SCIENTIFIC NOTE BOOK # 392E
Project 1402.562
Development of MULTIFLO code

by

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0. INITIAL ENTRIES

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Project Title: Development of MULTIFLO code

Project Staff: Stefan Mayer

Principal Investigator: Scott Painter

Cross-Reference: Scott Painter maintains the independent scientific notebook #282 for this project.

By agreement with the CNWRA QA, this notebook is to be printed at approximate semi-annual intervals. This computerized Scientific Notebook is intended to address the criteria of CNWRA QAP-001.

[Stefan Mayer, July 19, 2000]

1. General

Multiflo has a new boundary condition that allows to simulate free drainage under the effect of gravity. The scope is to run simple benchmarking simulations to verify that this boundary condition is implemented to yield reasonable results.
The source code is located on Vulcan in /home/spainter/bin. The version currently compiled there is MULTIFLO V1.2.2.
The input files and results of the simulations are stored on Vulcan in /home/smayer/Multiflo/gravitybc.

[Stefan Mayer, August 30, 2000]

CORRECTIONS to previous entry:
1) The scope is NOT a formal benchmarking, but rather an informal testing of the gravity drainage boundary condition.
2) The version used is NOT MULTIFLO V1.2.2, but is beta version MULTIFLO V2.0beta, which is located on Vulcan in /home/spainter/multiflo/mflo2.0/metra.

[Stefan Mayer, August 30, 2000]

Simulations are run on Vulcan, which is described in Table 1.1. Vulcan was accessed remotely from the PC Lemur, located in Bldg 189 in Rm A127.

Table 1-1. Computer and operating system used for the tests.

Machine Name	Machine Type	Operating System	Compiler	Location
vulcan	SUNW, Ultra-Enterprise; sparc; sun4u	SUNOS 5.6	Used compiled version supplied by S. Painter	Building 189

2. Testing of the gravity drainage boundary condition in metra

A simple test is to simulate a homogeneous porous medium with initial condition near saturation, to impose no-flow boundary conditions at the top and sides of the 2D domain, and to impose the gravity drainage boundary condition at the bottom side of the domain. This simulated medium should drain from top to bottom. Within round-off errors, the liquid saturation contour lines should remain horizontal at all times. The water flux should be in the vertical direction only. At equilibrium, the water flux should be zero and the porous medium should have a uniform residual water content.

The input file "intest1.dat" to run this simulation is stored on Vulcan in /home/smayer/Multiflo/BCgravity/test1.dir. A homogeneous porous medium having hydraulic porperties similar to those of the nonwelded paintbrush layer matrix (PTn) at Yucca mountain is simulated and discretized over a 20x20 grid, with grid nodes uniformly spaced 2 [m] apart from each other. The initial simulated water content is 90% (input as 10% residual air phase per volume).

Output files are obtained for the distribution of field data (such as relative water content) and for the distribution of water flow velocities at intermediate times. The final set of output files is obtained for the time at which the code converges, defined by the time at which cumulative relative changes of field properties are below a set threshold. The output files are stored on Vulcan in /home/smayer/Multiflo/BCgravity/test1.dir.

Figure 1 shows the simulated velocity vectors and the contours of the vertical (z) component of the drainage velocity. As expected, the contour lines are horizontal. Drainage velocities increase with depth, reflecting the increased level of saturation with depth at this early time (0.1 [yr]) in the simulation. They do not exceed 0.3 [m/yr]. Figure 2 shows the same contour lines at an intermediate time (1.0 [yr]). Overall, drainage velocities are reduced, reflecting an overall reduction in water content. Upon convergence, velocity values approach zero (on the order of 10^{-6} [m/yr]).

Figures 3 through 5 show contours of liquid saturation levels at early (0.1 [yr]) and intermediate (1.0 [yr]) times and upon convergence. As expected, the contour lines are horizontal, and levels of saturation decrease with time. After 0.1 [yr], water contents have not changed substantially from initial conditions. The same contour lines have shifted down markedly after 1 [yr], reflecting early drainage.

