```
*****************************************************************
****************      TOUGH2, Version 2.0      ****************
****************    Overview of Code Revisions    ****************
*****************************************************************
*****************************************************************
****************  http://www-esd.lbl.gov/TOUGH2/  ****************
*****************************************************************
****************         November 1999         ****************
*****************************************************************
```

Introduction

The TOUGH2 simulation program for multiphase non-isothermal flows was first released to the public in 1991, and was subsequently updated in 1994 through addition of a set of preconditioned conjugate gradient solvers. These notes provide a brief summary of the nature and scope of enhancements that were made in the new Version 2.0. An overview of the new version of TOUGH2 had been presented at the TOUGH Workshop '98 (Pruess et al., 1998). Full documentation and user's instructions for TOUGH2 V 2.0 are available in report LBNL-43134 (Pruess et al., 1999).

The specific objectives pursued in the development of the new Version 2.0 of TOUGH2 are the following: (1) add significant capabilities for simulating flow and transport processes, that will be useful for engineering and geoscience applications; (2) add features to improve the useability of the code, but avoid encumbering users with "feature creep;" (3) keep code changes to the minimum required to achieve desired capabilities; (4) remain as much as possible upward compatible with the earlier version; (5) stay with the FORTRAN77 language standard; (6) facilitate code maintenance by minimizing the number of independent modules and "minor" variations among them; (7) increasingly emphasize solved problems and internal documentation as a way of communicating code features and use.

The T2VOC code for modeling three-phase three-component flow of water, air, and a volatile organic chemical is now included as a module into TOUGH2. It provides all the process simulation capabilities discussed in the T2VOC User's Guide (Falta et al., 1995), but some of the new features added in Version 2.0 of TOUGH2 are not yet implemented with T2VOC. The T2DM module for strongly coupled flow and transport in 2-D systems with hydrodynamic dispersion has also been integrated into TOUGH2. Specialized reports are available that document features and input requirements for T2DM (Oldenburg and Pruess, 1993, 1995).

Code Revisions and Enhancements

We begin by briefly describing the process followed for making code changes. As an example, consider the implementation of a capability for flowing wellbore pressure corrections of geothermal (two-phase water-steam) wells. This required coding changes in the sink/source subroutine QU, as well as in subroutine RFILE in which assignment of GENER input data to data arrays is made. The modification process was started by extracting subroutines RFILE and QU from program file t2f.f, and copying these routines into a new source code file qumod.f. Modifications were then made to file qumod.f, while preserving the old versions of RFILE and QU intact in file t2f.f. During the development process, the compiled file qumod.o was linked in front of t2f.o. This creates a condition of “duplicate names” during linking, whereupon the linker on our IBM RS/6000 proceeds to use the first appearance of that name. (On some computers such a duplicate name would produce a fatal error condition. The easiest way to avoid this is to rename unwanted duplicate program units; in our example, subroutines QU and RFILE in t2f.f would be renamed something like QUX and RFILEX, respectively.) Preserving the unmodified versions of subroutines intact in their respective source code files makes it very convenient to continue using unmodified code versions for comparison runs. After all desired changes were implemented in qumod.f and new as well as “old” code capabilities were tested, the final code revision step consists of importing the new revised subroutines from qumod.f into t2f.f, and archiving the previous subroutines.

EOS Modules

The subroutines providing water properties (COWAT, SUPST, and SAT) were replaced with faster routines written by Michael O’Sullivan, University of Auckland, New Zealand. The speedups were achieved through coding changes such as using multiplication instead of exponentiation wherever possible. The correlation for temperature dependence of Henry’s law in the EOS2 module was replaced with a new formulation developed by Battistelli et al. (1997), which is accurate for $0\ ^\circ C \leq T \leq 350\ ^\circ C$.

