

Memorandum use of CCC models

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Mining Development & Compliance

Management summary

Following a review of the CCC report on cavern abandonment for Zuidwending, several color-plots (cross sections) show results at the cavern wall that appear non-continuous. These have been attributed to be the result of numerical instabilities in the 2D and 3D geomechanical simulations produced by Brouard Consulting using the LOCAS software. As a result, the validity of the model outcomes may be questioned. This could cause a debate on the validity of the overall generic abandonment-strategy that Nobian has described in the recent extraction plans for Zuidwending (submitted) and Heiligerlee (final preparations before submittance). This in turn could be an obstacle in the approval process of the extraction plans.

The cavern abandonment studies for the Delfzijl fields are partially based on the LOCAS 2D and 3D simulations. These simulations form a significant part of the scientific basis that shows that the deep/tall caverns in this field can indeed be abandoned safely. The simulations were performed with in-house developed software: LOCAS, a finite element based Thermo-Hydro Mechanical (THM) model. LOCAS simulates the deformation of the cavern as well as the surrounding host rock and is coupled with a thermodynamic model for the interior of the cavern. Within the overall CCC-report the LOCAS results are primarily used to assess the pressure buildup after abandonment and to estimate the risk of hydraulic fracturing, as the LOCAS results allow for small-scale (~meter scale) elements. Subsidence prognoses are also available out of LOCAS. However, these are only used to compare with the semi-analytical approach from DEEP.KBB. Subsidence effect studies are based on the prognoses from DEEP.KBB as they result in a higher subsidence after abandonment.

The current question is whether the numerical instabilities are due to a user error from Brouard Consulting or if they are a consequence of a deeper issue in LOCAS that might force us to reconsider its utilization altogether. Based on our technical expertise, Nobian estimates that the instabilities are unlikely to significantly affect the abandonment plan, at least from a technical point of view. First, the position of the instabilities near the bottom of the cavern means that they are less likely to affect the results at the roof of the cavern, which is the key region with a higher likelihood for hydraulic fracturing. Furthermore, simulation in LOCAS of pressure buildup after abandonment and estimation of hydraulic fracturing risk were validated by the independent LaMEM model from smartTectonics. This is a different modelling method which produces similar results. These models are also part of the CCC scope and can be used as a study-specific benchmark.

Moreover, field studies will be done as an important validation step. The CCC-report recommends such additional field studies to validate the numerical results. CCC argues that numerical results need this validation step to account for any things that the models may not have captured. The CCC model results do represent the forefront of research. However, they are still the result of a simplified geology, just less simplified than all previous approaches. Therefore, validation based on field studies is still needed.

Regarding the overall correctness and reliability of LOCAS, Nobian estimates that the validation and benchmarking of the software is in line with industrial standards. Therefore, Nobian estimates that LOCAS can still be trusted, and the numerical instabilities are caused by user errors.

To conclude, as Nobian technical experts, we express the following recommendations:

- Work in close cooperation with Brouard Consulting to solve these instabilities and produce updated results that have addressed the current questions.
- Communicate our position on LOCAS so that trust is maintained and that Nobian can continue to rely on Brouard Consulting for numerical simulation work.

- On the long term Nobian should diversify our modeling capabilities. This can be done by internalizing a part of it and/or fostering collaboration with universities and knowledge centers to develop innovative software solutions.

Why might the use of LOCAS not be trusted?

Several plots suggest numerical instabilities in simulation results presented in the CCC report. In a nutshell, such instabilities are the result of a solver within the FEM-code which has produced an outcome that is mathematically valid (i.e., withing acceptable error or tolerance) but does not make too much sense in terms of the physics involved. A detailed explanation on numerical instabilities is given later in this memo. The instabilities seem only present in the 2D and 3D cavern scale simulations, run by Brouard Consulting using the LOCAS software. The observed occurrences are found in the abandonment phase of the cavern lifecycle just after the hard shut-in moment. At the start of the abandonment phase a relatively sharp increase in cavern pressure is observed (see figure 1 below for an example). The instabilities only seem present in the rock salt surrounding the bottom of the cavern. It is not known whether the instabilities are caused by a user error or by an issue within the source code of the LOCAS software.

The simulation results have been used as scientific backbone for the general abandonment strategy and are incorporated as such in extraction plans for Zuidwending and Heiligerlee. Moreover, the CCC results have been shared with the regulator as a response to their questions regarding abandonment. The situation may be that the advisors to the minister of Economic affairs (evaluating the extraction plans) will have questions on the validity of the LOCAS models. Consequently, this could be an obstacle in the approval process of the extraction plan in its current form.

