The application of numerical modeling to geothermal investments

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Among numerous applications of numerical modeling in many different fields of science, there is numerical modeling applied to the issues related to geothermal investments [1]. A number of important parameters and properties can be estimated based on numerical modeling. In the case of geothermal investments, we can determine several factors, which may influence operation of the heating plants, e.g.: exploitation and size of extraction and/or injection of groundwaters, selection of an optimal spacing of boreholes (in the case of geothermal doublets), and water temperature or pressure [2].

This paper presents the issues related to the numerical modeling of geothermal reservoirs as well as a variety of computer software packages commonly used in creation of static and dynamic models, such as: Visual MODFLOW, TOUGH, FEFLOW or Petrel [3, 4]. The process of numerical modeling is presented in four general steps: (1) archival data collection and analysis (often using statistical methods), (2) creation of the static and (3) dynamic numerical models of a reservoir, and (4) environmental, financial and technical assessments based on a mathematical model of surface installation [5]. Each step is presented in details and the most important reservoir parameters, which influence the utilization of geothermal energy, are discussed.

At the end, the main directions in current utilization of geothermal waters in Poland and the future opportunities of geothermal heat generation, including the financial aspects related to geothermal investments, are discussed.

Keywords: numerical modeling, geothermal investments, geothermal heating plants.

1. INTRODUCTION

Dynamic modeling is used in various fields of science, e.g., geology, hydrogeology, reservoir engineering as well as in a wide spectrum of issues related to utilization of geothermal energy. The dynamic models enable us not only to project the geothermal reservoirs and the processes operating within them but also contribute to our understanding of their physical nature [1]. Depending on the scale of study area, the numerical models can be constructed as micro- (local scale, vicinity of geothermal doublets) or as macro-models (regional scale) [3]. Based on these models, we can estimate many important parameters, properties and factors which may influence the exploitation of groundwater reservoirs. The most important, from the point of view of geothermal investments, are: volumes of produced and injected waters, selection of the optimal spacing between production and injection wells (if geothermal doublets are used), determination of the radius of hydraulic swept area, water temperature or a breakthrough time of cold-water front to the reservoir. The advantages of modeling include the creation of multi-variant simulations of geothermal system operation and the analysis of problems which may emerge during this operation [3]. Thus, modeling may contribute to reduction of investment risk and running costs due to selection of optimal operation parameters. The currently available, specialized software widely used in dynamic modeling enables the operators to introduce many variables, which improves the accuracy of resultant models but also significantly extends the computation time of simulations [1]. The correctness of final model is strongly influenced by input data used in the modeling. Even the perfectly constructed models based on the averaged input datasets preclude the correct results. Important is also the professional experience of a person who operates the modeling procedure and interprets the results.

2. NUMERICAL MODELING PROCESS

In Poland, before the mid- 1960s the mathematical modeling of groundwater reservoirs has been usually conducted with the software related to the HYDRYLIB library [6]. The first calculation codes of numerical modeling applied to reservoir engineering have been developed in early 1970s. Before 2000, the numerical modeling has been used in over 100 geothermal fields [1].

The modeling itself is a complicated operation, which includes not only the determination of the objectives of the whole process but also involves the archival data acquisition and verification, the construction of conceptual model and its calibration, and the generation of numerical model used for simulations (Fig. 1).



Fig. 1. Main stages of modeling (after Murray-Darling Basin [7]).

Taking into account the complexity of numerical modeling from the point of view of its application to geothermal investments, we propose to divide the modeling process into the four main stages, which include not only the above mentioned operations but also embrace the design of surface installations (Fig. 2). The first three stages refer to scheme in Fig. 1 and include data preparation and interpretation (mostly, datasets available from deep wells and well logs) as well as conceptual and numerical models, which give a rise to an estimation of geothermal potential of a specific region.



Fig. 2. Modeling stages of geothermal reservoirs (authors' own data).

The last stage, which deals with the costs of surface installation, is the most important issue from the investor's point of view as it determines the economic efficiency of a given investment. The efficiency is controlled by the volume of extractable energy resources and the lifetime of installation [8] considering the most optimal prognostic scenarios.

Numerical modeling enables to approximate the solution of differential equations which describe the analyzed processes. The most commonly used numerical methods are:

- finite difference method (FDM),
- finite element method (FEM).

