Computers & Geosciences 65 (2014) 2–12

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

Advances in subsurface modeling using the TOUGH suite of simulators

Stefan Finsterle*, Eric L. Sonnenthal, Nicolas Spycher

Lawrence Berkeley National Laboratory, Earth Sciences Division, One Cyclotron Road, MS 74-120, Berkeley, CA, United States

ARTICLE INFO

Article history:
Received 17 April 2013
Received in revised form
12 June 2013
Accepted 14 June 2013
Available online 20 June 2013

Keywords:
Numerical simulation
Coupled processes
Multiphase flow
Reactive transport
TOUGH

ABSTRACT

The TOUGH suite of nonisothermal multiphase flow and transport simulators is continually updated to improve the analysis of complex subsurface processes through numerical modeling. Driven by research questions in the Earth sciences and by application needs in industry and government organizations, the codes are extended to include the coupling of relevant processes and subsystems, to improve computational performance, to support model development and analysis tasks, and to provide more convenient pre- and post-processing capabilities. This review paper briefly describes the history of the simulator, discusses recent advances, and comments on potential future developments and applications.

1. Introduction

Numerical modeling is applied to characterize, predict, and optimize subsurface systems of increasing complexity. This increase arises foremost from the technological challenges that need to be addressed to ensure the sustainability of water, energy, and environmental systems. To be able to reliably predict the response of these systems to natural or man-made changes in the subsurface properties and forcing terms, it is essential to consider coupled processes and to include many intricate hydrogeologic features. Advances in both process understanding and computational methods have enabled us to simulate such systems with a higher degree of realism. This increased model fidelity is accompanied by increased requirements for code developers, modelers, and end-users of simulation results, making it imperative that the capabilities and limitations of a code are clearly stated, that the assumptions underlying a site-specific conceptual model are understood and justified, and that confidence in simulation results are obtained through independent information and assessments. While most of these requirements need to be fulfilled by the user, some characteristics of the computer code itself and the way it is developed are essential for its successful application.

There are many computer codes for simulating flow and other, more complex processes in the subsurface. They differ in the features and processes being modeled, the method used to couple them, in the numerical approach, and in the support provided for setting up and post-processing models and their results. It is often difficult (and beyond the scope of this paper) to compare the capabilities of these codes and to make a decision on which code is most suitable for a given application. We refer the reader to review papers and code-comparison studies, which often provide a good overview of simulator capabilities (Baca and Seth, 1996; O'Sullivan et al., 2001; Oldenburg et al., 2003; Pruess et al., 2004; MDH Engineered Solutions Corporation, 2005; Hudson et al., 2009; Birkle, 2011).

This paper focuses on the TOUGH codes, which simulate nonisothermal flow of multiphase, multicomponent fluids in porous and fractured geologic media (Pruess et al., 1999; http://esd.lbl.gov/TOUGH2). The simulator's long history, its scientific underpinnings, its vibrant developer and user community, and—most importantly—its widespread application to a large number of relevant scientific and engineering projects are considered key to making it suitable for addressing the next level of subsurface flow and transport problems.

This paper summarizes some advances of the TOUGH suite of codes, supplementing previous reviews (Pruess et al., 1997; Finsterle, 2004; Pruess, 2004; Finsterle et al., 2008, 2012a) and the research papers in this special issue of *Computers & Geosciences*. The review is very limited in that it focuses on recent code developments rather than providing a comprehensive overview of code applications.

2. History

Developed at the Lawrence Berkeley National Laboratory in the early 1980s primarily for geothermal reservoir engineering, the

* Corresponding author. Tel.: +1 510 486 5205; fax: +1 510 486 5686.
E-mail addresses: SAFinsterle@lbl.gov (S. Finsterle), ELSonnenthal@lbl.gov (E.L. Sonnenthal), NSpycher@lbl.gov (N. Spycher).

0098-3004/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.cageo.2013.06.009

suite of TOUGH simulators (Table 1) is now widely used at universities, government organizations, and private industry for applications related to geological carbon sequestration, nuclear waste disposal, energy production from geothermal, oil and gas reservoirs as well as methane hydrate deposits, environmental remediation, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and geomechanical processes in permeable media. While the fundamental concept of writing the governing mass- and energy-balance equations in integral form and solving them fully coupled using the integral finite difference method has been preserved over the years, the TOUGH suite of simulators is continually updated, with new equation-of-state (EOS) modules being developed, and refined process descriptions implemented into its framework. Moreover, the code's multi-physics capabilities have been significantly widened, and linkages to related subsystems (such as wellbores, surface water bodies, and the atmosphere) have been established. Finally, the numerical performance of the simulators is being improved through parallelization and the use of state-of-the-art linear equation solvers. The following paragraphs provide an overview of the various members of the TOUGH family of codes.