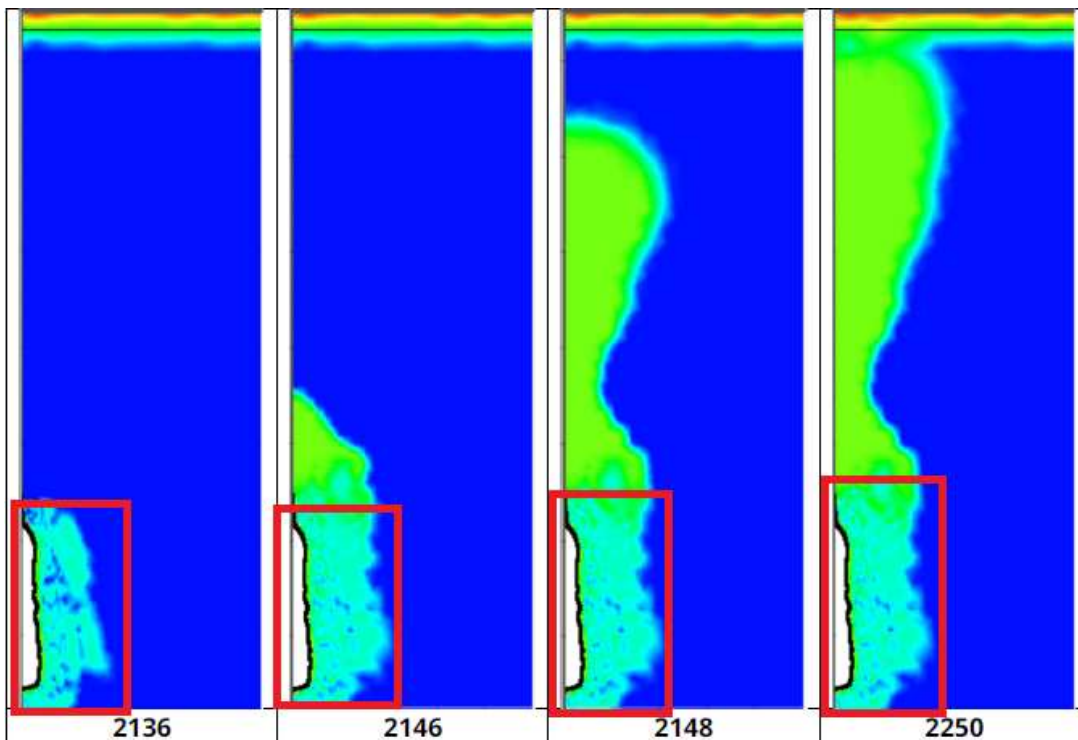


Figure 1: Example of numerical instabilities in the cavern wall in 2D axisymmetric models (CCC 2024)

What are numerical instabilities?

In FEM codes used for geomechanical analyses work as follows (in a nutshell): a displacement field is calculated based on the rheological properties of the material, and the stresses it is subjected to. This is achieved by solving a relatively large set of linear equations for each timestep. Such models use “solvers”, which are mathematical algorithms that are used to approximate solutions to complex differential equations and can also be used to solve a large matrix-inversion problem, which is at the functional core of FEM models. The solver approximates the “real result”. This is known by testing the solver with relatively simple differential equations of which analytical solutions are available. For the FEM-type matrix problem solved within the model, no analytical solution is available. The validity of the result is based on expert judgement of the user. This can be achieved by evaluation of the result through plots. The solver can produce results that are suspicious in terms of validity, if the variation in the results is too large. Moreover, in the case of finite elements, if there are large differences in the results for adjacent elements (without a direct cause), this may also point to numerical instability.

Numerical instabilities thus refer to a type of undesirable behavior that can occur during computational simulations due to various factors. These instabilities manifest as erratic or non-physical results, convergence issues (i.e., the simulation never reaches a result), or solution divergence (i.e., the solution is not reproducible by rerunning the simulation). These issues can be “local”, meaning that it only occurs in one part of the model, but not in others. This is also seen in the models Brouard has run for Nobian, where small instabilities are observed in limited areas of the simulation (Figure 1). It can also occur “global”, where the entire simulation solution is inconsistent.

What is the possible cause of numerical instabilities?

