U.S. Department of Energy
Office of Civilian Radioactive Waste Management

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Idaho National Laboratory Technical Review of INFIL 2.0

Presented to:
Nuclear Waste Technical Review Board

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Predecisional—Preliminary

Outline

- Overview of INFIL 2.0 review
- Quality assurance (QA) objectives
- QA issues
- INFIL 2.0—Flow chart of codes
- Examples of QA issues
- Simple test case comparing INFIL to Excel
- New graphical user interface in INFIL 2.2
- Summary

Overview of INFIL 2.0 Review

- **Why review INFIL 2.0?**
  - **In light of U.S. Geological Survey (USGS) e-mails, decision was made to conduct QA software review and technical review of INFIL codes**
- **What was done?**
  - **Idaho National Laboratory (INL) software engineers conducted QA review of INFIL 2.0 code and 11 pre- and two post-processors, per Yucca Mountain Project (YMP) QA procedures**
  - **Other YMP staff conducted technical review of INFIL code**
  - **Reviews conducted from Oct. 2005 through Aug. 2006**
  - **No contact with INFIL originators during the reviews**

Overview of INFIL 2.0 Review (continued)

- **What was done by INL?**
  - **Conducted software QA review of INFIL 2.0 and eleven pre- and two postprocessors using 68 test cases**
  - **Updated code to current Fortran standards with explicit initialization of variables and dimension statements**
  - **Implemented a graphical user interface (GUI)**

Overview of INFIL 2.0 Review (continued)

- **What was done in YMP technical review?**
  - **Primary focus was reproduction of 9 infiltration maps in Technical Data Management System (TDMS), produced using INFIL and all pre- and postprocessors**
  - **Develop and run model test cases to verify INFIL 2.0 coding and conceptual model**
    - **Simplified INFIL calculations were replicated using a Microsoft Excel spreadsheet with macro to test that conceptual model described in infiltration analysis and model report (AMR) was consistent with code calculations**

