

INSTALLATION INSTRUCTIONS FOR MICROSOFT® WINDOWS® VERSION OF *xFlo*

1 INTRODUCTION

xFlo is an integrated finite volume model developed by the Center for Nuclear Waste Regulatory Analyses (CNWRA®) (Painter, 2006). *xFlo* was originally developed in a Linux® environment and was recompiled to be able to operate in Microsoft® Windows®. This document provides instructions for installing *xFlo* in the Windows operating system.

2 OPERATIONAL ENVIRONMENT

The *xFlo* code for Windows requires the following support utilities to be installed on the host machine.

Windows 7—host operating system used to run the support utilities and the *xFlo* scripts and executable file.

WinZip—used to unzip (unpack) the ZIP file containing the code distribution file set.

Lahey/GNU Fortran—Fortran compiler that creates the *xFlo* executable file from the Fortran code files.

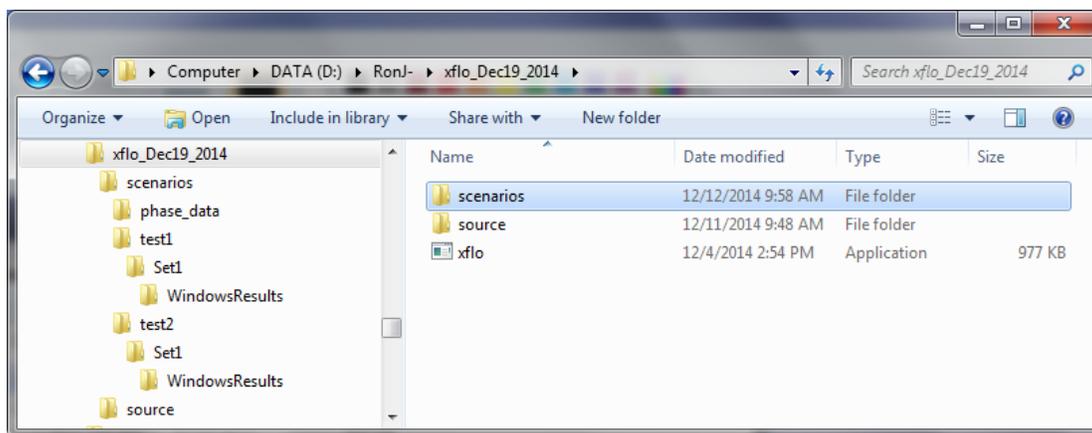
3 CODE DISTRIBUTION

The *xFlo* code is distributed in a single ZIP file called *xFlo_Dec_19_2014.zip*. The file is 2.06 MB and is archived on the N: shared drive.

This file may be unpacked using the WinZip application. The directory structure used to create the ZIP file is discussed in the next section. If WinZip is installed on the host machine, it can be invoked by right clicking the ZIP file name in the Windows Explorer window.

Directory Structure

This is a screen snapshot of the directory structure that was used to create the *xFlo* distribution ZIP file.



DRAFT

xflo_Dec19_2014 is the main directory, which contains two subdirectories and the *xflo.exe* executable file. As a convenience for the analyst, the executable file is also in the *test1* and *test2* subdirectories.

scenarios contains no files other than its three subdirectories. Each problem or test run will have its own subdirectory relative to this level.

phase_data contains seven data files with the enthalpy and viscosity relationships relative to pressure and temperature conditions for water. The path to this directory must match the path supplied in the first line of the *physics.dat* file discussed below.

test1 contains the working directory for the running of the first installation test. The two script files for creating single and multiple sets of *xFlo* output files are provided with the distribution package. One “set” subdirectory is provided, which contains the necessary data files to complete the performance of test 1.

Set1 contains four data files with the problem initial conditions and the main *xFlo* input file called *Set1.flo*. It also contains the *WindowsResults* subdirectory.

WindowsResults contains the result files for *Set1* as they were created on the Windows development machine at the CNWRA. In addition to the *aflux**, *hflux**, *mass**, *results**, *secondary**, and *wflux**, *run.out* and *Set1.out* output files from *xFlo*, four *.dat* and the *Set1.flo* input files were placed here during the execution of the ‘*runset.bat*’ batch script.

test2 contains the working directory for the running of the second installation test. The two script files for creating the *xFlo* output files are provided with the distribution package. The subdirectory structure is the same as that described for *test1*.

source contains 25 Fortran 90 code files and three batch files used in the compilation and running of the *xFlo* code.