Upon convergence - the code approached near equilibrium after 4 x 10^6 [yr] - the simulation yields a remaining vertical gradient of water saturation levels, ranging from 0.21 to 0.225. The residual saturation input for the porous medium is 0.14. The discrepancy of values and remaining gradient could be attributed to a number of reasons, and the interpretation remains speculative at this point. Given the high "alpha" values of the porous medium, the asymptotic approach to equilibrium may be extremely small.

A similar simulation, where the convergence criterium is more stringent (STEADY values from 10^{-7} to 10^{-9}) and where the "alpha" VanGenuchten parameter is increased from 10^{-6} to 10^{-4}, still yields a gradient of saturation levels. Results for the converged contours are shown in Figure 6.

[Stefan Mayer, September 6, 2000]

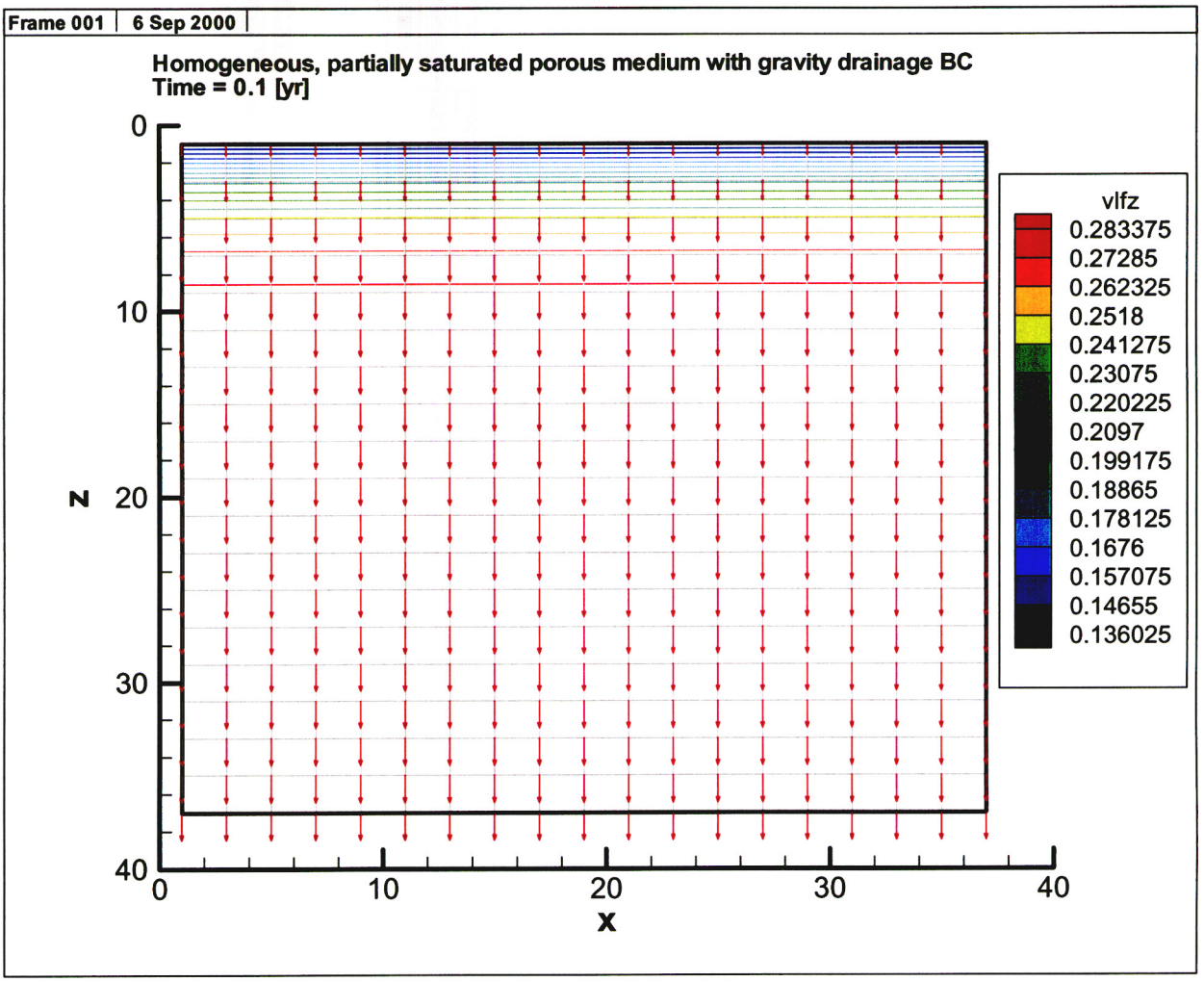

Figure 1: Velocity contours and vectors at initial stage of gravity drainage.