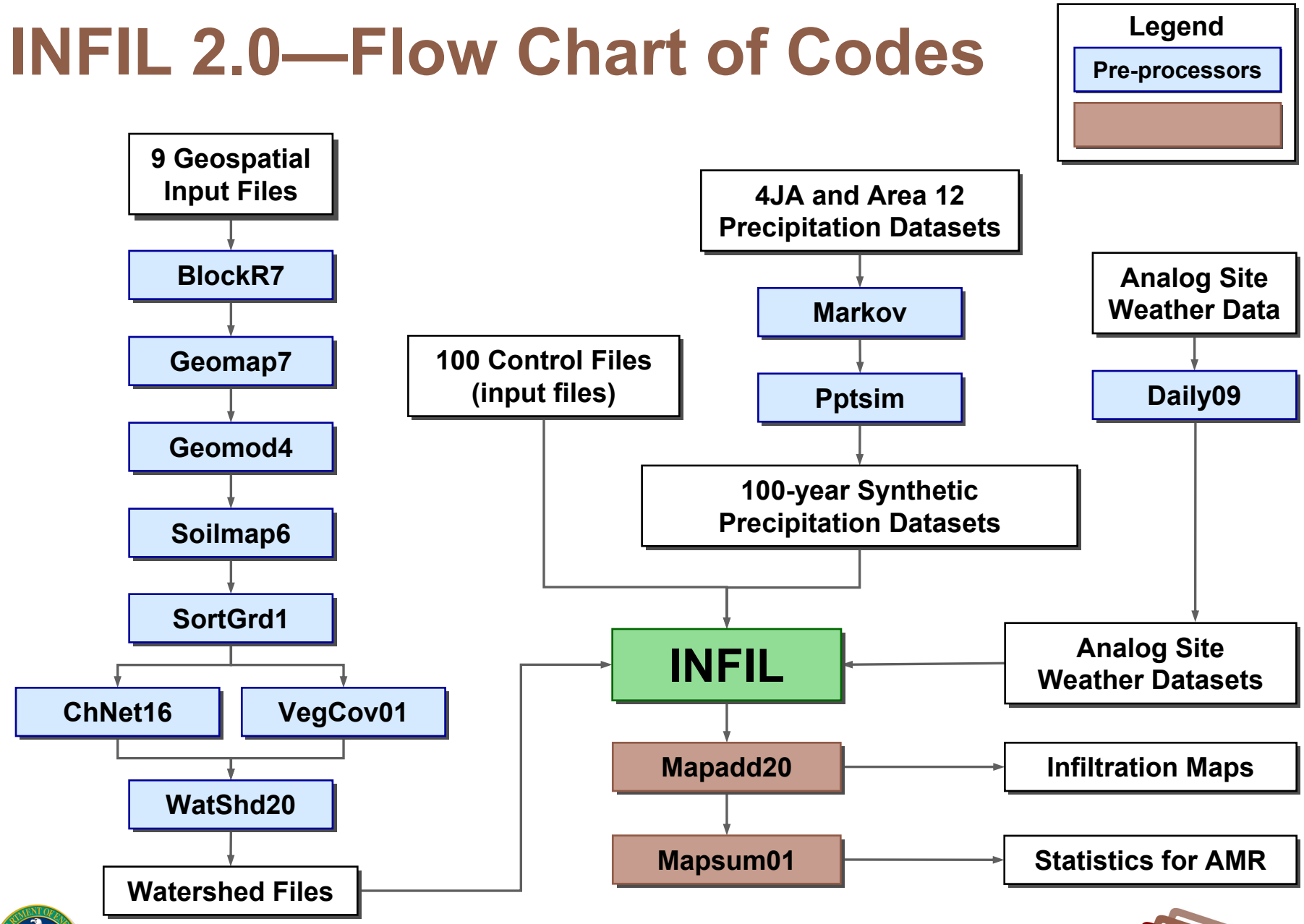
QA Objectives

- **Transparency**
  - **A document that is sufficiently detailed as to purpose, method, assumptions, inputs, conclusions, references, and units, such that a person technically qualified in the subject can understand the document and ensure its adequacy without recourse to the originator**
- **Traceability**
  - **The ability to trace the history, application, or location of an item and like items or activities by means of recorded identification**
- **Reproducibility**
  - **Record of files must be complete for reproducibility**

QA Issues

- **Instances of lack of transparency and traceability identified**
  - **Apparent coding error identified**
  - **Documentation was not always sufficient to reproduce original calculations**
  - **Certain input files missing from records packages**
  - **Software version control problems**

INFIL 2.0—Flow Chart of Codes



Examples of QA Issues

- **Instances of lack of transparency—code error**
  - **"Apparent" error in code was discovered**
    - **Reviewers believe transpiration from 2nd and 3rd soil layers should be multiplied by vegetative cover fraction (as was done for 1st layer)**
    - **Justification for this implementation was not included in the available documentation**
    - **"Apparent" error is insignificant because root-zone weights were adjusted during model calibration**
    - **INFIL 2.2 includes option to include vegetation cover factor in layers 2 and 3**

Examples of QA Issues (continued)

- **Instances of lack of transparency—documentation and reproducing infiltration maps**
  - **INFIL User's Manual states that 1996 version of file "30msite.inp" should be used**
    - **If this file is used, watershed files are reproduced, but with some minor exceptions**
    - **Effect on predicted net infiltration rates is insignificant (i.e., 1.702 versus 1.706 mm/yr for SC1 watershed)**
  - **If first pre-processor (BlockR7) is used with 9 geospatial input files to generate "30msite.inp", watershed files cannot be exactly reproduced**
    - **Many differences in blocking ridge values (used for calculation of potential ET)**
    - **Effect on infiltration is small (3% to 4%)**

Examples of QA Issues (continued)

- **Instances of lack of traceability—missing files**
  - **File required for pre-processor Geomap7 was missing**
    - **File was successfully re-created using available geology data found in TDMS**
  - **Shape files missing for calculation of infiltration over unsaturated zone (UZ) flow model area and repository area**
    - **Successfully re-created repository shape file ("Repos8.dat") for a test case**
    - **Did not re-create UZ shape file ("UZmod2.dat") (not required for the test case)**
  - **Required missing files could be re-created**

Examples of QA Issues (continued)

- **Instances of lack of traceability—version control**
  - **Pre-processor Markov is not the same code that produced Markov output files in TDMS**
    - **Differences in the number of digits reported**
  - **Differences in IMSL libraries used with WinNT and WinXP platforms**
    - **Caused minor numerical differences**

Results using Markov/Pptsim in INFIL v2.2 Workbench

		Markov/Pptsim version:	Infil v2.0 *	Infil v2.2 **	
			Avg annual infil. (mm/yr)		Diff. (%)
Mean Present-Day	Avg of mod3 & 4JA	JR1	7.4718	7.4133	-0.78
Upper Present-Day	Avg of mean PD & Area12	JR1	18.5104	18.8485	1.83

* Results in TDMS (DTN: GS000308311221.005)
** Results generated using INFIL v2.2 (exe file timestamped 6/1/06)

JR1 = Jet Ridge 1 watershed

Examples of QA Issues (continued)

