

Activity report on postprocessing and evaluation of data model in pilot area Bratislava-Hainburg

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1. Executive summary in English language

This report provides an overview of the post processing steps of the geological and numerical models in the pilot area Bratislava-Hainburg. We elaborated our models with special software systems, SKUA-GOCAD for geological modelling and FEFLOW for numerical modelling. Furthermore, we used more commonly applied software systems such as e.g. ArcGIS and MS Excel for post processing. Post processing of exported data from the models was necessary to derive secondary maps, such as resource maps, and to provide the data in the harmonized GeoPLASMA-CE standard for uploading to the GeoPLASMA-CE webportal. This mainly involved adapting and changing the file structure. Furthermore, post processing also included visualization of modelling results, which we achieved with ArcGIS.

We were able to finalize all post processing steps for both models as planned within the project runtime of GeoPLASMA-CE. The numerical model will provide initial conditions for a detailed model within the new Horizon 2020 project MUSE - Managing Urban Shallow geothermal Energy. As of now, there are no activities planned for the geological model outside of GeoPLASMA-CE.

Detailed information about all post processing steps, model uncertainties and error estimations are included in D.T3.3.1 - Activity report on 3D modelling - Part 1 and Part 2.

2. Deutsche Zusammenfassung

Gegenständlicher Bericht gibt einen Überblick über die post-processing Schritte des geologischen und numerischen Modells im Pilotgebiet Bratislava-Hainburg. Die beiden Modelle wurden mit den speziellen Softwaresystemen SKUA-GOCAD, für die geologische Modellierung, und FEFLOW für die numerische Modellierung, erarbeitet. In der post-processing Phase kamen mit ArcGIS und MS Excel zusätzliche Softwaresysteme zur Anwendung. Die aus den Modellen exportierten Daten mussten aufbereitet werden, um weitere Projektergebnisse, wie Ressourcenkarten, daraus erstellen zu können und die Daten im harmonisierten GeoPLASMA-CE Standard zur Verfügung stellen zu können. Es wurden nur Daten im GeoPLASMA-CE Webportal aufgenommen, die dem GeoPLASMA-CE Datenstandard entsprechen. Dafür war eine Reihe von Adaptierungen und Änderungen der Dateistruktur notwendig. Außerdem wurde in der post-processing Phase die Visualisierung der Modellergebnisse mit der Software ArcGIS durchgeführt.

Wir konnten alle notwendigen post-processing Schritte während der Projektlaufzeit erfolgreich abschließen. Das numerische Modell wird erste Voraussetzungen für ein detailliertes Modell im Rahmen des Horizon 2020 Projekts „MUSE - Managing Urban Shallow geothermal Energy bieten. Für das geologische Modell sind momentan keine weiteren Aktivitäten außerhalb GeoPLASMA-CEs geplant.

Detaillierte Informationen über alle post-processing Schritte, Modelunsicherheiten und Fehlerabschätzungen sind in D.T3.3.1 - Activity report on 3D modelling - Part 1 and Part 2 zu finden.

3. Zhrnutie v slovenskom jazyku

Tento článok poskytuje prehľad krokov pri následnom spracovaní geologického a numerického modelu v pilotnej oblasti Bratislava-Hainburg. Modely boli vytvorené pomocou špeciálnych softvérových systémov, konkrétne SKUA-GOCAD pre geologické modelovanie a FEFLOW pre numerické modelovanie. Pre následné spracovanie boli taktiež použité ďalšie bežné softvérové systémy, ako napr. ArcGIS alebo MS Excel. Následné spracovanie údajov exportovaných z modelov bolo nevyhnutné pre vypracovanie odvodených druhotných máp, ako sú napr. mapy zdrojov, a tiež pre sprístupnenie údajov na webovom portáli GeoPLASMA-CE vo formáte zodpovedajúcom štandardu GeoPLASMA-CE. Tento proces zahŕňal najmä úpravy a zmeny štruktúry súborov. Okrem toho sa v procese následného spracovania vizualizovali výsledky modelovania, na čo bol použitý softvér ArcGIS.

Všetky potrebné kroky následného spracovania pre oba modely sme boli schopní dokončiť načas, tak ako boli plánované v rámci projektového obdobia GeoPLASMA-CE. Numerický model poskytne iníciaľne podmienky pre podrobnejší model v rámci nového projektu Horizon 2020 MUSE - Managing Urban Shallow geothermal Energy. Pokiaľ ide o geologický model, v súčasnosti nie sú plánované žiadne ďalšie aktivity mimo GeoPLASMA-CE.

Podrobné informácie o všetkých krokoch následného spracovania, neistotách modelu a odhadoch chýb nájdete v D.T3.3.1 - Správa o činnosti pri 3D modelovaní - časť 1 a časť 2.

4. Introduction

4.1. Aim and scope of this report

This report describes post processing steps performed on the model of the pilot area Bratislava-Hainburg, which have been created within the frame of Activity A.T3.3. These reports summarize activities on post processing and evaluation of 3D model of the pilot areas. It identifies strong and problematic points of preparation of the model.