4 COMPILATION

After the distribution files have been unzipped from the ZIP file, the source code files must be compiled to generate the *xFlo* executable file. This is done by opening a “Command Prompt” window and setting the current working directory to the “...*xflo_Dec19_2014*\source” directory and invoking the “*compile_xflo.bat*” script. This will create an *xflo.exe* file in the ...*source* directory. This executable file should be copied to the *test1* and *test2* directories, as well as any future scenario directories developed by the analyst.

5 VERIFICATION TESTS

The following one-dimensional test problems are considered:

- Thermal conduction—Thermal process only with specified influx
- Isothermal unsaturated flow—Moisture flux only with specified influx

Boundary Conditions and Sources in *xFlo*

xFlo inherently uses an unstructured grid built on several input files, although a built-in preprocessor builds some of the input files for structured grids. The verification testing directly defines the unstructured grid files in order to preserve flexibility in defining the gridding.

By default, *xFlo* imposes a zero-flux boundary condition on all boundaries and assumes that there are no sources. As currently implemented with the unstructured grid files, boundary conditions are imposed using boundary condition cells. Boundary condition cells can be linked to more than one interior cell, at the cost of significantly increasing memory demand, so best practice attaches each boundary condition cell to a single interior cell. Multiple boundary condition cells can be attached to a single interior cell. Sources are applied to interior cells, and multiple source definitions can be applied for each interior cell.

Values of the state variables and mole fluxes are interpolated to the start of each time step in each boundary condition and source definition. These values remain fixed through the time step, lagging the boundary condition and source information by one time step. This approach has no impact when the boundary conditions are fixed in time, but is inconsistent with fully implicit time stepping. A future enhancement may be desirable to make the boundary conditions consistent with the time stepping scheme.

There are two types of boundary conditions coded in *xFlo*: the DIRICHLET and INFILTRATION conditions. In both boundary conditions, all three state variables are defined in the boundary condition cell and all three are used to define fluxes to the interior cell. The DIRICHLET boundary condition is limited to the definition of the boundary state variables, but the INFILTRATION boundary condition also adds a boundary flux to the interior cell as an equivalent source term.

The preprocessor routines also define an INFILTRATION boundary condition for structured grids. The preprocessor routines convert specified volumetric water flux, pressure, and temperature into the corresponding state variables plus mole flux of air, mole flux of air plus water, and enthalpy flux required for the boundary condition input file.

There is no explicit method for defining mixed conditions, such as a specified temperature or energy flux with no mass flux, but *xFlo* can accommodate mixed conditions by appropriately redefining material properties in boundary cells. This method is not documented and will be described in future revisions to the *xFlo* Manual (Painter, 2006). To turn off mass flux, the boundary cell must be assigned zero permeability (which turns off gas and liquid flow), zero porosity (which turns off vapor diffusion), and zero liquid diffusion coefficient (which turns off diffusion of air in water). To turn off thermal conduction, the boundary cell must be assigned zero dry and wet thermal conductivities.

In the test problems, all *xFlo* boundary cells were assigned zero volume and zero thickness. Note that this approach would fail for models that implement Dirichlet boundary conditions as an extremely large reservoir, but is permissible for *xFlo* boundary cells. In the test problem with the INFILTRATION boundary condition, the material properties in the boundary cells were redefined to shut off mass and energy exchange with the interior. Sources were not used for either of the problems.

One linear dimension

The linear model domain is similar to a DECOVALEX column test. The model domain is 50 cm long. The entire model domain is filled with the porous medium, which has a uniform initial saturation throughout. An initial temperature of 6 °C is applied everywhere except for a linear ramp in temperature over 1 cm at the top boundary. The boundary value is 16 °C for the DIRICHLET condition and 50 °C for the flux boundary. A DIRICHLET bottom boundary condition maintains all state variables at the initial conditions for the duration of the test.

Table 1 provides the parameters used for verification testing of the thermal and Richards-based equations.