Several new EOS-modules have been added to the TOUGH2 package. These provide simulation capabilities for variably saline brine and non-condensible gas; dissolving and precipitating salt (NaCl) with porosity and permeability change; three-phase flow of water, air and oil; parent-daughter radionuclide tracers that may dissolve in the aqueous and volatilize in the gas phase; and saturated-unsaturated flow according to Richards’ equation.

User Features

Common block /TIMES/ was renamed /TIM/ to avoid a name conflict with the systems timing routine on IBM RS/6000 workstations. Subroutine SECOND is now active for timing runs on the RS/6000.

Time series data for graphing can be generated by means of a new data block "FOFT" for selected grid blocks, by means of a new data block "COFT" for connections, and for sinks and sources by means of a new data block "GOFT." The corresponding data files named FOFT, COFT, and GOFT, respectively, are written in a new subroutine FGTAB following CYCIT.

A number of user features and conveniences were added. The previous (1991) release of TOUGH2 allowed records in the input file that did not begin with a keyword signaling the beginning of a data block. Such records could be informally used as comments to document noteworthy features of the input data. If present, each such record triggered printing of an output statement `HAVE READ UNKNOWN BLOCK LABEL "     " --- IGNORE THIS, AND CONTINUE READING INPUT DATA`. These records are now formally recognized as comments and, if present, the first 50 of them will be printed to the output file. No warning messages will be printed when unknown block labels are encountered.

Radiative Heat Transfer

Subroutine MULTI was upgraded to (optionally) include radiative heat transfer. For grid blocks with interface area A and absolute temperatures T_1 and T_2, radiative heat flow rate is given by

$$F_{rad.}^{heat} = A \cdot s \cdot \sigma \cdot \left(T_2^{\,4} - T_1^{\,4}\right) \quad (1)$$

Here, σ is the Stefan-Boltzmann constant, $\sigma = 5.6687 \times 10^{-8}$ J/(m^2 K^4 s), and s is the relative "radiant emittance" which, for a perfect "black body," is given by s = 1. Radiative heat transfer between two grid blocks is engaged simply by specifying $s \neq 0$ at the appropriate connection.

Sinks and Sources

The coding for sinks and sources, chiefly in subroutines QU and RFILE, was completely re-written. QU was restructured as an exectuive routine with modular structure for different generation types. Most of the numerical work in assembling generation terms is now performed by a number of satellite routines. Previously available GENER-options were maintained or enhanced in an upwardly compatible manner, and new sink/source options are available. For example, timedependent sink/source rates, specified by tabular data, can now be handled in such a manner that cumulative mass or heat exchanges are rigorously maintained, regardless of time steps taken. This "rigorous step rate" capability can be selected by setting MOP(12) = 2.

Coupled Wellbore Flow

Chiefly of interest for geothermal reservoir studies is a new capability to produce single- and two-phase wells with specified wellhead pressure. The coupling between flow from the reservoir into the well, and flashing (boiling) flow up the wellbore, is automatically performed during the simulation. Well behavior is described by tabular data of bottomhole pressures as a function of flow rate and flowing enthalpy. The well tables must be generated by wellbore simulation prior to a TOUGH2 run. The option of producing with specified wellhead pressure is selected by specifying a GENER-type starting with the letters `'F'` or `'f'`. For example, `'f-209'` is a valid GENER-type that will associate the host element with a production well. The user must supply a disk file named `f-209` in which TOUGH2 can find appropriately formatted data relating wellhead to flowing bottomhole pressures. Multiple data sets for flowing wellbore pressures may be used, e.g., for wells with different diameter, feed zone depth, and wellhead pressure. At present, no provisions are made for possible changes in the composition of produced fluids (non-condensible gases, dissolved solids). Full details are given in section 7.3 of the TOUGH2 User's Guide.

Multiphase Diffusion

Diffusion of all components in all phases was added. The formulation allows for strong coupling between diffusion and phase partitioning of water-soluble and volatile species. Diffusion coefficients are provided through a new data block DIFFU. In order to engage diffusion, the user must set the number of secondary parameters NB ≥ 8 in data block MULTI. Diffusion coefficients can be specified to remain constant, or to depend on phase saturations to represent saturation-dependent tortuosity effects. An option for enhanced vapor diffusion is also available. Details are given in Appendix D of the user's guide.