Causes of numerical instabilities can be put in two broad categories:

1. user driven instabilities
resulting from inadequate use of the simulation software for a given problem and;
2. software driven instabilities
resulting from bugs in the software or software implementations that are not robust enough to work on certain problems.

User driven numerical instabilities in finite element modeling can arise from factors such as irregular element shapes, inappropriate time step sizes, inaccurate material properties, unsuitable solver settings, and improperly defined boundary conditions. These numerical instabilities are very well understood mathematically and are extensively described in any good textbook on numerical simulation (Liu and Quek, 2013). These issues can be addressed through careful meshing of the simulated space, accurate material characterization, appropriate time step selection, adequate solver parametrization, and rigorous verification of boundary conditions. In practice, identifying these instabilities and resolving them can be a challenging task that can only be undertaken by experienced simulation engineers with a good command of the software used and a thorough understanding of the problem modeled.

Software driven numerical instabilities are usually much harder to identify. The users that encounter them rarely have knowledge of the implementation details of the software. The state-of-the-art approach to prevent such issues from arising is to have a large panel of tests and benchmarks of the software against analytical solutions or results from other trusted software packages. This approach has its limits, and to solve software driven numerical instabilities a software editor relies on users reporting issues when they encounter them. Therefore, only time and a large user base can ensure trust in a scientific modeling software package.

Perspective on numerical instabilities in LOCAS

The simulations using LOCAS in 2D and 3D (see example in figure 1) show clear signs of numerical instabilities. It is impossible to fully rule out that these instabilities influence the overall results of the simulations. Therefore, all simulations containing instabilities can be questioned in terms of validity. However, these instabilities are not considered to completely invalidate the results. Through additional work, it is possible to identify their causes, correct them and rerun the simulations so that the instabilities are gone.

Below we make suggestions of the potential sources of these instabilities and how to correct them. We must point out that these suggestions are only based on the experience of numerical modelers. Extended investigation and testing by Brouard consulting will be needed to reliably identify the sources of the instabilities and correct them. We have identified two potential sources of numerical instabilities. Both are user driven sources for numerical instabilities.

1. 2D numerical simulations use linear elements in the model. This might be the source of the instabilities due to the non-linear nature of the deformation in simulation. In general, it is not advised to use linear elements in models of these complexity as they might underestimate deformation or diffusion effects. This cannot be the cause for 3D numerical simulations as according to the CCC report (section 4.1.2) quadratic elements are used in those simulations.