- **Reproducibility (generation of watershed files)**
  - **If the first pre-processor (BlockR7) is not used, and the 1996 version of "30msite.inp" is used (as specified in Users Manual), then 8 out of 10 watershed files can be exactly reproduced**
    - **YW1 watershed has a different rock type for one grid cell (out of 46,716 grid cells)**
    - **SC1 watershed has differences in 83, 64, and 141 grid cells for soil depth class, soil depth, and rock type, respectively (out of 14,095 grid cells)**

Examples of QA Issues (continued)

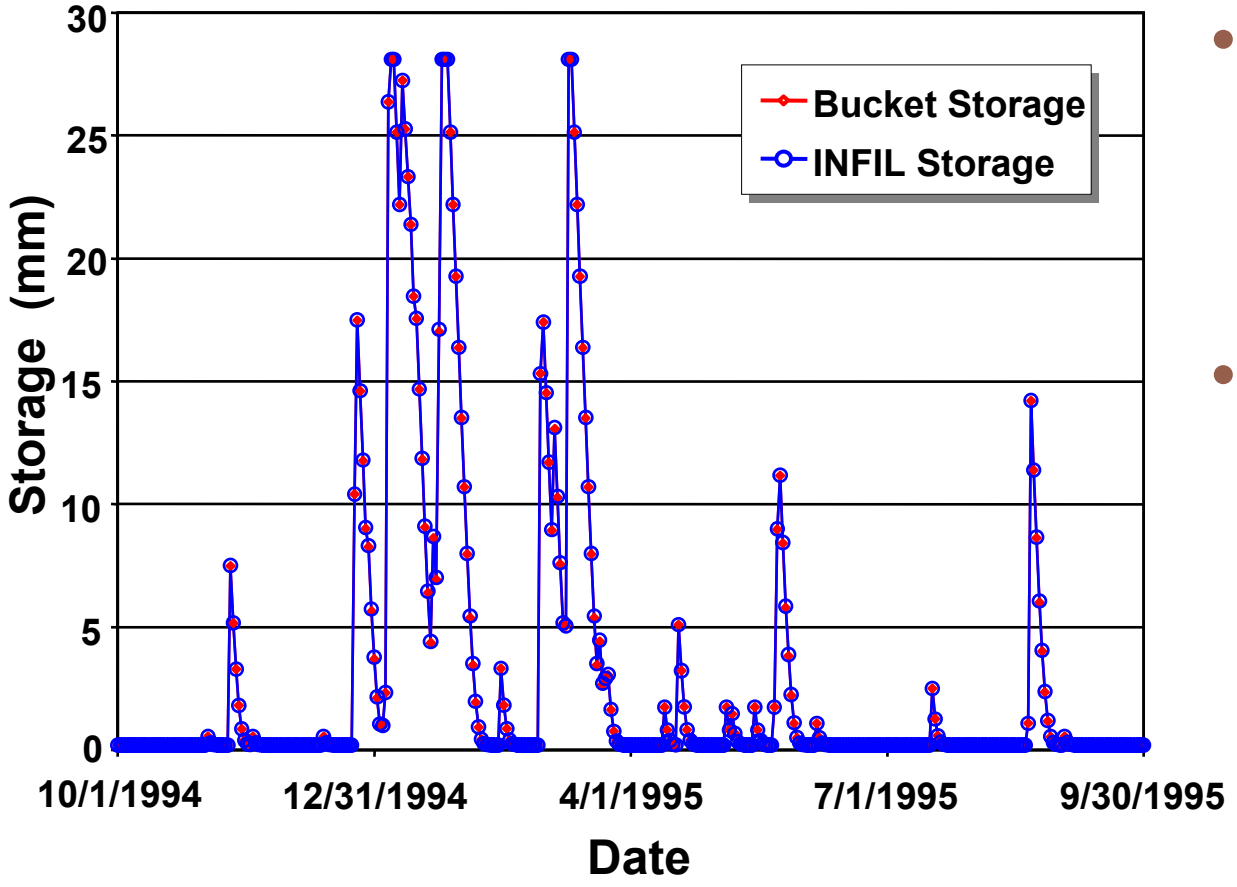
- **Reproducibility (generation of watershed files)**
  - **Effect of lack of exact reproducibility is very small**

Results using INFIL v2.2 Pre-processors and 1996 30msite.inp file

		Model:	Infil v2.0 *	Infil v2.2 **	Infil v2.2 **
		W'shed files:	Infil v2.0 ***	Infil v2.0 ***	Infil v2.2 **
Climate	W'shed:		Infiltration (mm/yr)		
Lower Glacial-Transition Climate	SC1		1.70272	1.70272	1.70614