Recently, the modeling operations have used a specialized software, which not only generates the models but also verifies them and evaluates the errors (Table 1). Taking into account a plethora of available numerical modeling software, the most important selection criterion is the problem subject to modeling. In the case of hydrogeological models, the MODFLOW is usually a choice as it enables the operator to determine the dynamics of groundwaters, to verify the hydrogeological parameters and to evaluate the recharge of aquifer (including the safe yield), and the optimal production parameters [3]. Similar to MODFLOW is the MT3D99 mainly applied to the modeling of filtration and migration of pollutants [6].

SOFTWARE	
Finite Difference Method (FDM)	Finite Element Method (FEM)
MODFLOW family (Visual MODFLOW, Processing MODFLOW)	AQUA [6]
TOUGH	FEFLOW [6]
GMS [6] (groundwater modeling system) depending on version	GMS [6] (groundwater modeling system) depending on version
MT3D99 [6]	
MIKE.SHE [6]	

 ${\bf Table \ 1.} \ {\bf Recently \ used \ dynamic \ modeling \ software.}$

A widely used modeling software is also the transport of unsaturated groundwater and heat (TOUGH) software dedicated to generation of joint mass and heat transfer models in both the porous and fractured reservoirs [9]. This software produces models of both the geological and hydrogeological conditions then used in construction of thermal models enabling us to estimate the energy generation [10]. Other popular software [6] are: MIKE.SHE – a Danish development suitable for solving hydrogeological and hydrologic problems, somewhat similar GMS (groundwater modeling system) – a US-originated system dedicated to hydrogeological and water management issues, FEFLOW developed by a German-Danish joint venture and designed for modeling of filtration, migration and heat transfer in aquatic environments, and a less-popular AQUA from Iceland, used in modeling of heat transfer in groundwaters.

Input data and structural model

The development of static 3D model is a joint effort of geologists, seismic and well log geophysicists, petrophysicists, sedimentologists and geostatisticians. Recent trends in software development for 3D modeling include a deeper integration of various datasets, more comprehensive usage of geophysics [11–14] as well as modeling of uncertainty resulted from the limited accuracy of seismic data interpretation as well as modeling of velocity and reservoir properties, all very important from the point of view of exploration economics [14–19] (Fig. 3).



Fig. 3. Principal stages of geological static modeling.

The construction of structural model starts with the geological data acquisition necessary for determination of geological and hydrogeological conditions as well as geothermal parameters (Fig. 3). Particularly important is the information obtained from deep wells together with a full range of the results of studies and laboratory analyses collected during the drilling. Crucial is also the relevant recognition of geological structure of the area, including the orientation of discontinuities (faults, tectonic zones) and directions of groundwater flows [3], their recharge zones and drainage patterns. Apart from the geological information obtained during the drilling, the results of archival mappings and 2D/3D seismic interpretations are also valuable in modeling [4, 20]. Modern developments in geological modeling aim at a very close integration of structural, facial, parametric and tectonic models combined with reservoir and geomechanical simulations [21] using the 3D seismics and seismic attributes analysis, which enables us to position the tectonic discontinuities [22] as well as to correlate the results of many variants of seismic inversion with the laboratory measurements of porosity and geomechanical properties of rocks, and with the well log data.

When data integration is completed, the geometric control points of 3D structural model are generated in relation to stratigraphic information from the wells. Usually, the control point network is based on archival structural maps and/or on the results of seismic data interpretation. Depending on the used software and the complexity of geological structure, the spatial 3D model can be either structured, e.g., composed of regular or irregular hexagons or can be unstructured, e.g., built of triangles spatially transformed into tetrahedrons.

The next stage is the generation of principal parametric models, successively: lithofacial, claycontent, porosity or permeability. The static models of geological formations can be generated directly with the software used for dynamic modeling, e.g., TOUGH, MODFLOW, ECLIPSE and others. However, better results are obtained with the application software dedicated especially to static modeling such as PETREL, GOCAD, SKUA or RMS, as they provide geologically more correct spatial distribution of discrete parameters, e.g., facial and/or lithological variabilities, or those showing the continuous variability, e.g., petrophysical parameters, which define the quality of reservoir rock [4]. Detailed static models can be used either directly or after adjustment (usually after simplification) [20, 23].

