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Numerical modelling in research on geothermal systems

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Abstract. Nowadays, numerical modelling is a common tool for supporting the research of geothermal systems. Due to the development of computer sciences and access to software dedicated to numerical modelling of hydrogeological processes this is possible. Research can schematise hydrogeological conditions and simulate the work of geothermal systems and thermal water intakes. Research creates numerical models of geothermal systems at the regional and local scale for simulating work of specific thermal waters for example.

In connection with the economic development of the use of thermal waters in Poland there are many research projects where numerical modelling occurs as a primary tool. This paper provides an overview of research issues where the solution to the problem was found by using computer applications and numerical simulators.

Key words:
numerical modelling,
geothermal systems,
thermal water,
computer simulation

A Few Words about Creating Numerical Models

With the computer applications dedicated to hydrogeology it becomes possible to predict the temperatures of thermal waters and changes in operating of geothermal systems for many years (30-50 years). This is particularly important in the time assessment of cold water movement inside a rock matrix by the reinjection process into the aquifers. Possibilities of forecasting changes in pressures, groundwater levels and changes in discharge of the wells are also very important.

The huge advantage of numerical modelling is that it is possible to find an easy solution to research problems where finding a solution with analytical methods, field studies and laboratory investigations would take many years. Another advantage is that it is a comfortable way to create the graphic presentation of the modelling issue. Mathematical modelling is a good tool not only for forecasting changes in thermal water temperatures inside a reservoir. This model of geothermal systems helps to determine the mining area and allows rational decisions to be taken in processes of thermal water formation and energy management (Kapuściński 2011).

Available applications allow scientists to create models with many variables. Unfortunately, it causes an increase in the complexity of the models in some cases and requires extra time for calculations and difficulties during the validation of the models (Miecznik 2010). Another problem pointed out by researchers is also a small amount of reliable hydrogeological data (Szczepański, Szklarczyk 2006; Kapuściński 2011).

Geological data are the basis for creating numerical models. Information about results of the exploration works, field investigations and monitoring of the work of individual thermal water formation and intakes is particularly useful. During the calibration/validation of numerical models it is important to use the monitoring data consisting of the exploitation of thermal waters. With numerical models researchers can better understand processes occurring during the exploitation of the thermal waters.

For creators of numerical models the challenge is an appropriate mapping of directions of the fissures and faults recognizing the discontinuity surfaces that determine the permeability of rocks and thermal water flow directions. In such cases the structure of porous rock aquifers and dual porosity using the MINC method (Multiple Interacting Continua) or mapping accurately identified fissures and fault systems are taken into consideration (Ganguly, Kumar 2012).

Research on Polish Geothermal Systems Supported by Numerical Modelling

Use of the PHREEQC and related applications

PHREEQC application (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/index.html) and related simulators are used primarily in the studies of the chemical composition of thermal waters and chemical processes related with the technology of exploitation of thermal waters.

This program was used for the modelling of the thermodynamic equilibrium of the water-rock interaction and to predict the scaling process of secondary minerals in thermal waters (Kania 2003; Tomaszewska 2008; Bujakowski 2010; Kępińska, Bujakowski 2011; Kleszcz, Tomaszewska 2013). In this research an assessment was made of the risk of the decline in injection possibilities. This phenomenon is caused by clogging of the well active zone (Tomaszewska, Pająk 2012). Finding solutions to these kinds of problems is a key to taking actions to ensure trouble-free work during the exploitation in the geothermal systems.

Applications like PHREEQC, PHREEQCI, SEAWAT, HYDROTHERM and WATEQ4F are used to calculate the thermodynamic equilibrium. All of these applications work based on a free licence. Simplicity of use and the possibility of applying different thermodynamic databases are the major advantages of the PHREEQCI type programs. Unfortunately, Phreeqc.dat default database is not good for modelling hydrogeochemical processes of high saline thermal waters. These problems touch thermal waters located in the Polish Lowland. To solve such problems researchers used databasespitzer.dat, and/or wateq4f.dat and llnl.dat which contain many kinds of minerals (Bujakowski 2010).

