SOFTWARE REQUIREMENTS DESCRIPTION FOR SOILGEN VERSION 1.0

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1 SOFTWARE FUNCTION

The SoilGen program is intended to be a special-purpose code used to estimate soil thicknesses over Yucca Mountain and perhaps analog sites. SoilGen will use a balance of dust deposition, bedrock entrainment, creep, and intermittent overland water transport of sediment to calculate soil thickness, using a rectangular computational grid such as the grids used in a Digital Elevation Model. This Software Requirements Description describes the basic principles and functions that are to be incorporated in the SoilGen Version 1.0 code.

Versions of the code have been created to examine methodology, starting in 1995 (see CNWRA Scientific Notebook #163, chapter entitled Geomorphology of Mountain Erosion), and have provided the estimates of the soil thickness above the Yucca Mountain repository used in ITYM, a preprocessor code for the Total-system Performance Assessment code used in performance assessment activities. Soil thickness is a parameter necessary to estimate mean annual infiltration at Yucca Mountain. Because of its use in performance assessment activities, the code is being enhanced, formalized, and placed under configuration control.

The first version of the test code was based on a kinematic routing approach to model water, sediment, and bulk soil from highest elevation to lowest elevation. The routing approach was found to be appropriate where significant topographic relief exists without local hollows. Ridges and hillslopes were handled well at Yucca Mountain, but channels and washes were plagued with numerous hollows (usually due to resolution issues). As explicit routing eliminates the need to solve large systems of simultaneous equations, quite large grids (several hundred grid blocks on a side) can be handled when the topography is appropriate. The entire Yucca Mountain repository area was considered with a resolution of about 7.5 m on a side (800 by 1200 pixels).

Although the routing approach is robust and computationally efficient for hillslopes, difficulties with channels and low-relief alluvium have provoked investigation of another approach that implicitly solves for the unknowns, at the cost of solving systems of simultaneous equations. A second test code has been developed to use an alternate numerical technique (a diffusion approach often used in surface water modeling) with the same set of mathematical models describing the physical system. Since an implicit system of simultaneous equations is solved, the diffusion approach more robustly handles local hollows; however, matrix solution costs limit the number of unknowns that can be considered by at least an order of magnitude relative to the routing approach. A domain-decomposition approach was adopted in the diffusion-approach test code to overcome this limitation, and it is possible (albeit slow) to address problems with an 800 by 1,200 grid on a personal computer.

The second test code is to be formalized into SoilGen Version 1.0 code.

2 TECHNICAL BASIS: PHYSICAL AND MATHEMATICAL MODEL

The following features are to be included in SoilGen Version 1.0 code:

- Dust input. Dust is the primary soil component at Yucca Mountain under present-day conditions. Dust deposition is an important driver for soil redistribution.
- Bedrock entrainment. Bedrock also provides a component of the soil column. The bedrock source depends on soil thickness, with entrainment assumed to be

exponentially decaying with increasing soil thickness. The exponential decay is related to the increasing shelter from environmental cycles provided by the soil.

- Soil creep. Soil slowly moves downslope through gravity. This slow movement may be described as viscous film flow. The viscosity of the soil can change by many orders of magnitude (consider a landslide versus a stable hillslope).

- Overland water flow. Water flow is assumed to be governed by Manning's equation. A small set of "typical" storms are used to generate equivalent steady streamflow used for sediment transport, with storm frequencies used to estimate the fraction of the time that the flow occurs.

- Sediment transport. One or a few sediment sizes are considered for transport. Each steady streamflow is used to calculate carrying capacity, erosion, and deposition. Deposition is based on a particle settling rate. Kinetic erosion is assumed to occur, with a rate proportional to the difference between carrying capacity and actual concentration. The steady sediment transport rates are multiplied by the time fraction that the streamflow occurs.

Primary sources for the overland flow and sediment transport mass-balance and constitutive equations (the most complex part of the formulation) are the KINEROS (Woolhiser, et al., 1990) and WEPP documentation (Flanagan and Nearing, 1995).

The computational approach is an implicit staggered-grid finite-volume method, where all properties are defined as piecewise constant within cells and state variables are linearly interpolated between nodes. Control volumes are node centered, with volume and surface integrals evaluated piecewise within cells.

The model will be able to run bulk soil, water, and sediment transport independently. The model will also allow the transport components to be coupled through iteration (although not solved for with a simultaneous solution of linear equations). A typical coupled solution would define an initial soil thickness, obtain the equivalent steady flow conditions for the typical storms, and step through time by sequentially iterating on soil thickness and time-averaged sediment concentration.

A domain-decomposition technique will be available for large numbers of unknowns. The technique divides the rectangular domain into 2 sets of parallel same-width strips, with the strips as wide as feasible. Within each set, the strips touch but need not overlap, while the 2 sets are offset by half the strip width. The strips are solved independently, with all strips from one set solved before any from the other. The most-recent value is held fixed along interior edges; alternating between strip sets updates the interior edges.

3 COMPUTATIONAL APPROACH

3.1 Data Flow and User Interface

The SoilGen program is a collection of Matlab routines. Program execution is started through a call to the driver routine from the command line of a Matlab session. The driver routine is given the name of a command file responsible for providing all parameters needed for execution.

Storage of variables within SoilGen is through several global structures. Each structure is self-documenting, with a text description for each variable and a label regarding intended use (e.g., cell data, node data, scalar value, control string).

Each command file is a Matlab-interpreted routine that returns a single variable in the form of a list of name/value pairs. Each name corresponds to the name of a field in the global structures. The list is used to override default values for internal variables. Distributed input values can be specified in the form of a single value, an array of values of the correct size (such as a Digital Elevation Model grid), or as a Matlab-interpreted function of the coordinates. And as the command file is a Matlab-interpreted routine, the user is free to load additional input files and use programming techniques to generate the input values.

Output is in the form of periodic storage of the global structures, in a Matlab-interpreted binary format. These structures can be retrieved from within the Matlab environment for further processing.

3.2 Hardware and Software Requirements

The controlled version of SoilGen is to be coded in the Matlab programming language. To increase computational speed, some of the routines in the application may be converted into ANSI C or C++ using the converter provided with the Matlab compiler toolbox. Although conversion is not necessary for program execution, certain routines may be execution bottlenecks that are far more efficiently executed using a compiler than in Matlab's interpreted language. The generated C or C++ code requires use of an external compiler.

Because SoilGen is to be coded in Matlab, it is generally independent of computational platform. SoilGen should execute on all hardware platforms that support Matlab.

3.3 Graphics Requirements

Graphics are not intended to be a formal part of the code, although Matlab-intrinsic plotting routines may be used for debugging.

3.4 Pre- and Post-Processors

No formal pre- and post-processors are required to run the software. However, each command file may be used like a preprocessor, and it is necessary to use a conversion routine to transfer the generated soil thicknesses into a standard Digital Elevation Model format for use in the ITYM code.

3.5 Software Validation

This software develops data used as input to the net infiltration process model and abstracted performance assessment model. As such it will be validated using measured data and comparison with empirically-based equations developed by the U.S. Geological Survey. A recommended date for submittal of the software validation plan is June 30, 2003.

4 REFERENCES

Flanagan, D.C. and M.A. Nearing. "USDA—Water Erosion Prediction Project Hillslope Profile and Watershed Model Documentation." NSERL Report No. 10. USDA-ARS National Soil Erosion Research Laboratory. 1995.

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