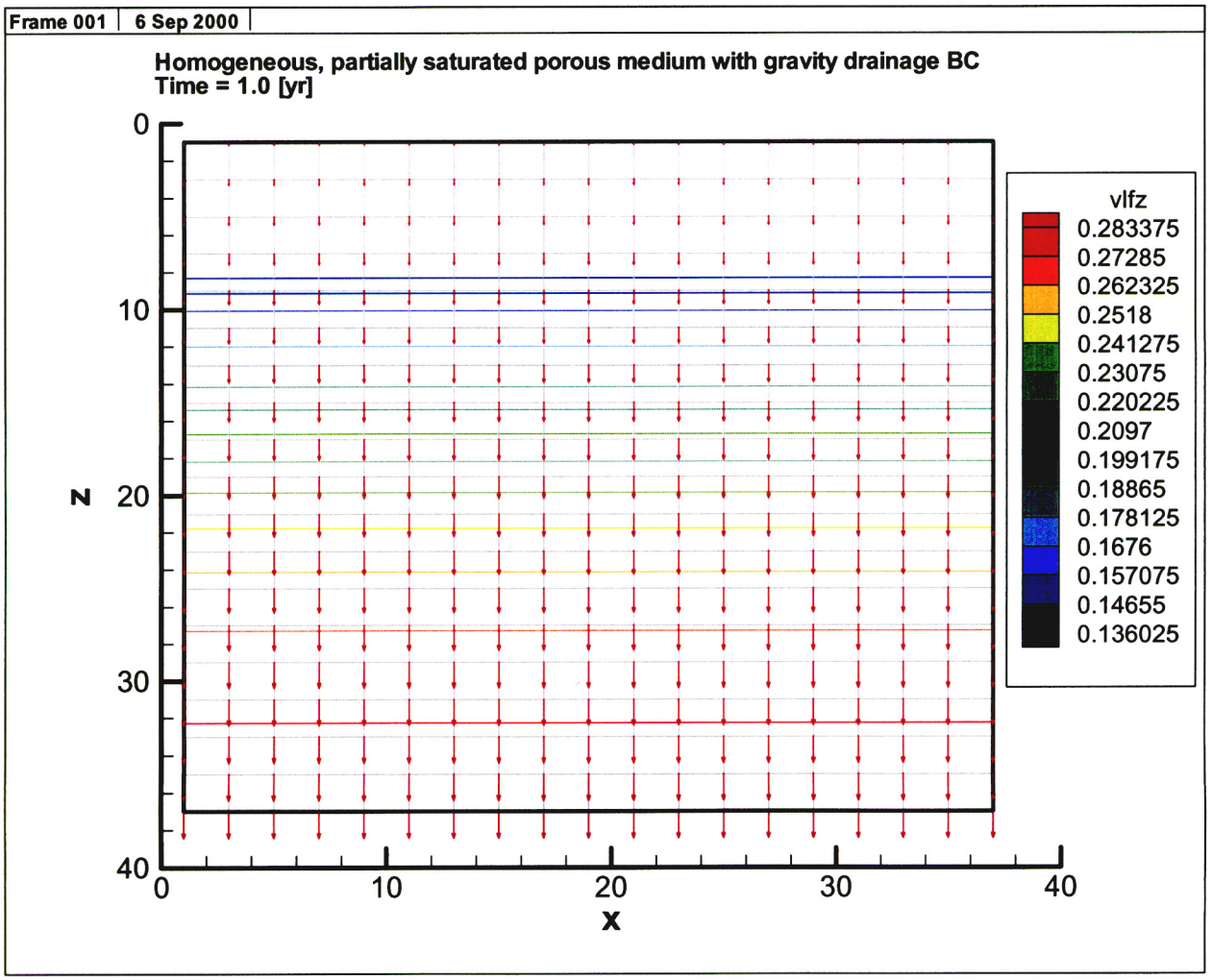

Figure 2: Velocity contours and vectors at intermediate stage of gravity drainage.