PHREEQCI was used for the identification of the chemical composition of the thermal waters and evaluation of the chemical equilibrium in the Busko C-1 borehole in Busko-Zdrój town. In Busko-Zdrój groundwaters in areas of thermal waters occur which are defined as thermal and medicinal waters (Gała 2011). Assessment processes determined the chemical composition of water in the Busko C-1 borehole and its origin was a result of a hydrogeochemical analysis carried out with the use of the PHREEQCI program.

In a similar purpose the PHREEQCI program was used in studies of the Łódź Trough area thermal waters. The result of hydrogeochemical modelling was determined by forming conditions of the chemical composition of thermal waters in that area (Wiktorowicz 2014).

Geothermal formation issue – software used

AQUA (Vatnaskill Consulting Engineers of Reykjavik) was one of the first programs used in thermal water investigation in Poland. This program based on the finite element method was used to predict the exploitation of the Lower Jurassic thermal water intakes in Pyrzyce, the Szczecin Trough. By this numerical model it was possible to outline the stability of the temperature forecast, interaction between production and injection wells and determination of the mining area. Researchers created two models: the hydrodynamic model of filtration and dispersion and the heat flow model (Kapuściński 2011).

Currently, there are many programs which are commonly used for simulations of groundwater flows and other processes in the deep aquifer systems, for example: TETRAD (Vinsome, Shook 1993), STAR (Pritchett 1995), SHEMAT (Wellmann et al. 2012), CHILLER (Reed 1998) or TOUGH (Pruess et al. 1999) with its updates (Table 1). TOUGH2 is a numerical simulator which is the most popular among Polish researchers and helps them to solve problems of thermal water exploitation.

Table 1. Review of TOUGH simulators (based on Finsterle et al. 2014)

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 modelling, 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-condensable 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 and Xu et al., (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 well bore–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 and Zhang et al., 2009
TOUGHREACT-ROCMECH	Adds rock mechanical deformation to TOUGHREACT, including new formulation for deformation using MINC	No public release	Kim et al., 2012a and Kim et al. 2012b
EOS7C-ECBM	Enhanced coal-bed methane	2013	Webb (2011)

[a] NAPL, non-aqueous phase liquid
[b] NCG, non-condensable gas; VOC, volatile organic compound
[c] Key references in Finsterle et al. (2014)

TOUGH2 numerical simulator (Transport of Unsaturated Groundwater and Heat) is used in modelling of the combined heat and mass transport in porous aquifers, modelling mixed compound and multiphase fluids (Pruess et al. 1999). TOUGH2 is especially useful in the modelling processes in geothermal systems (Ganguly, Kumar 2012; Lei, Zhu 2013; Arnaldsson et al., 2014; Finsterle et al. 2014). Moreover, by this program researchers can create the design of the radioactive waste landfill (Rechard et al. 2014), models of HDR systems (Hot Dry Rocks), the EGS (Enhanced Geothermal System) (Borgia et al. 2012; Zeng et al. 2014) and the carbon dioxide sequestration (Audigane et al. 2011). TOUGH simulators have been developed since 1980 by Lawrence Berkeley National Laboratory (http://esd1.lbl.gov/research/projects/tough/).

The TOUGH algorithm is based on the finite difference method. Numerical models created in TOUGH were used for the assessment of interaction between Skierniewice GT-1 and Skierniewice GT-2 wells as regards thermal water hydrodynamic, heat transfer and exploitation conditions (Kępińska, Bujakowski 2011). Modelling was performed using an EWASG simulator. It was possible with the EWASG simulator to model the impact of fluids with high NaCl content on the density, viscosity and enthalpy of thermal waters. Numerical modelling of the Skierniewice area with EWASG was created by Battistelli and Nagy (2000).

