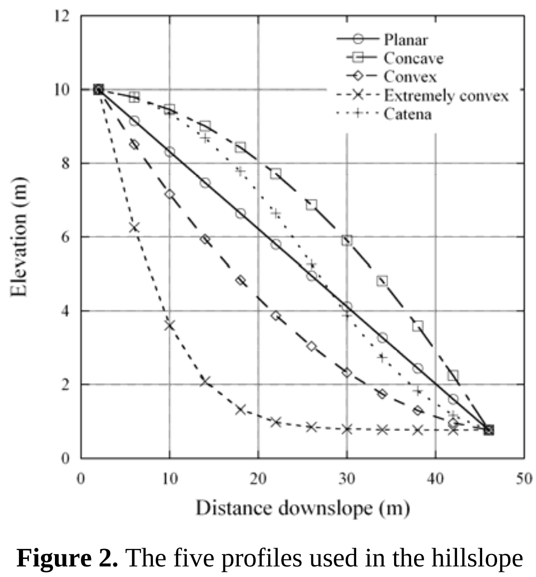

Figure 2. The five profiles used in the hillslope scale simulations.

100 000 years using two sets of hillslope profiles. These profiles are an extended and modified version of the 1D hillslopes used in the ARMOUR and later in the mARM1D experiment (Willgoose and Sharmeen, 2006 and Cohen et al., 2009a respectively). Here we present two sets of hillslope scale simulations. Each set contains five different hillslope profiles (Figure 2): (a) planar, (b) concave, (c) convex, (d) extremely convex and (e) catena. The profiles are 48m long and divided into 12 equal length nodes with an average slope of 21%. In one set we ran mARM using the exponential weathering function and in the second we used the humped equation.

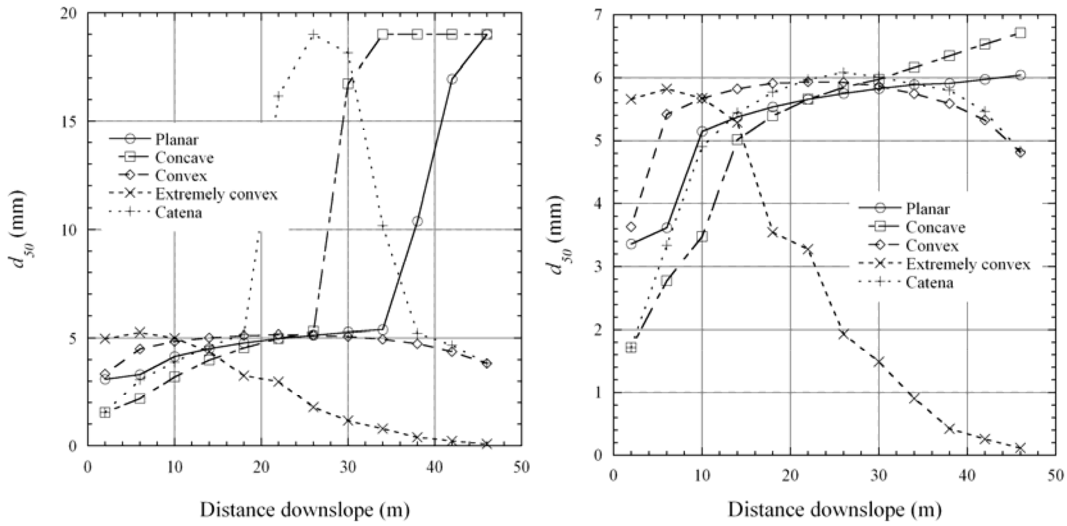

Figure 3. Surface d_{50} distribution along the five hillslope profiles using the exponential (left) and humped (right) weathering equations. Initial surface d_{50} values are 3.34mm.

Figure 3 shows the surface d_{50} distribution in all five profiles from the exponential and humped sets. The planar profile resulted in downhill coarsening caused by the increased erosion as a function of increased contributing area downhill (slope is constant). This trend is even stronger for concave profile due to the increasing slope downhill. The extremely convex profile resulted in downhill fining due to the significant decrease in slopes downhill which reduce transportability. In the convex profile grading is relatively similar at the top and the bottom of the hillslope with a shallow arc distribution in between. This suggests the existence of a balance between area, slope and soil grading and a potential analytical solution to this relationship. The catena profile shows a trend of top to middle downhill coarsening followed by downhill fining. This trend generally resembles natural catenary soil distribution.