The final stage of construction of geometric control points for static model is the implementation of model's internal architecture, e.g., its layering, in such a way that it would reflect sedimentation conditions and structural-tectonic evolution of the area. The vertical density of layering of particular rock complex is controlled by vertical variability of recorded parameters. The vertical density of layering can be matched to the vertical variability of petrophysical parameters observed in the input data derived from well logs [24].

The geometric control points of structural model provide a basis for parametric modeling. Generally, this procedure can be divided into the three main substages [24]:

- creation of well model, e.g., model of geological parameters in single cells distributed along the well trajectory,
- creation of discrete parametric model reflecting the geological, paleographical, facial or lithological conditions,
- creation of continuous parametric model reflecting the spatial distribution of parameters showing continuous spatial variability (e.g., petrophysical properties, temperature, pressure, mineralization, etc.).

The well model is constructed by so-called "upscaling" of well data [12], e.g., by application of one of many averaging methods of input data [24] in the cells distributed along the well trajectory. In a vertical plane, the number of cells in well model depends on density of layering in particular stratigraphic succession of 3D model. Datasets used in creation of the well model include continuous geophysical logs, results of laboratory measurements irregularly distributed along the well trajectory as well as discrete data: digitally coded lithology, facial variability or stratigraphy.

The discrete parametric model (e.g., lithological or facial) is usually estimated based on the lithological and facial interpretation of geophysical logs calibrated with the descriptions of cuttings and drill-cores. It may also result from integrated seismic interpretation of 3D volume and geophysical logs. In the latter case, spatial interpretation is based on selection procedures, which apply artificial neural nets. The principal lithological (facial) datasets, no matter if they contain laboratory point observations or continuous records of geophysical logs, are transformed into discrete format, in which specific lithologies, facies or stratigraphic subdivisions are digitally coded [11, 12,

25, 26]. In the case of still used modeling based on point well models, the raster (pixel-based) simulation techniques are recommended [12], which use deterministic and stochastic algorithms. The deterministic algorithm enables us to obtain only one, repeatable result of modeling for unchanged geometry of 2D/3D model. Models computed with the deterministic techniques generally show significant continuity of obtained distributions of parameters. The stochastic simulation process is controlled by variograms and statistical analyses of input datasets. Stochastic algorithms most commonly used in discrete modeling are based on iterative, sequential or direct attempts [11]. For iterative algorithms, the philosophy of modeling is the same for object models and for indicator models. The first computed model reveals entirely random distribution of lithologies (facies), and when subjected to a sequence of iterations, the modeled values better and better approximate the input boundary values (shapes and geometries of objects or calculated indicator variograms and shares of specific facies). The difference between the object and indicator modeling is that in the former method, the changes of successive iterations are applied to specific objects whereas in latter one these are applied to voxels of 3D model [11].

In discrete modeling, the most common are deterministic algorithms, e.g., nearest neighbor method and indicator kriging [27, 28], or stochastic algorithms, e.g., sequential indicator simulation or truncated Gaussian simulation. The newest simulation techniques used in parametric modeling include the algorithms which combine deterministic solutions with stochastic (commonly object) modeling and neural nets, e.g., the multipoint facies pattern algorithm.

In the case of continuous parametric models, the computation techniques are similar but the algorithms ensure continuous approximations of variability of mapped parameters. The most commonly used are deterministic algorithms representing the inverse-distance family, e.g., inverse distance, weighted average, moving weighted average or universal, simple and ordinary kriging [11, 12, 28, 29].

For both the discrete, lithological-facial models and the continuous models of reservoir parameters, the stochastic techniques are a valuable alternative for deterministic computation methods of parametric models. In both cases, the realistic results will be obtained only when a full geological information on the study area is included in the modeling, e.g., the spatial distribution of sedimentary environments, the presence of vertical and/or horizontal trends in variability of facies and reservoir parameters, the correct statistical recognition of variability of analyzed parameters, etc.

One of the recent and most popular stochastic algorithms is the sequential Gaussian simulation (SGS) [11, 27, 30] developed from the kriging. The algorithm accepts, among others, the input data, the statistical distributions of input data, the variability trends (1D, 2D, 3D) and, particularly, the variograms. During the estimation, the software randomly generates positive and negative anomalies accepting the distributions of input data. In order to understand the range of risk of this model, it is recommended to compute from several to a dozen of variants. The credible resultant model can be obtained by averaging the variants of parametric model [20].