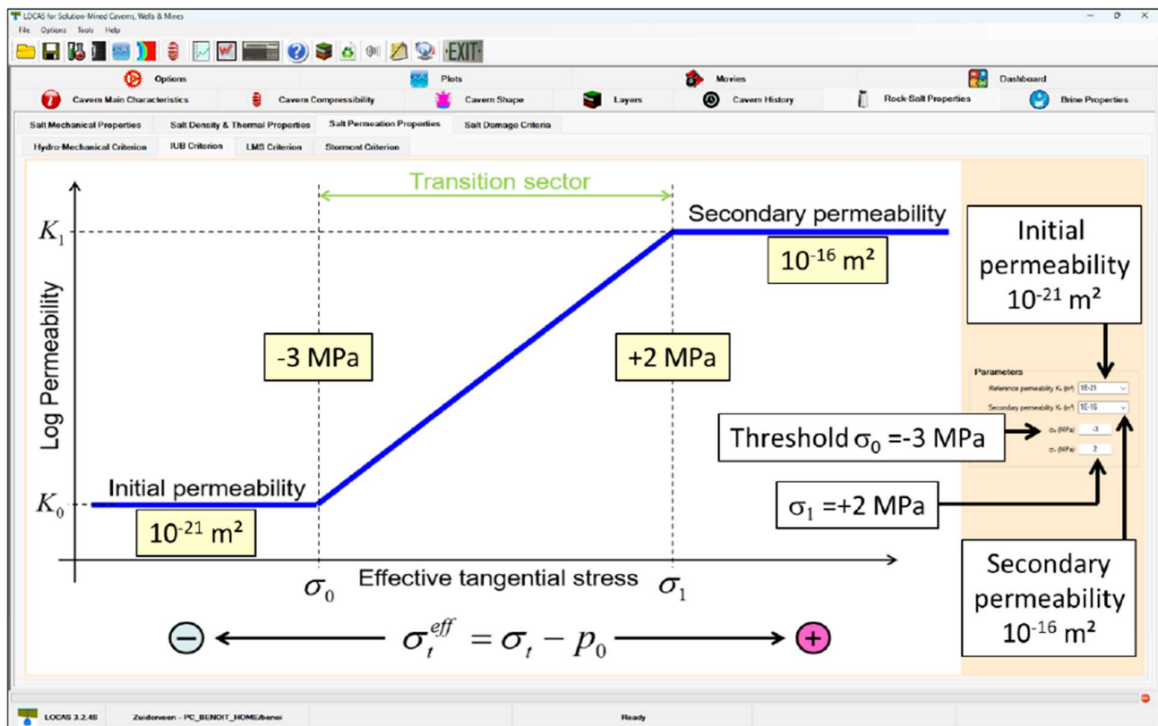


Figure 66. Coupling between permeability and effective stress: IUB criterion.

Figure 2: description of the implementation of the effect of pressure on permeability. A step function with a linear transient zone is used.

2. The source of instabilities could come from the current implementation of the non-linear effect of pressure on rock salt permeability (e.g., the permeation effect). In the LOCAS software permeation is implemented as a step function with a linear transition zone between two levels of effective stress. This causes discontinuities in derivative between the plateau (before and after the transition zone) and the transient zone in between (see Figure 2). This can be seen as an abrupt change of slope in the graph. As brine-pressure at each element is dependent on the permeability (Darcy flow) there is a coupling loop between permeability and pressure. A discontinuity in this coupling is likely to negatively affect the convergence of the software solver (Liu and Quek, 2013). Replacing this implementation with a C1 continuous function such as a logistic function - as it was done in LaMEM (CCC report section 5.4.1) - could resolve the instability problem. SmartTectonics has implemented such a curve for this very reason within the CCC work.

Perspective on the use of LOCAS software in general

It has been pointed out that LOCAS is not published in a peer-review journal. This raises the question of whether it can be considered reliable and accurate as the code has not been directly checked by a third-party nor is it open for investigation.

We argue that a software's reliability is not all given by the presence or absence of a peer-reviewed status. Commercial software developers and users have a compelling reason to protect their core intellectual properties. This goes straight against the openness needed for peer-review. This situation has been accepted in most fields of Engineering where accuracy of software simulation is critical. In fact, most reference software packages for simulations are not peer-reviewed nor open-source as can be seen in the examples below.

in Optical Engineering, there are two reference simulation software codes:

- Zemax (<https://www.ansys.com/products/optics/ansys-zemax-opticstudio>) and;
- codeV (<https://www.synopsys.com/optical-solutions/codev.html>).

Neither of these codes is peer-reviewed. They are often considered the only acceptable software for mission critical applications (Personal communication from TNO and the European Space Agency). Even more, the company that makes those software codes goes through great lengths to not communicate the internal implementations and working of their product which are considered essential IPs and trade secrets.

In computational fluid dynamics, there is one reference software code:

- Ansys Fluent (<https://www.ansys.com/products/fluids/ansys-fluent>)

This code is also not peer reviewed. They are a little open about the implementation details of their software, but the code is fully closed source.

The key factor to evaluate the accuracy and reliability of a simulation software code or package is the existence of a large set of published benchmarks and use cases applications. LOCAS has been used in a large number of peer-reviewed studies (Asgari et al., 2020; Habibi et al., 2021; Karimi-Jafari, 2007; Serbin et al., 2015) and three benchmarks against other existing software are published (Djizanne et al., 2022). It should be noted that references to SMRI conference papers are to a lower level of academic scrutiny compared to the peer review process of internationally well-ranked scientific journals. However, these papers are reviewed by editors from the scientific committee of the SMRI.

Therefore, given the maturity of LOCAS (> 20 yrs of usage, see for example Brouard et al., 2006, 2018) and the number of benchmarks it is in good faith that Nobian can assume that results provided by it can be trusted. Moreover, the use of the coupled model (cavern internal and external) is one of the key recommendations that came out of the KEM-17 report (Brouard et al., 2019). It is important to point out that

this does not warrant Nobian against erroneous results produced by user errors or usage outside of the advised applications of the software.

How did Nobian use the models in the extraction plan?

The main use of the cavern-scale models (based on LOCAS results) is projections of the stress state after abandonment, particularly focusing on the cavern roof. These models are able to calculate on a relatively fine mesh (compared to dome scale models of smartTectonics within the CCC scope), meaning detailed estimates are available that capture the cavern shape as projected from leaching models and sonar measurements. Particularly the development of large shear stresses compared to the mean stress is of importance. A situation with low mean stress and high shear stress could imply the dilatation threshold is crossed and a fracture could initiate. The ratio between shear and normal stress can be compared to the threshold value (known from lab tests / literature) and calculated for each point within the model. It is presented as a factor, with a value of zero meaning a stress state that is equal to the dilatation threshold. Higher values imply the stress state is further away from the threshold.