This report describes the following post processing steps:

General post processing steps

- Harmonization of attributes
- Transformation of the reference system and parameter units to GeoPLASMA-CE standards

Geological 3D modelling

- Change the model representation (e.g. 3D/2D, unit tops)
- Change data structure (e.g. grids, triangulated surface)
- Quality control, validation and error estimation
- Visualisation of modelling results and derivation of secondary maps

Numerical modelling

- Quality control, Validation and error estimation
- Changes of the file structure (e.g. ESRI database, shapefile)
- Visualisation of modelling results and derivation of secondary maps (e.g. calculation of resource maps for open loop systems)

5. General postprocessing steps

5.1. Harmonisation of attributes linked to modelling

Please list the parameters of the joint output dataset list, which refer to modelling (geological or process modelling), did you apply any joint data standards defined in GeoPLASMA-CE referring to the output parameters

We applied all joint data standards defined in GeoPLASMA-CE to the output parameters. The common reference system chosen is ETRS-UTM33N for the pilot area Bratislava-Hainburg. The harmonized standards for all output parameters can be found in the annexes of D.T2.3.1 - Set-up of harmonized data management infrastructure (for GeoPLASMA-CE).

See Table 1 for all output parameters related to modelling in the pilot area Bratislava-Hainburg. Geological modelling was used to derive the bases of geological units. The remaining four output parameters related to modelling were based on the numerical model and they are all resource parameters for open loop systems and borehole heat exchangers.

Table 1. Output parameters related to modelling in the pilot area Bratislava-Hainburg.

| Output-ID | Parameter | Relation to modelling |
|-----------|---|---|
| 1 | Base of geological unit | Derived directly from geological model |
| 2 | Bulk thermal conductivity (for depth intervals 0 - 100 and 0 - 150 m) | Calculated in ArcGIS with IEGeothermie plugin and MS Excel based on outcomes of numerical model |
| 7 | Thermal capacity at peak load | Calculated in ArcGIS and MS Excel based on outcomes of numerical model |
| 9 | Energy content (for cooling, heating and balanced use) | Calculated in ArcGIS and MS Excel based on outcomes of numerical model |
| 10 | Hydraulic productivity at peak load | Calculated in ArcGIS and MS Excel based on outcomes of numerical model |

5.2. Transformation of the reference system and parameter units to GeoPLASMA-CE standards

Please specify local coordinate systems and parameter units, which were used for modelling and needed to be transferred to joint coordinate systems or physical units;

We did not use local coordinate systems during geological and process modelling in the pilot area Bratislava-Hainburg. All input data was adapted following the GeoPLASMA-CE standards for the coordinate system and the physical units prior to modelling. This harmonization process at the beginning of modelling was necessary, since some of the input data sets referred to different coordinate systems, but the modelling software requires all input data sets to use one common coordinate system.

6. Geological modelling

6.1. Overview of applied products

Please list the software products you have used;

Table 2 lists the software products, which we applied for geological 3D modelling.

Table 2. Applied software products for geological 3D modelling.

| Version | Software | Activities related to numerical model |
|-------------|------------|--|
| 18 | SKUA-GOCAD | 3D geological modelling |
| 10.6.1.9270 | ArcGIS | Geodata preparation and georeferencing |

6.2. Changes of the model representation

Please any transformation of the geological model, which needed to be applied regarding the dimension (3D to 2D) and geological references);

No transformations were carried out regarding the 3D geological model prior to the implementation into the GeoPLASMA-CE portal. At the GeoPLASMA-CE webportal (<https://portal.geoplasma-ce.eu/>) virtual boreholes are automatically generated for location specific queries, which extract depth information for respective stratigraphic horizons from the 3D model and the webportal also links to the interactive 3D GST Web Viewer developed by GiGa (PP10), where the model can be explored in full detail.

6.3. Changes of the data structure

Please describe any changes in the data structure for later post processing, which includes transformation from surfaces to voxels or triangulated surfaces to regular grids;

The 3D model was generated using triangulated surfaces. No transformation from surfaces to voxels or grids was performed for the implementation into the GeoPLASMA-CE portal.

6.4. Quality control, validation and error estimation

Please describe all measures executed for quality control (e.g. plausibility checks), validation and error estimation;

Geostatistical methods have not been applied for quality control of the 3D Model. However, as abundance of well data in the pilot area are usually prevalent in the shallow subsurface decreasing with depth, so is the reliability of modelled horizons decreasing with depth below surface. Furthermore, geological descriptions of borehole profiles proved to be defective due to various interpreters, resulting in heterogeneous well databases. Absolute height values of well locations were often not accurate and therefore did not coincide with the surface of the digital terrain model imported into the 3D model. However, we performed quality checks of semantics,

plausibility and data consistency checks on input data sets by visualizing the spatial relationships of all available subsurface features in a 3D environment in depth domain.

6.5. Visualisation of modelling results and derivation of secondary maps

How were the models visualized, do you use data viewers for publishing the models outside the GeoPLASMA-CE portal? Which postprocessing steps have you undertaken to create secondary maps (e.g. thickness maps or structural maps); please also indicate the services on the GeoPLASMA-CE web portal linked to your 3D model

The 3D model can be explored interactively via a Web 3D Viewer, which can be accessed on the GeoPLASMA-CE portal. The Web 3D Viewer is operated by GIGA Infosystems. Thickness maps or structural maps have not been calculated based on the modelled horizons.