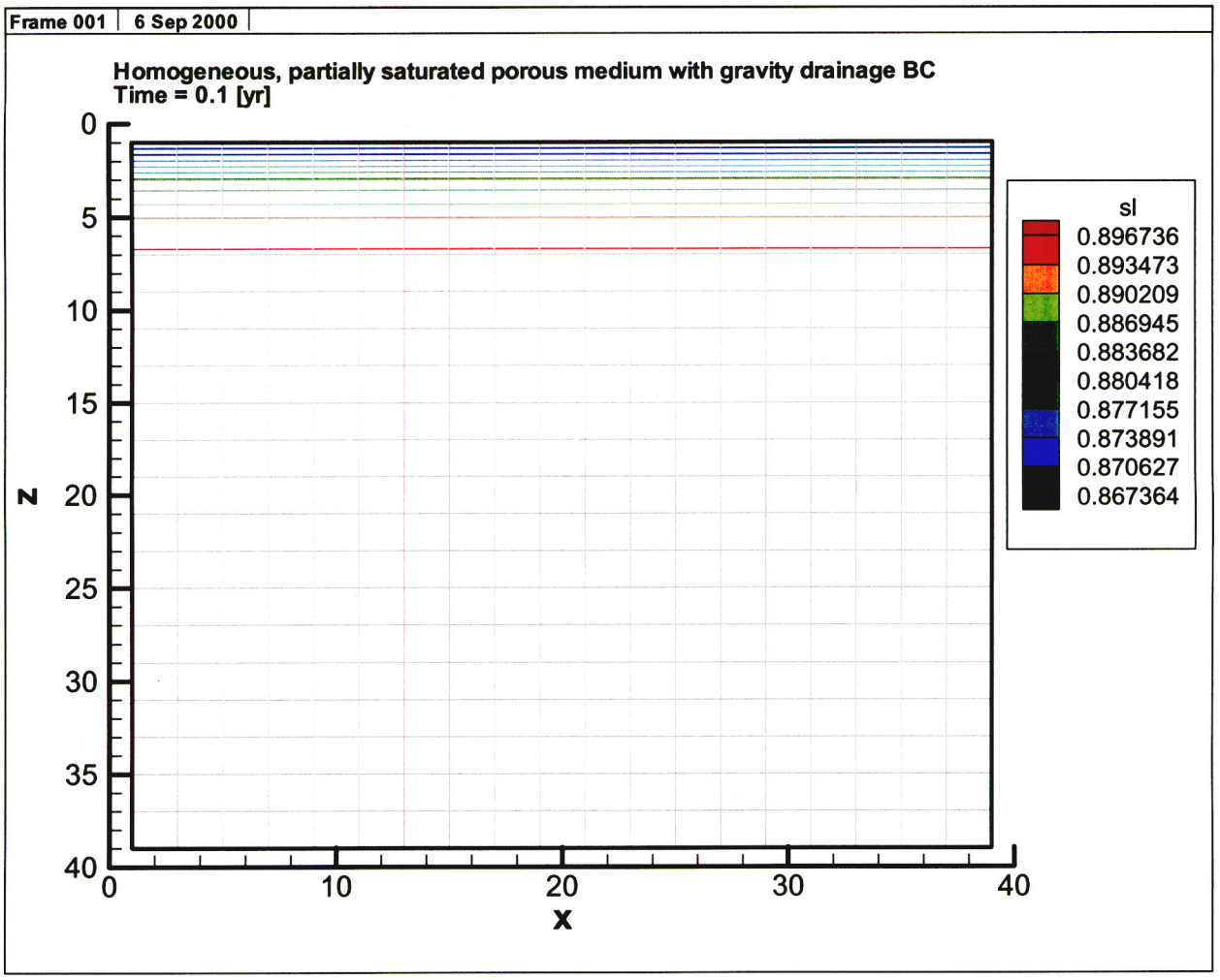

Figure 3: Water content contours at initial stage of gravity drainage.