Table 1. Parameters Used for Verification Testing			
Description	Units	Bentonite	Steel*
van Genuchten alpha	1/Pa	3.5×10^{-8}	NA
van Genuchten lambda (= m)	—	0.512	NA
Liquid residual saturation	—	0	NA
Liquid minimum saturation	—	0	NA
Saturation transition (S*)	—	0.9995	NA
Linear parameter a for relative permeability	—	-17.2375	NA
Linear parameter b for relative permeability	—	129.16	NA
Linear parameter a for capillary pressure	—	9.59882	NA
Linear parameter b for capillary pressure	—	-60.5027	NA
Matrix permeability	m ²	4.9×10^{-21}	0
Matrix porosity	—	0.444	0
Dry thermal conductivity	W/m-K	0.105	16.2
Wet thermal conductivity	W/m-K	0.137	16.2
Solid specific heat	J/kg-K	640	500
Solid density	kg/m ³	1,530	8,030
Diffusion coefficient for gas in liquid	m ² /s	0	0
Vapor pressure lowering	—	Off	Off
Klinkenberg parameter	—	0	—
Initial saturation	—	0.22	—
Initial temperature	°C	6	6

*Upstream boundary condition zone for thermal problems

Thermal Problem

The first test problem considers a fixed and uniform moisture state with a mild thermal change imposed at one boundary. The properties of the porous medium are based on the bentonite material considered in the tests modeled for DECOVALEX. A specified energy flux of 50 J/m²/s is applied at the top boundary.

Isothermal Unsaturated Flow

The unsaturated flow simulation repeats the test used for the thermal problem, using the same porous medium and model dimensions, and using the same strategies for applying initial

DRAFT

conditions and boundary conditions. At the start of the simulation, water is introduced at the top of the column at a flux rate of 2×10^{-10} m/s. Additional aspects of this model include:

- A uniform temperature is specified throughout the model (isothermal condition),
- The *xFlo* option for vapor-phase lowering was turned off to minimize vapor diffusion, and
- The diffusion coefficient for dissolved air in water was set to zero to eliminate dissolved-air diffusion.

6 INSTALLATION VERIFICATION PROCEDURE

Verification Procedure for Test 1

The problem provided in the *test1* directory should be prepared and executed to verify the installation of the *xFlo* code by comparing the output files generated to those created on the Windows development machine at CNWRA. The verification procedure is listed here.

1. Copy the *xflo.exe* file created in the compilation step above to the *test1* directory.
2. Open a 'Command Prompt' window.
3. Change the current directory to ...*test1*.
4. Execute the *runset.bat* script file using this command.

```
>runset Set1 Set1\initial.dat
```

5. Compare several of the output files in the *Set1* directory to their respective files in the ...*WindowsResults* subdirectory. Some informative files to compare are: the most recent *results** file created, the *Set1.out* file, and the *run.out* file. The files should be identical to those provided in the ...*WindowsResults* subdirectory.

Verification Procedure for Test 2

The problem provided in the *test2* directory should be prepared and executed to verify the installation of the *xFlo* code by comparing the output files generated to those created on the Windows development machine at CNWRA. The verification procedure is listed here.

1. Copy the *xflo.exe* file created in the compilation step above to the *test2* directory.
2. Open a 'Command Prompt' window.
3. Change the current directory to ...*test2*.
4. Execute the *runset.bat* script file using this command.

```
a. >runset Set1 Set1\initial.dat
```

5. Compare several of the output files in the *Set1* directory to their respective files in the ...*WindowsResults* subdirectory. Some informative files to compare are: the most recent *results** file created, the *Set1.out* file, and the *run.out* file. The files should be identical to those provided in the ...*WindowsResults* subdirectory.

DRAFT

CONVERSION FACTORS

Name	SI Unit	Conversion
Density	1 kg/m ³	= 0.06243 lb _m /ft ³
Length	1 cm	= 0.394 in
	1 m	= 3.28 ft
Permeability	1 m ²	= 10.76 ft ²
Power	1 W	= 3.412 Btu/h
Pressure and Stress*	1 N/m ² (1 Pa)	= 0.000145 psi
Specific Heat	1 J/kg-K	= 238.9 Btu/lb _m .°F
Thermal Conductivity	1 W/m-K	= 0.57782 Btu/h.ft.°F
Temperature	T °C	°F = 1.8 × T °C + 32

*The SI name for the quantity pressure is Pascal (Pa) having units N/m² or Kg/m.s²

REFERENCE

Painter, S. "xFlo Version 1.0β User's Manual." ML061940065. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2006.