7. Numerical modelling

7.1. Overview of applied products

Please list the software products you have used;

Table 3 lists the software products applied for numerical modelling.

Table 3. Applied software products for numerical modelling.

| Version | Software | Activities related to numerical model |
|----------------------|--------------------------------------|--|
| 7.1.9.18108 - 64 bit | FEFLOW | Numerical modelling |
| 7.1.9.2701 - 64 bit | FEFLOW Parameter Estimation (FePEST) | Calibration of numerical model |
| 2.1 | T-PROGS | Geostatistical modelling of lithology distribution |
| 10.3.0.4284 | ArcGIS | Pre and post processing of numerical model |
| 2010 - 32 bit | MS Office (Access, Excel) | Pre and post processing of numerical model |
| 2.7.10.0 | Python | Assignment of thermal properties to model grids |

7.2. Changes of the file structure

Please describe any changes of the file structures including data formats, which needed to be applied for postprocessing steps

In the post processing phase, we calculated the above mentioned output parameters for open loop systems and borehole heat exchangers. ArcGIS and MS Excel provided useful tools for the potential calculations. Application of these software programs only required one little change of data exported from FEFLOW. The exported shapefiles do not have a coordinate system assigned and this has to be adjusted in ArcGIS. Other than that, the results from FEFLOW could be used directly in ArcGIS for further post processing steps, which are explained briefly in chapter 7.4. and in more detail in D.T2.3.4 - Evaluated guidelines on harmonized workflows and methods for urban and non-urban areas.

7.3. Quality control, validation and error estimation

Please describe all measures executed for quality control (e.g. plausibility checks), validation and error estimation;

We performed the following quality checks for the numerical model of the pilot area Bratislava-Hainburg:

1. In the early stages of numerical modelling, we calibrated the hydraulic model. FePEST automatically adapted the hydraulic conductivities of the model to reach a good fit of the measured groundwater levels and the modelled hydraulic heads. FePEST also automatically provides an error estimation for the best fit of the calibration.
2. Within the process of modelling the groundwater temperatures, we compared time series of measured groundwater temperatures at certain observation wells and simulated groundwater temperatures at the same locations. This was a plausibility check to see if the temperatures are in a reasonable range and more importantly in doing so we were able to adapt thermal properties (thermal conductivity and thermal capacity) of the model.

7.4. Visualisation of modelling results and derivation of secondary maps

Has the numerical model been visualized? Please briefly describe any statistical analyses or other mathematical operations applied to modelled data; if applicable, please explain why the modelled data could not directly be used for creating the output parameters shown on the web services;

D.T3.3.1 - Activity report on 3D modelling - Part 2 describes all results of the numerical model in detail. Results of the numerical model were visualized in ArcGIS and these maps are part of D.T3.4.2 - Thematic maps showing potentials and conflicts at the pilot areas. Technically, the potential calculations could have been performed in FEFLOW, however we decided to use a combination of MS Excel and ArcGIS to derive the maps. This workflow does not depend on the software FEFLOW, which is a very specific modelling program, instead, to reach as many potential users as possible, we decided to prepare the workflow for more commonly used software systems.

We derived the maps using the outputs from the numerical model and joined them with additional input data in ArcGIS into one table. We exported this table into a text file and calculated the potential parameters in MS Excel. Annex 15 of D.T2.3.4 - Evaluated guidelines on harmonized workflows and methods for urban and non-urban areas, describes these steps and mathematical equations in more detail. It also provides an MS Excel template for all potential calculations for open loop systems. We imported the data from the text file into this template, which calculates the output parameters automatically, and transformed the data into maps with ArcGIS.

8. Conclusions and outlook

Please refer to the following points regarding post processing:

- *General aspects: was the workflow efficient and are there any pitfalls which need to be avoided; what are the strengths and weaknesses of the applied workflow - what is missing or could not be realized (e.g. error estimation);*
- *Are there any specific aspects you would like to mention, which refer to individual output parameters (e.g. unification of legends not possible for some parameters across the different pilot areas);*
- *Are there any activities concerning postprocessing of data planned after the end of GeoPLASMA-CE (e.g. additional focus on error estimation and validation)*

The workflow for geological 3D modelling was very efficient and we could apply it without problems in the pilot area Bratislava-Hainburg. For numerical modelling, the GeoPLASMA-CE team did not elaborate a workflow. Instead, we discussed specific modelling issues of the different pilot areas in numerous meetings and telephone conferences. The team at LP-GBA appreciated this approach, because in this way we could focus on current problems and topics.

There are no additional post processing activities scheduled for the geological or the numerical model after GeoPLASMA-CE. However, there are ideas to refine the models further. As of now, however, there are no new projects in the planning stage in which these tasks are considered. We will further work with the numerical model of the pilot area Bratislava-Hainburg in the Horizon 2020 project MUSE - Managing Urban Shallow geothermal Energy. It is planned to use the existing groundwater model to serve as input for the new more detailed model.