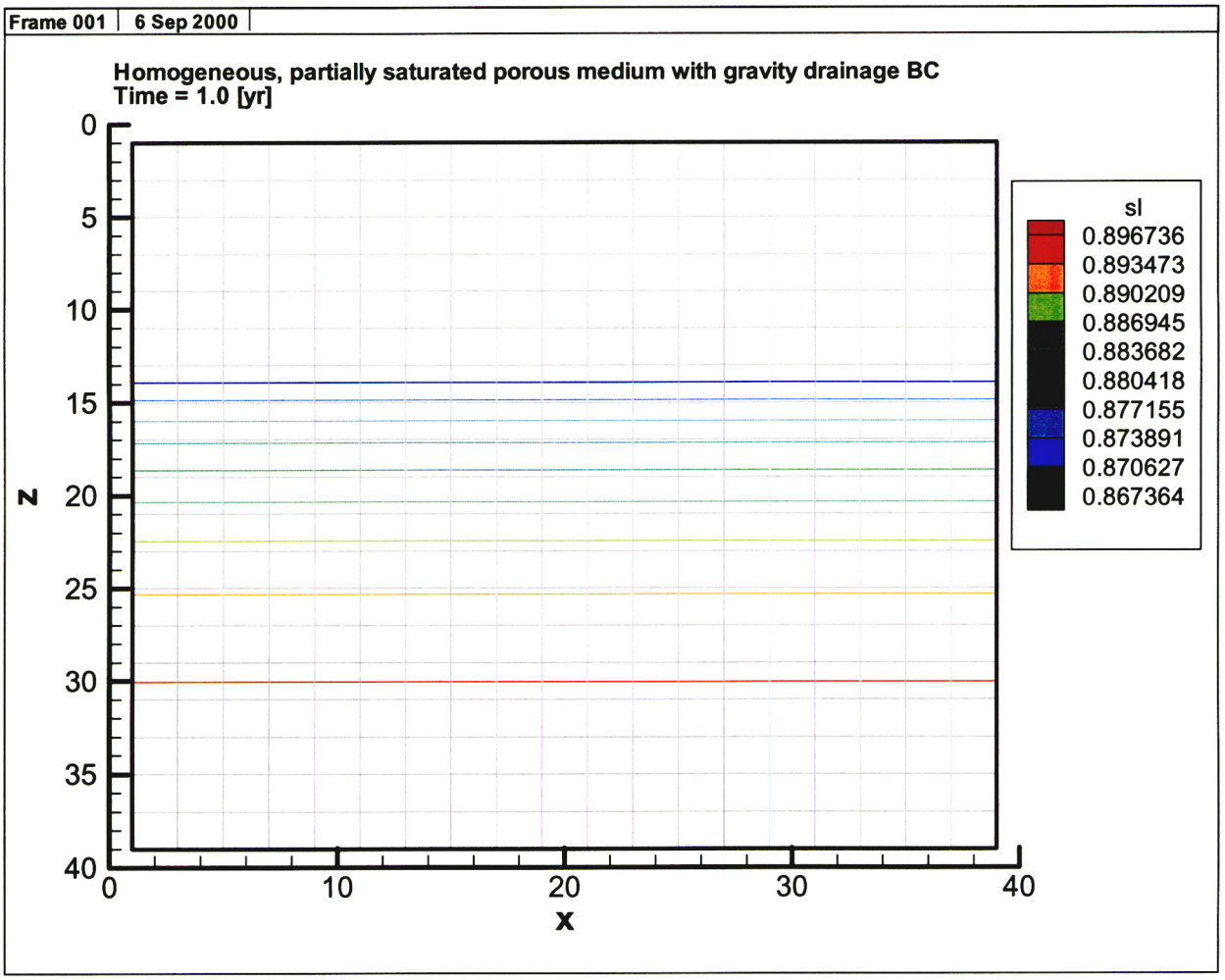

Figure 4: Water content contours at intermediate stage of gravity drainage.