Numerical model

The numerical model is developed from structural model supported by the results of parametric models and the archival data, e.g., the measurements ran during the drilling of deep wells and the interpretations of 2D/3D geophysics. The first step is conceptualization, usually in the form of a chart, into which we include all factors important for modeling, which would influence the water balance (including the groundwater resources) [6]. Then, using the positions of geological formations known from the stratigraphic model, we generate the 3D model of geothermal reservoir on which we superimpose the interpolation grid (depending on the used software). The grid geometry and the density of cells for which the calculations will be run influence both the accuracy (denser grid = more accurate results) and the time of computation. The latter can be quite long when a dozen of thousands of calculations cells is considered.

The next and very important step is the determination of uniqueness conditions for solutions of differential equations, e.g., the initial and boundary conditions projecting the true conditions within the modeled space. When the uniqueness conditions are established we run the modeling in order to obtain the steady-state conditions which represent the current state of geothermal system. Subsequently, we introduce to the model the wells which are involved in operation of the designed installation. Taking into account geological and hydrogeological conditions faced in Poland (e.g., considerable depths and high total dissolved solid-TDS values), there are usually production and injection wells working as geothermal doublet. The commonly used method is densification of an interpolation grid around the specific wells in order to obtain a better projection of reservoir zone [1]. Important is also the fact that locally densified grid enables us to obtain the modeling results that are better matching the observations. For instance, the finite value of hydraulic permeability of geological formations causes that a densification of grid discloses the local, abrupt pressure increase in the filter zone of production well. Proper determination and introduction of uniqueness conditions of differential equations solution into the computed model influences the results of analyses and the prognoses concerning the three principal natural processes [1]:

- accumulation (retention) of surface and groundwaters,
- migration (circulation) of water through the boundary surfaces (recharge/drainage), also within a groundwater aquifer,
- changes in quality of waters circulating within the analyzed aquatic system.

The boundary conditions (Fig. 4) represent real objects important for the functioning of an aquatic system. The most commonly used are [31]:

- first-type (Dirichlet) boundary condition constant (predefined) pressure (hydraulic head) and temperature values in a node or nodes (e.g., at the surface) of grid superimposed on a study area, H = const and t = const,
- second-type (Neuman) boundary condition constant (predefined) value of groundwater flux and density of heat flow perpendicular to the boundaries of a study area, V = const and Q = const,
- third-type (Cauchy) boundary condition determination of pressure and temperature in the vicinity of a boundary surface and determination of heat and mass transfer coefficients between this surface and the surrounding space.



Fig. 4. An example of boundary conditions superimposed on a discrete grid of a model [32].

After a correct definition of boundary conditions, the calibration of our model (if relevant comparative datasets exist) to verify its quality and to reduce possible errors is invaluable. Calibration is a comparison of natural state (e.g., prior to production) and conceptual models. The matching of models is accomplished mostly by changes of petrophysical parameters (including permeability and heat transfer coefficient) such that the natural state model only insignificantly differs from the conceptual one (e.g., from observed/measured values) [1]. The calibrated model of natural state is a starting point for generation of production model followed by numerical simulations of various production variants.

There are many reasons why the numerical models are so widely applied in reservoir engineering. Such models can be the suitable tools for construction of geological cross-sections, for imaging the distribution of temperature and pressure, for visualization of geothermal waters reservoir or directions of groundwater flows and many others. The results of numerical modeling of geothermal aquifers can be useful also for determination of particular parameters:

- groundwater production potential $[m^3/h]$,
- wastewater injection potential $[m^3/h]$,
- optimal spacing of production and injection wells [m],
- hydraulic conductivity [m/year],
- radius of hydraulic interaction [m],
- reservoir temperature [°C],
- temperature of injected water [°C],
- breakthrough time of cold-water front [years],
- pressure in production well [Pa],
- required injection pressure [Pa].

Considering a wide spectrum of practical applications, the results of numerical modeling can be used at the stage preceding the localization of geothermal heat plant, as it was in the case of the Pyrzyce installation [8] and for optimization of existing installations, as in the case of production model generated for the Mszczonów heat plant [33], which helped to estimate the possible production increase of the installation. The modeling-based optimization of installation was also carried on for the Uniejów heat plant [34] and for installations in the Podhale region [1].

