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Author

Doughty, C

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Introduction to the Special Issue on Simulation of Geologic Carbon Sequestration with the TOUGH codes

As a leading candidate technology to mitigate greenhouse gas (GHG) emissions, geologic carbon dioxide sequestration (GCS) has been intensively studied over the last 15+ years. Because there have been relatively few field projects, and these have mainly been of limited size and duration, numerical simulation has taken on a critical role for improving our understanding of the processes accompanying CO₂ injection into geologic formations. Of the reservoir simulators that have been developed and used extensively for GCS, the TOUGH family of codes stands out for its long history and large user base. The TOUGH codes were originally developed in the early 1980s for geothermal reservoir simulation at the Lawrence Berkeley National Laboratory (LBNL) (see <http://esd.lbl.gov/TOUGH>). The TOUGH codes (TOUGH is an acronym for Transport Of Unsaturated Groundwater and Heat) have been applied to a large variety of problems, including geothermal energy reservoir engineering, nuclear waste isolation, subsurface environmental remediation, methane gas hydrate production, compressed air energy storage, and many other energy and environmental applications in addition to GCS, the subject of this Special Issue. The long history and wide range of application areas of the TOUGH codes comes with a large number of users around the world in academia, government research labs, and industry.

The LBNL TOUGH development group organizes and hosts a triennial TOUGH symposium in Berkeley to bring the community together to share research results and applications of the TOUGH codes. During 28-30 September 2015, LBNL hosted its 8th triennial TOUGH symposium since 1990, at which approximately 100 attendees from 19 countries gathered over three days to present more than 80 papers in oral and poster formats about their applications and enhancements related to the TOUGH codes. The philosophy behind the LBNL's development and distribution of the TOUGH codes is to make new developments available to the community at low cost, either as executable or source code, or both. Access to source code means that users can customize the code for their specific purposes. When these researchers allow the LBNL to incorporate their improvements and distribute the new capabilities, even more people to benefit from the development work. So while the TOUGH codes are not formally a community code, many of the developments find their way back to the LBNL and public distribution.

As for past TOUGH symposia, some of the authors who presented papers across a range of subject areas at the TOUGH Symposium 2015 were invited to submit full journal papers for inclusion in peer-reviewed journal special issues. This Special Issue of *Greenhouse Gases: Science and Technology* contains six papers by authors from four countries (Australia, Italy, Taiwan, and the USA), which are the invited papers in the area of GCS. (The full TOUGH Symposium 2015 proceedings can be found on the TOUGH website.) Two of the papers in this special issue focus on thermodynamic properties of fluids relevant for GCS (CO₂, CH₄, brine), while the remainder examine factors such as formation heterogeneity, hysteretic multi-phase flow properties, and fault self-sealing, which control CO₂ trapping in the subsurface.