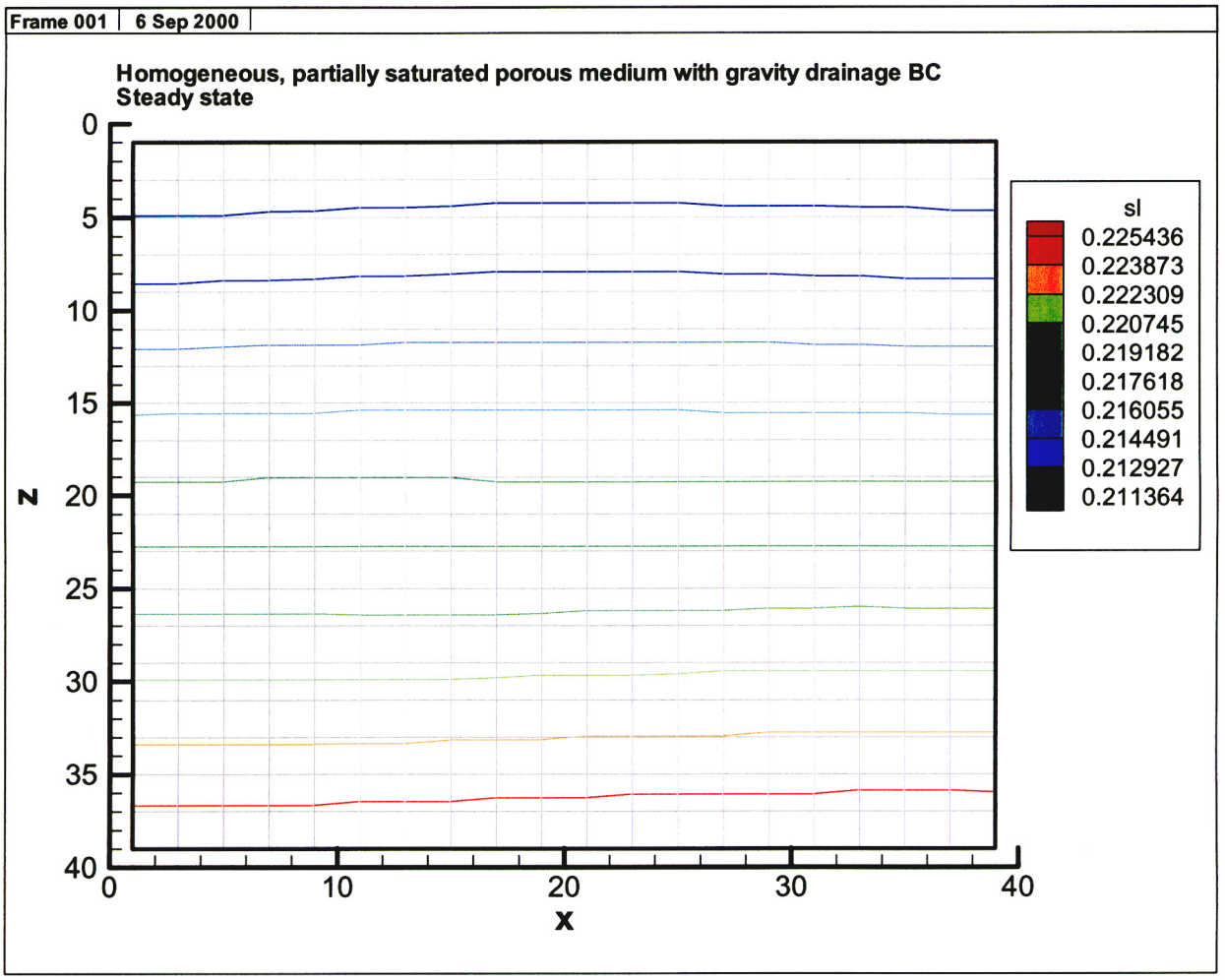

Figure 5: Water content contours after convergence of simulation to equilibrium.