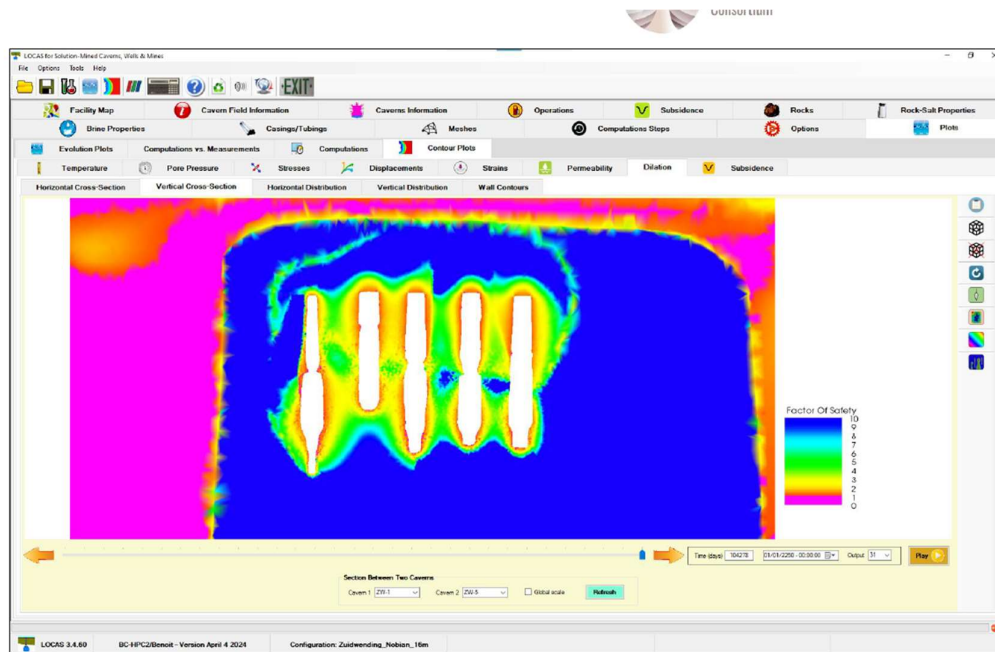


Figure 127. LOCAS 3D Model - Nobian caverns - Vertical section, in a plane passing through the axes of the ZW-1 and ZW-5 caverns, of dilation FOS contours in year 2250. The effective stress tensor is considered to evaluate the possible onset of dilation and a Biot coefficient of 1 is taken into account.

Figure 3, example of the FOS (factor of safety) plots assuming a worst-case pore pressure coupling (in this case simple effective stress law or a Biot-coefficient of 1 which is unlikely for rock salt). Values for outside of the salt dome are calculated and plotted, but should be omitted from the plot, as the dilatation threshold for rock salt does not apply to the side- and overburden rocks, being different rock types.

In figure 3 an assumption is made on how the pore pressure (brine infiltrating between individual crystals that make up the host rock salt) affects the stress tensor. Here the assumption of a Biot-coefficient of 1 is made, implying a simple effective stress law can be applied. In simplified terms, this assumption means that the mean stress is reduced by the value of the pore pressure, but the shear stress is not affected (pore pressure only affects principal components). This is a conservative approach, Biot-coefficients for rock salt are typically

assumed to be 0 (no effect of pore pressure at all), or in some cases 0.3 (see the CCC report for more details).

Even with the conservative approach, the LOCAS results show a relatively large zone in the cavern roof where the FOS value remains high. In other words, in this zone high shear stresses (compared to the mean stress and dilation threshold) do not appear to occur. Since the inferred numerical instabilities do not occur in this zone, the results seem plausible. It should be noted that numerical instabilities observed at the cavern sump-level could affect overall cavern pressure and thus still indirectly influence the results at the cavern roof. However, the results are qualitatively backed up by the results of the (coarser) dome scale model.

The general trend from both models for the cavern roofs is as follows. As the pressure in the cavern increases so does the stress state in the cavern roof. Thus, the mean stress is higher as well and the dilatation threshold is higher. Because the pressure increase is occurring gradually (order of magnitude of some bars per year), this does not produce high shear stresses. This could be the result of considering pressure solution creep in the numerical models. The rock salt at the cavern roof appears viscous enough to dissipate high differential stresses.