Block-by-block Permeability Modification

Various improvements have been made for initializing geometry data and providing information about mesh data in printed output. New routines were written to provide a capability for block-by-block permeability modification, as needed to model flow systems with multi-scale heterogeneity. Permeability modification coefficients ζ can be applied to each grid block to change permeability according to $k' = k * \zeta$, while strength of capillary pressure will be simultaneously scaled according to $P_{cap}' = P_{cap}/\sqrt{\zeta}$ (Leverett, 1941). The permeability modifiers ζ can either be internally generated or externally supplied by the user. Internal generation capabilities are currently available for randomly heterogeneous fields; if spatially-correlated heterogeneity structure is desired, users will have to provide their own routines for generating such fields.

Linear Equation Solvers

Linear equation solution capabilities were considerably enhanced (Moridis and Pruess, 1998). A new direct banded solver and a conjugate gradient solver DLUSTB using the BiCGSTAB algorithm (van der Vorst, 1992; Sleijpen and Fokkema, 1993) were added to the previously available direct and iterative solvers. DLUSTB provides improved convergence behavior when iterations are started close to the solution, i.e., near steady state. A variety of new preconditoning algorithms are available that can cope with difficult problems in which many of the matrix elements on the main diagonal are zero, such as "two waters" problems. The selection of solvers by means of the parameter MOP(21) is still available, but it can be overwritten with a new optional input data block SOLVR that allows selection of preconditioners, as well as iteration and convergence criteria.

References

Battistelli, A., C. Calore and K. Pruess. The Simulator TOUGH2/EWASG for Modeling Geothermal Reservoirs with Brines and Non-Condensible Gas, *Geothermics,* Vol. 26, No. 4, pp. 437 - 464, 1997.

Falta, R.W., K. Pruess, S. Finsterle, and A. Battistelli. T2VOC User's Guide, Lawrence Berkeley Laboratory Report LBL-36400, March 1995.

Leverett, M.C. Capillary Behavior in Porous Solids, *Trans. Soc. Pet. Eng. AIME*, 142, 152-169, 1941.

Moridis, G. and K. Pruess. T2SOLV: An Enhanced Package of Solvers for the TOUGH2 Family of Reservoir Simulation Codes, *Geothermics,* Vol. 27, No. 4, pp. 415 - 444, 1998.

Oldenburg, C.M. and K. Pruess. A Two-Dimensional Dispersion Module for the TOUGH2 Simulator, Lawrence Berkeley Laboratory Report LBL-32505, September 1993.

Oldenburg, C.M. and K. Pruess. EOS7R: Radionuclide Transport for TOUGH2, Lawrence Berkeley National Laboratory Report LBL-34868, November 1995.

Pruess, K., C. Oldenburg and G. Moridis. Overview of TOUGH2, Version 2.0, in: K. Pruess (ed.), Proceedings of the TOUGH Workshop '98, pp. 307 - 314, Lawrence Berkeley National Laboratory Report LBNL-41995, Berkeley, CA, May 1998.

Pruess, K., C. Oldenburg and G. Moridis. TOUGH2 User's Guide, Version 2.0, Lawrence Berkeley National Laboratory Report LBNL-43134, Berkeley, CA, November 1999.

Sleijpen, G.L.G. and D. Fokkema. BiCGSTAB(m) for Linear Equations Involving Unsymmetric Matrices with Complex Spectrum, *Electronic Transactions on Numerical Analysis,* Vol. 1, pp. 11 - 32, 1993.

van der Vorst, H.A. Bi-CGSTAB: A Fast and Smoothly Converging Variant of BiCG in the Presence of Rounding Errors, *SIAM J. Sci. Statist. Comput.*, Vol. 13, pp. 631 - 644, 1992.