The basic TOUGH2 code is a serial, general-purpose simulation program that considers flow of multiphase fluid mixtures and heat in fractured porous media for select components and phases. The considered combination of components and related fluid properties are calculated by the particular EOS fluid property module that is linked to the main flow and transport core, which sets up and solves the mass- and energy-balance equations. All EOS modules contain water, and may include non-condensable gases, solutes, volatile organic compounds, tracers, and radionuclides. These components are transported through the geologic media in one, two, or three fluid phases (gaseous, aqueous, and non-aqueous phase liquids). Some components may also precipitate and dissolve, or adsorb and desorb, i.e., become part of or interact with an immobile solid phase. The partitioning of each component in each phase and the appearance or disappearance of

Table 1
Overview of TOUGH simulators.

Simulator	Phases[a], components[b], processes	Released	Key references[c]
MULKOM	Research code for nonisothermal multiphase, multicomponent flows of Newtonian and non-Newtonian fluids	No public release	Pruess (1983)
TOUGH	Nonisothermal flow of water and air in aqueous and gaseous phase	1987	Pruess (1987)
AUTOUGH	Enhanced version of TOUGH(2) developed by the University of Auckland, New Zealand	No public release	Bullivant (1990)
TOUGH2	Nonisothermal flow of water and NCG in aqueous and gaseous phase	1991	Pruess (1991)
M2NOTS	Nonisothermal flow of water, air, multiple organic contaminants in aqueous, gaseous, and NAPL phase	No public release	Adenekan et al. (1993)
T2VOC	Nonisothermal flow of water, air and VOCs in aqueous, gaseous and NAPL phase	1995	Falta et al. (1995)
ChemTOUGH	Nonisothermal multiphase flow and reactive transport	No public release	White (1995)
EOS7R	Nonisothermal flow of water, brine, and parent–daughter radionuclides (released with TOUGH2 V2 in 1999)	1995	Oldenburg and Pruess (1995)
iTOUGH2	Inverse modeling, sensitivity analysis, and uncertainty propagation analysis for TOUGH2 and additional EOS modules	1997	Finsterle (2004)
EWASG	Nonisothermal multiphase, multicomponent flow of saline fluids and a non-condensible gas with salt precipitation	1999	Battistelli et al. (1997)
EOS9nT	Saturated/unsaturated flow and decaying solute/colloid transport	1999	Moridis et al. (1999)
TOUGH2 V2	Nonisothermal multiphase, multicomponent flow	1999	Pruess et al. (1999)
T2R3D	Radionuclide transport module with hydrodynamic dispersion (released with TOUGH2-MP in 2008)	No public release	Wu (1999)
T2LBM	Landfill bioreactor model	No public release	Oldenburg (2001)
TMVOC	Nonisothermal flow of water, air, multiple VOCs and NCGs in aqueous, gaseous, and NAPL phase	2002	Pruess and Battistelli (2002)
TMVOCBio	Nonisothermal flow of water, air, multiple VOCs and NCGs in aqueous, gaseous, and NAPL phase	No public release	Battistelli (2004)
EOSN	Nonisothermal flow of water, air, and noble gases	No public release	Shan and Pruess (2004)
TOUGHREACT	Nonisothermal multiphase flow and reactive transport including equilibrium and kinetic mineral dissolution and precipitation, chemically active gases, intra-aqueous and sorption reaction kinetics and biodegradation	2004	Xu and Pruess (2001) and Xu et al. (2006, 2011)
EOS7C	Nonisothermal flow of water, brine, CH_4–CO_2 or CH_4–N_2 in aqueous and gaseous phase	2007	Oldenburg et al. (2003)
Hysteresis	Hysteretic relative permeability and capillary pressure functions	2007	Doughty (2007)
TOUGH+	Re-engineered and expanded version of TOUGH2 simulator, specifically for the simulation of hydrate-bearing geologic media	2008	Moridis et al. (2008)
TOUGH-FLAC	Research code for coupled multiphase flow and thermal–geomechanical processes; links TOUGH2 and FLAC3D Itasca Consulting Group Inc., (1997)	No public release	Rutqvist et al. (2002)
TOUGH2-MP	Massively parallel version of TOUGH2	2008	Zhang et al. (2008)
TMGAS	Nonisothermal flow of mixtures of inorganic gases and hydrocarbons	No public release	Battistelli and Marcolini (2009)
T2Well	Coupled wellbore–reservoir simulator	2011	Pan and Oldenburg (2013)
ECO2M	Multiphase flow of sub- and supercritical CO_2	2011	Pruess (2011)
TOUGHREACT-Pitzer	Adds Pitzer-type formulation for high ionic strength brines to TOUGHREACT	2012	Zhang et al. (2006, 2009)
TOUGHREACT-ROCMECH	Adds rock mechanical deformation to TOUGHREACT, including new formulation for deformation using MINC	No public release	Kim et al. (2012a, b)
EOS7C-ECBM	Enhanced coal-bed methane	2013	Webb (2011)

[a] NAPL, non-aqueous phase liquid.
[b] NCG, non-condensible gas; VOC, volatile organic compound.
[c] For a complete list and download of all available manuals, see the documentation tab at http://esd.lbl.gov/TOUGH.