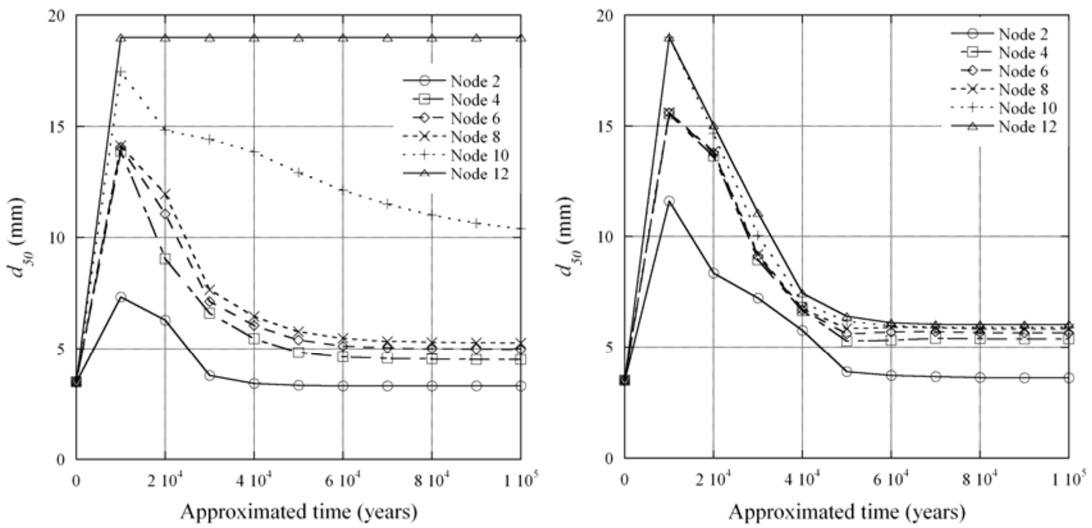

Figure 4. Surface d_{50} evolution in 6 of the 12 nodes (node numbering increase downhill) of the planar profile using the exponential (left) and humped (right) weathering equations.

The differences between the results of the two weathering functions are most apparent in the planar, concave and catena profiles. In the exponential function at least one of the nodes in these profiles reached the maximum d_{50} value (19mm) which indicate a near total removal of soils particles (19mm is the largest size class in this case). The evolution of surface d_{50} on the planar profile is presented in Figure 4. It shows that the lower nodes (10 and 12) evolve to an armouring dominated regime (where erosion is supply limited) in the exponential simulation. The remaining nodes tend toward a weathering dominated regime (where erosion is transport limited) and have a slightly lower equilibrium d_{50} value relative to the humped simulation. These results are repeated on the concave and catena profiles (not presented here). In the humped simulation all the nodes reach a weathering dominated equilibrium.

3.2. Large scale simulations

In the ARMOUR study Willgoose and Sharmeen (2006) used a one-dimensional hillslope from the Ranger Uranium Mine spoil site. We used mARM3D to simulate soil evolution on this entire artificial landscape over a time spend of about 50 000 years. Similar to the hillslope scale simulation above, we used both exponential and humped weathering equations.

Figure 5 shows the equilibrium surface d_{50} maps of these two simulations. The soil distribution in the two maps is generally similar with coarser values on high slope areas and positive correlations between the density of the elevation contours and coarser soils. The average d_{50} is lower on the exponential relative to the humped (2.85 and 3.22mm respectively). However the exponential map has more mass transport pixels (maximum d_{50} is 19mm) which account for 1.61% of the dataset compared to just 0.55% in the humped. In the humped map these pixels only appear when a combination of high slope and drainage area (along main drainage paths) resulted in extremely high transportability. These results correspond well with the hillslope scale simulations where nodes with similar trends were slightly finer in the exponential model and mass transport occurred only in the exponential simulation. The landscape simulation shows that nodes can evolve to an armoured dominated regime in the humped equation but at a much lower extent.