TOUGH2 was also used in the work of the study "Atlas of the possible use of geothermal waters for combined production of electricity and heat using binary systems in Poland" (Bujakowski, Tomaszewska 2014). For 10 selected zones models were created of thermal characteristics of the orogen on a local scale as were models of exploitation conditions of geothermal systems in a long time scale (50 years). The area of each zone was about 150 km^2. By using data from models the amount of energy production was assessed which obeyed principles of the sustainability of natural resources (Bujakowski, Tomaszewska 2014).

The TOUGHREACT simulator is an extended version of the TOUGH simulator. Using this simulator researchers can model chemical reactions between liquid and rocks in porous and fracture reservoirs (Xu et al. 2006). This type of modelling is very important in forecasting the permeability of the reservoir rocks in the long time scale. A result of the precipitation of secondary minerals might be the reduction in the porous space in reservoir rocks and the decline in aquifer permeability. Such phenomena occur especially in the active zone of the production wells (Kępińska, Bujakowski 2011) and during the exploitation of highly mineralized thermal waters (Tomaszewska 2008).

The complexity of hydrogeological processes and geothermal conditions and/or the variety of problems in geothermal issues are reasons why researchers also use other applications in numerical modelling. Szczepański and Szklarczyk (2006) used in their research project the MODFLOW application. The MODFLOW algorithm is developed by the U.S. Geological Survey and since 1984 is available as an open-source licence (http://water.usgs.gov/ogw/modflow/).

Modelling was a tool which helped to review resources of thermal waters in the Upper Jurassic aquifer geothermal systems in the Piła region, Rogoźno and Wągrowiec wells (Szczepański, Szklarczyk 2006). The MODFLOW algorithm is based on the finite difference method. In that case researchers determined groundwater circulation by MODFLOW and MT3D (http://hydro.geo.ua.edu/mt3d/) simulators and checked out hydrogeological parameters and assessed resource sustainability, disposable resources and optimal exploitation conditions of the thermal waters in prospective areas. The task was solved in a few steps: in the first one researchers created a numerical model of the regional water circulation systems, the next was to cut down the regional model to the local area with Rogoźno and Wągrowiec wells and the last point was a detailed mass transport modelling. The mass transport model was necessary for the assessment of cold water movement inside a rock matrix.

In the Wiśniowa massif the problem of the optimalization of geothermal doublet work was solved with the Eclipse (Schlumberger) simulator (Machowski et al. 2013) and others (Botor et al. 2012; Botor et al. 2013; Papiernik et al. 2013). The working time for geothermal doublet was determined for 50 years. Thermal waters in this area are characterized by a high temperature, high discharge from a well and anomalous formation pressure. Researchers created a three-dimensional hydrodynamic model using applications like: TEMP – heat transport, THCONR –rocks and liquids thermal conductivities, SPECHEAT – fluid specific heat data and SPECROCK – rock specific heat data.

Summary

Numerical modelling is a common tool used in characterizing geothermal systems from the recognition stage to the utilization of thermal waters. Creation of reliable numerical models depends upon available geological data and information as well as the level of details of the conceptual and numerical model and is related to results of calibration and validation. Monitoring of the geothermal systems allows the numerical models to be validated. Numerical models help also to forecast changes in the structure of geothermal systems caused by actions during the exploitation of thermal waters, re-planning wells, existing time and/or drilling new wells.

Characteristics of the research problem determine the possibility of choosing the best modelling applications. Chemical composition of thermal waters might be determined with the PHREEQC application. This application is also a good tool in resolving problems related with the clogging of geothermal system installations. Researchers used the Eclipse simulator in attempt to optimize cooperation of the geothermal doublet. In the assessment of resources and groundwater circulation in geothermal systems MODFLOW applications were used. Generally, TOUGH2 is the most often used application by Polish researchers in their work.

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