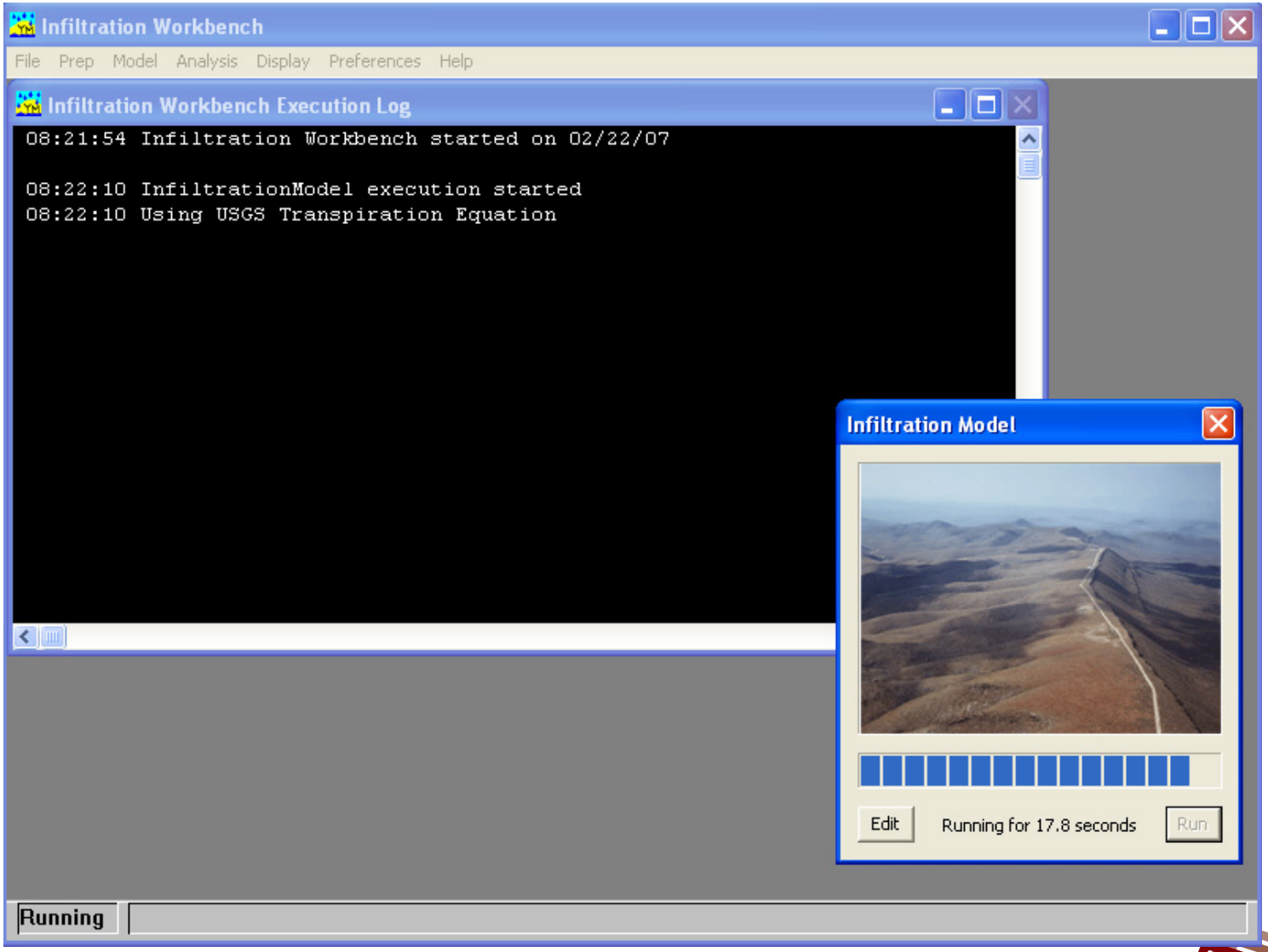
* Results in TDMS (DTN: GS000308311221.005)
** Results generated using INFIL v2.2
*** Watersheds files in TDMS (DTN: GS000308311221.004)

Reproducibility
Simple Test Case



- Simplified INFIL calculation can be exactly reproduced using Excel
- INFIL coding is consistent with conceptual model described in the infiltration AMR

INFIL 2.2—Graphical User Interface



Summary

- QA problems were discovered in the form of instances of lack of transparency and traceability
- Exact reproduction of 9 infiltration maps was not achieved because of issues with Markov and reproduction of watershed files, but differences are small
- INFIL code was found to be consistent with conceptual model described in the infiltration AMR
- Errors found in codes were not considered to be significant to calculations of infiltration

Summary (continued)

- **A *nuclear culture* demands strict attention to detail**
  - **Problems identified with INFIL 2.0 and infiltration AMR exemplify areas for which improvements are needed**
  - **The new infiltration AMR is being developed with strict adherence to QA requirements**