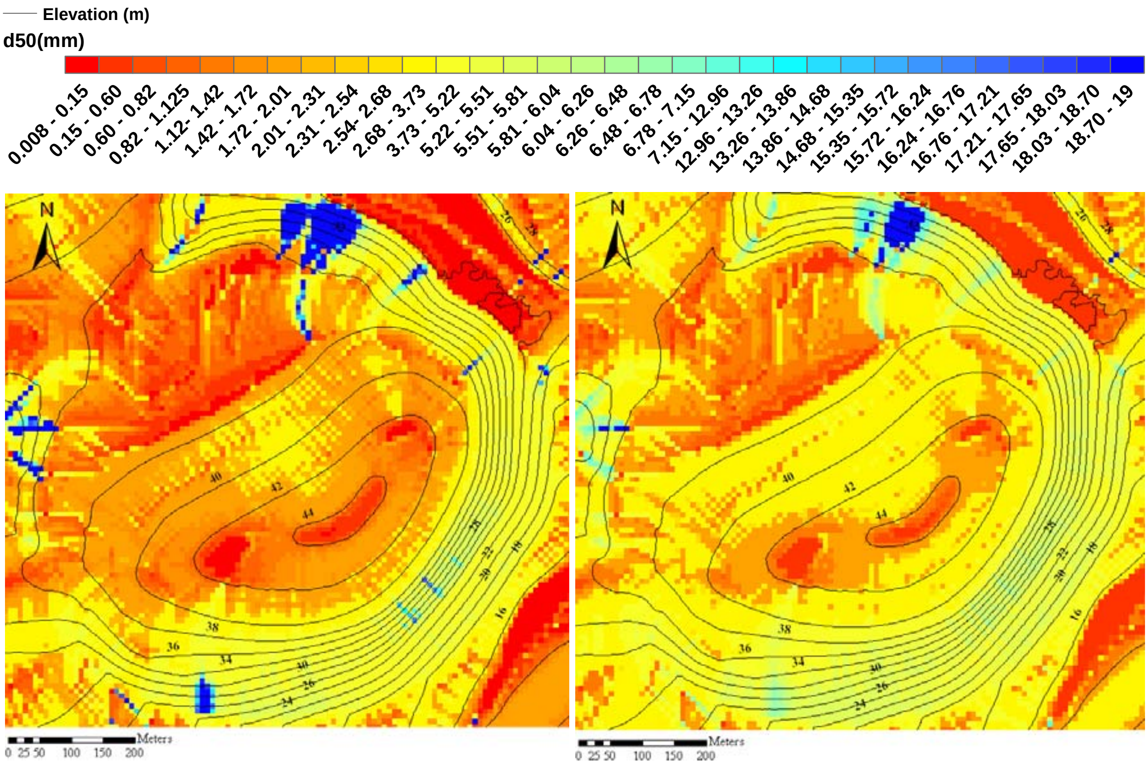

Figure 5. Surface d_{50} maps of the Ranger Uranium Mine spoil site simulations using the exponential (left) and humped (right) weathering equations. Initial surface d_{50} values are 3.34mm.

4. DISCUSSION AND CONCLUSIONS

Soil properties and their spatial distribution are of great importance. In planning a mine spoil site, for example, the evolution of soil can have a huge impact on the erodability of different parts of the structure. In natural landscapes better understanding of soil evolution will allow better description of its spatial distribution and prediction of potential impacts of environmental changes (e.g. climate). In the mARM model we were able to create a framework which allows simulations of complex soil processes in a computationally efficient manner. Even without fully describing the pedogenesis process, mARM3D showed great potential as a virtual laboratory of soil processes.

By simulating the impact of two depth-dependent weathering functions (exponential and humped) we found that while the exponential resulted in a generally slightly finer surface it is significantly more inclined toward armouring dominated surface in high erodibility areas (relative to the humped equation). The general finer soil of the exponential simulation can be explained by the fact that its surface weathering rate is significantly higher (Figure 2). The higher armouring tendency is however counterintuitive. It can be explained by examining the differences between the resulting soil profiles. The humped equation resulted in a thicker and better defined B horizon with extremely fine soil grading (clay texture). Our hypothesis is that this large reservoir of fine material significantly reduced the likelihood of an armour dominated regime. This idea needs to be further examined and may be of great significance.

The mARM modelling framework and results, as presented here, are at this stage mainly a proof of concept. The modularity of the algorithm allows the integration and easy manipulation of many processes and relationships. We believe that mARM holds great potential for soil studies, landform evolution modelling, environmental management etc. Its mathematical concept may be of use to modelling efforts of other processes and disciplines.

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REFERENCES

Ahnert, F., (1977), Some comments on the quantitative formulation of geomorphological process in a theoretical model. *Earth Surface Processes,* 2, 191–201.

Cohen, S., Willgoose, G.R., and Hancock, G.R. (2009a), The mARM spatially distributed soil evolution model: a computationally efficient modelling framework and analysis of hillslope soil surface organization. *Journal of Geophysical Research-Earth Surface*, In press.

Cohen, S., Willgoose, G.R., and Hancock, G.R. (2009b), The mARM spatially distributed soil evolution model: three-dimensional model framework and analysis of soil hillslope processes, in preparation. *Journal of Geophysical Research-Earth Surface*, In preparation.

Gilbert, G.K., (1877), Report of the Henry Mountains (Utah), US Geolgraphical and Geologicla Survay of Rocky Mountains Region. US Government Printing Office, Washington DC. 169pp.

Henderson, F. M (1966), *Open channel flow*. MacMillan.

Legros, J.P. and Pedro, G. (1985), The causes of particle-size distribution in soil profiles derived from crystalline rock, France. *Geoderma,* 30, 15-25.

Minasny, B., and McBratney, A.B. (2006), Mechanistic soil-landscape modelling as an approach to developing pedogenesis classifications. *Geoderma*, 133: 138-149.

Minasny, B., McBratney, A.B., and Salvador-Blanes, S. (2008), Quantitative models for pedogenesis- A review. *Geoderma*, 144: 140-157.

Salvador-Blanes, S., Minasny, B. and McBratney, A. B. (2007), Modelling long-term in situ soil profile evolution: application to the genesis of soil profiles containing stone layers. *European Journal of Soil Science,* 58, 1535-1548.

Willgoose, G. R. and Sharmeen, S. (2006), A One-dimensional model for simulating armouring and erosion on hillslopes: I. Model development and event-scale dynamics. *Earth Surface Processes and Landforms,* 31, 970-991.