Title
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Publication Date
2017-11-01

DOI
10.1016/j.cageo.2017.09.001

Peer reviewed

Preface to the Special Issue on TOUGH Symposium 2015

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The TOUGH Symposium 2015 was held in Berkeley, California, September 28-30, 2015. The TOUGH family of codes, developed at the Energy Geosciences Division of Lawrence Berkeley National Laboratory (LBNL), is a suite of computer programs for the simulation of multiphase and multicomponent fluid and heat flows in porous and fractured media with applications in many geosciences fields, such as geothermal reservoir engineering, nuclear waste disposal, geological carbon sequestration, oil and gas reservoirs, gas hydrate research, vadose zone hydrology and environmental remediation. Since the first release in the 1980s, many modifications and enhancements have been continuously made to TOUGH and its various descendants (iTOUGH2, TOUGH+, TOUGH-MP, TOUGHREACT, TOUGH+HYDRATE, TMVOC...), at LBNL and elsewhere. Today, these codes are used worldwide in academia, government organizations and private companies in problems involving coupled hydrological, thermal, biogeochemical and geomechanical processes. The Symposia, organized every 2-3 years, bring together developers and users for an open exchange on recent code enhancements and applications. In 2015, the Symposium was attended by one hundred participants, representing thirty-four nationalities. This Special Issue in Computers & Geosciences gathers extended versions of selected Symposium proceedings related to (i) recent enhancements to the TOUGH family of codes and (ii) coupled flow and geomechanics processes modeling.

In this special issue, a paper by Jung et al. provides a new base version of TOUGH, TOUGH3. This latest version addresses the computational robustness and efficiency needed for the increasing complexity of the simulated processes and the growing size of model domains. Moreover, it consolidates the serial and parallel versions into a single code, hence, inconsistencies between different versions are less likely to occur, and code maintenance and development become more efficient. *Finsterle et al.* present a review of the capabilities of iTOUGH2 and illustrate the workflow of an integrated simulation-optimization framework. *Liu et al.* present an approach to reduce the computational cost of performing Bayesian inverse modeling and demonstrate their approach using a synthetic experiment simulated with TOUGH2. Regarding the mesh generation process, the paper by *Doughty* presents a generalization of the grid-generation algorithm embedded in TOUGH2 (MESHMAKER) to create one-column grids with fractal dimension, useful for representing flow through fractures or highly heterogeneous media with fractal geometry, and also for inverse methods. *Sentís and Gable* present a module to interface the open source code Lagrit with TOUGH2, that assists in the processes of mesh generation and model setup, and that can be particularly useful for complex geometries and large models. *Bonduà et al.* present a pre-processing tool

(VORO2MESH) that features a full 3D Voronoi approach for structured and unstructured grids, and an enhanced post-processor (TOUGH2Viewer) for the visualization of 3D Voronoi grids.

The literature review shows that coupled fluid flow and geomechanics has gained increasing attention in the last years in many geosciences fields. In this context, several codes of the TOUGH family have been successfully coupled with geomechanics software. The paper by *Rutqvist* presents a review of some of these TOUGH-based geomechanics models, of which the TOUGH-FLAC simulator – presented for the first time in the TOUGH Symposium 2003 – is well-known worldwide and has been used in a large variety of applications, encompassing the application domains of the TOUGH codes. *Blanco-Martín et al.* present an extension of TOUGH-FLAC to the finite strain framework, motivated by the existence of large strains associated with rock salt deformation in the context of heat-generating nuclear waste disposal. Following a paper published in the Special Issue of the TOUGH Symposium 2012 in this journal, *Kim et al.* present the current status of the TOUGH-RSBN simulator for coupled hydro-mechanical modeling of hydraulic fracturing using a discrete fracture network approach, and present some validation and demonstration cases. *Rinaldi and Nespoli*present TOUGH-SEED, an injection-induced seismicity modeling approach using TOUGH2 and a geomechanics stochastic model, and apply it to the Basel EGS project. Finally, *Rinaldi et al.* use the PEST protocol implemented in iTOUGH2, combined with TOUGH-FLAC as the forward model, to perform inverse modeling for the In Salah CO_2 demonstration site in Algeria. Using pore pressures and InSAR displacements as observations, this approach allows for a multi-physics joint inversion and takes advantage of the inverse capabilities of iTOUGH2 (parameter estimation, sensitivity analysis, uncertainty estimation …), applied to coupled fluid flow and geomechanics.

On behalf of the members of the TOUGH Symposium 2015 Organizing Committee, I hope that this collection of papers will provide the readers of Computers & Geosciences with a recent view of the capabilities of the TOUGH family of codes, as well as with current modeling research domains in the geosciences. Last but not least, I would like to express my gratitude to all the reviewers who kindly contributed to this Special Issue, as well as the Journal staff who have made this publication possible.