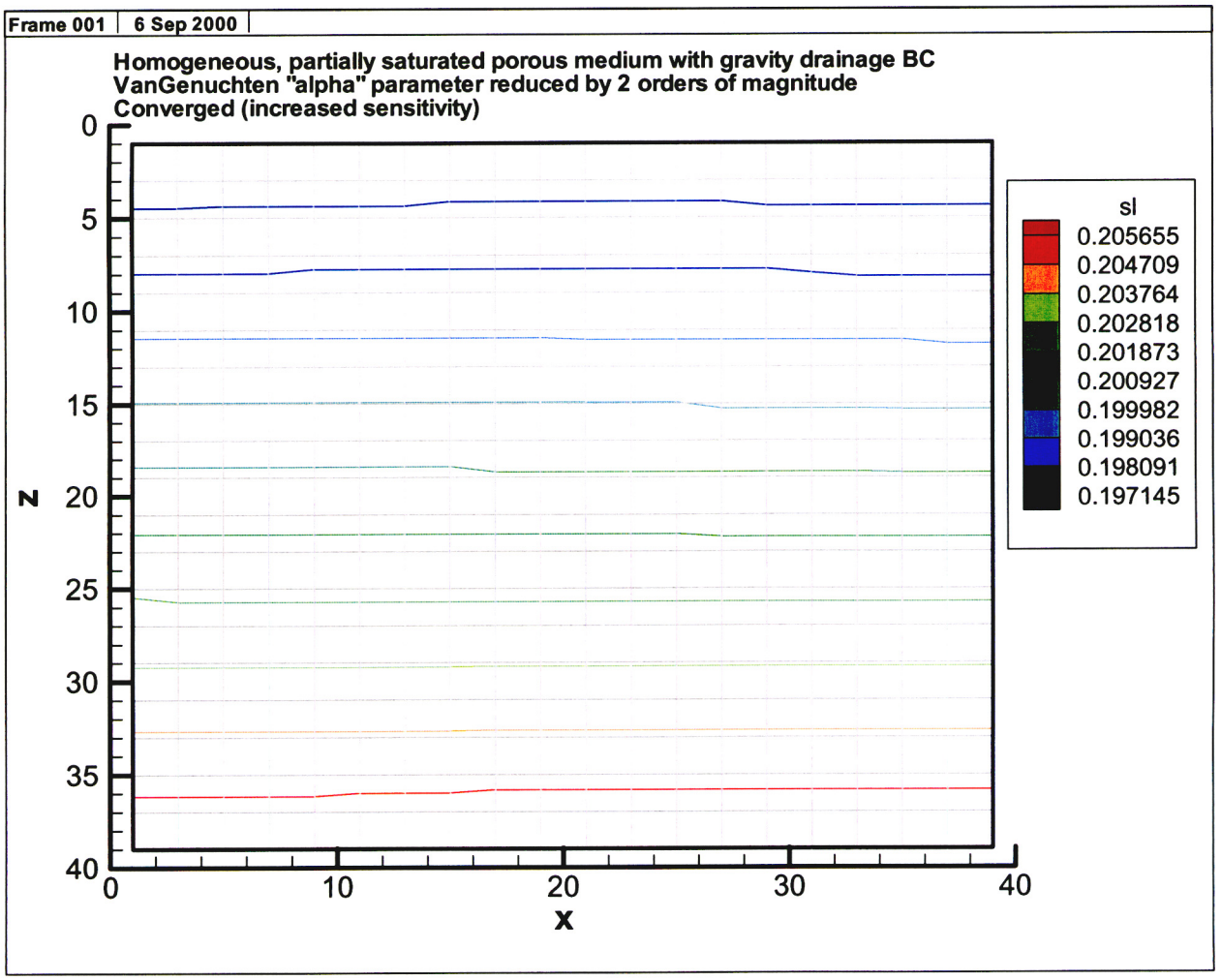

Figure 6: Water content contours for reduced alpha, after convergence of simulation to equilibrium.

[Stefan Mayer, September 6, 2000]

3. Conclusion

The simple preliminary test documented here suggests that the gravity drainage boundary condition is implemented properly. Observed simulation results appear reasonable. Qualitatively, this BC is considered to function as expected.

Note that no explanation is offered for the simulated residual water saturation distribution. A future check is required, possibly in form of a comparison to analytical results for residual water under gravity drainage, to establish if this is a correct result.

[Stefan Mayer, September 6, 2000]

Entries into Scientific Notebook No. 392E for pages 1 to 12

have been made by Stefan Mayer/ S. Mayer /September 15, 2000.

No original text entered into this Scientific Notebook has been removed.

S. Mayer, 9-15-2000