Modeling the effects of surface installations

The production parameters of geothermal well estimated with the numerical modeling are then applied for determination of the data important for operation of surface installation, according to the scheme in Fig. 5. The most important reservoir parameters obtained from the production modeling of geothermal waters are:

- temperature of geothermal fluid at the production wellhead (taking into account the temperature drop of fluid flowing from filter zone through casing to wellhead),
- available flux of reservoir fluid and its phase composition,
- position of groundwater table during production (so-called dynamic water level).



Fig. 5. Modeling chart for operation of a surface geothermal installation based on the results of numerical modeling of reservoir production.

Unfortunately, the very important parameters such as chemical composition and physical properties of reservoir fluids are rather rarely determined at the wellhead. The numerical modeling usually estimates the temperature and pressure of geothermal fluid in a filter zone. Hence, these values must be recalculated to those at the wellhead because such values determine the utilization of geothermal energy. When flowing to the surface through still cooler geological formation, the geothermal fluid also cools and its pressure decreases due to flow resistance [35].

The recognition of reservoir fluid composition is crucial for proper selection of construction materials used in the geothermal installation, which will be in contact with the fluid. Usually, we design the fluid circulation system to be as short as possible, which eliminates the flow of atmospheric air into the fluid. This is very important because atmospheric oxygen causes corrosion of installation elements being in contact with geothermal fluid. Moreover, the materials used in construction of installation elements which are in contact with the fluids are non-standard and usually very expensive. The installation elements in contact with the fluids are: casings of production and injection wells, water pump impellers and pipes, geothermal water distribution pipes, fluid/cold water heat exchangers and impellers of injection pumps.

Some output parameters obtained in numerical modeling characterize the reservoir engineering problems, e.g., the breakthrough time of cold-water front because temperature at production wellhead depends on the distance between production and injection zones. Other such parameters can be interrelated and their determination during the production modeling may disclose such links. An example is the relation between the yield and the position of dynamic water level or the required injection pressure: with the increasing yield the wellhead temperature usually increases, but dynamic water level lowers in a production well, which requires the higher power and the deeper sinking of production pump assembly in the well. Moreover, the increasing yield results in the rise of required injection pressure of geothermal water left after energy conversion.

Apart from the reservoir parameters, the modeling of operation of surface geothermal installation provides also important parameters characterizing the energy distribution system and the heating installations assembled in a consumer's infrastructure (Fig. 5). The instantaneous power of heating installation required during the heating season depends on parameters characterizing the atmospheric conditions (air temperature and humidity, wind speed). Furthermore, the operation of any energy distribution system transferring energy from the source to the consumer generates costs controlled by investment expenditures (influenced mostly by pipeline length and diameter), energy loss during transfer and fluid flow resistance.

Comparison of available power of geothermal water intake versus a consumer's demand provides important information about the use of auxiliary energy sources (so-called "peakers"), which are necessary during a peak demand for power. In common practice, "peakers" must be used not only due to power deficit of geothermal installation during the peak hours but also due to low temperature of geothermal fluid, which is insufficient to meet the thermal energy demand of a consumer.

The examples of numerical modeling of surface installation operation can be found in the literature [5]. The modeling of particle separation from geothermal fluid and their settling on filter in the injection well was presented by Tomaszewska & Pająk [36] and Pająk [35].

3. SUMMARY

The dynamic modeling is currently applied even at the initial designing stage of a project, even before the key decisions are made concerning the start of new drillings for geothermal aquifer or the usage of existing wells [6]. The dynamic modeling may play a crucial role in both the selection of wells localization and the improvement of effectiveness of already operating geothermal installations. However, the investments in deep geothermics are affected by high expenditures necessary for construction of plants and auxiliary infrastructure, by geological risk related to drilling of wells (usually two wells: production and injection) and by high costs of drillings.

The proposed modeling process includes also the design of surface installation and enables us to preliminarily evaluate the economic efficiency of geothermal investment, which is the key information for potential investors. Considering the current legislation and financial support programs for investments in unconventional energy utilization, the numerical modeling may contribute to reduction of investment risk and, consequently, to reduction of very high expenditures of geothermal installations. The optimization of geothermal system, which enables us to design such parameters of installation that would ensure its long live and stable operation, is also important. Moreover, the importance of localization of geothermal heat plant cannot be neglected as this factor controls its economic effectiveness.

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