The second main use of the models is to assess the pressure buildup curves, both in terms of pressurization rate and maximum pressure level. This is also a result of the dome-scale model. Also, regarding this topic the results are comparable between LOCAS and LaMeM.

For subsidence prognosis (and potential subsequent effects at the surface) the results of the semi-analytical model of DEEP.KBB has been used, instead of the results out of the deterministic models from CCC. Note that these deterministic models show a surface rebound phase after abandonment which can be thought of in a simplified manner as a buoyant cavern-shaped brine bubble that rises in the high-viscous rock salt. These results may cause a topic of debate, as for example Hunfeld et al. (2022) show that such a rebound phase may be the result of a too-large volume of rock salt which is mobilized at low differential stresses. In that work they use this as an argument that a low-stress threshold for pressure solution creep must exist. A theoretical basis for such a threshold does exist (e.g., van Oosterhout et al, 2022), but so far, no experimental results have been able to prove its existence (note the philosophical consideration of proving something doesn't exist is impossible, but in this case the threshold may be shown by narrowing down the range through a set of well-defined and constant experimental conditions). The models from smartTectonics (dome-scale models in the CCC report) have also shown that a rebound phase is likely to happen, whether a threshold is implemented or not.

The DEEP.KBB model shows continuous subsidence at a reduced rate after cavern abandonment (hard shut-in), and therefore can be thought of as a conservative approach to study the post-mining effects. While rebound may reduce the maximum subsidence, it could lead to more varying deflection of the surface compared to the regular bowl-like shape that is assumed in the DEEP.KBB model. However, the gradients (and curvature) at surface in the CCC-model for subsidence (i.e., the rebound scenario) fall below the levels observed in the DEEP.KBB models.

Verification from the field

Nobian's position in the extraction plans is that both models need verification from the field. This is also recommended by the CCC team themselves. They argue that any model will need validation from the field. All models thus far are simplifications, which are needed to approach the bulk behavior result of complex micro-scale to dome-scale processes. Small scale details which could affect the model results may not be captured by the model approach. In other words: the only way to know for sure if the models can be relied upon is to try it in the field and measure. Monitoring of cavern pressure and outflow behavior at different pressures is the plan for each cavern that is no longer actively leached (e.g., max minable volume is reached). In this post-

leaching phase, cavern pressure is allowed to build up naturally to a maximum of 0.18 bar/m at the last cemented casing shoe depth.

Such a test does not give direct information on what occurs at higher cavern pressures, which are likely to occur after abandonment, when pressure measurement is no longer an option. Nobian has been granted funds from the Solution Mining Research Institute (SMRI) to perform field tests which will address this. With sufficient safeguards in place, and permission from authorities granted, field tests will be done where the 0.18 bar/m threshold is exceeded. Within the scope of this research project, Brouard Consulting is also involved in providing a numerical twin of the target cavern using 3D LOCAS software. This approach allows for finetuning of parameters to best explain the pressure build up curve. This also enables further calibration of LOCAS and LaMeM based on field results.

Conclusions

Regarding the numerical instabilities, our assessment is that they are likely to have limited effect on the simulations. They are mostly centered around the lower segment of the cavern wall (sump level). Therefore, the results for the cavern roof area are likely unaffected by instabilities and seem reliable. Indirectly there may be a slight effect in overall cavern pressure. However, both for cavern pressure and stress state in the cavern roof area the LOCAS model results are qualitatively backed up by the results out of the dome-scale model (LaMeM / smartTectonics). Finally, the subsidence prognosis listed in the extraction plans are based on the DEEP.KBB model, which is more conservative than the CCC subsidence prognosis.

Field tests will be done to validate and further improve the reliability of the forecasting ability of LOCAS, LaMeM and the overall CCC results. This forms the basis of a continuous improvement loop. Such a loop is already applied to subsidence prognoses, where the input (from leveling campaigns) is used to track and improve the quality of the prognoses.

Nonetheless, Nobian has asked Brouard Consulting to further investigate the numerical instability issue in LOCAS, such that the results are on a level that future simulations are judged as plausible scenarios.

What are the possible steps forward?

Nobian continues to work with Brouard Consulting within the CCC team. This team currently provides us with a high-quality software solution specifically designed for cavern-field analysis. Brouard is open to improvement of the code. He is working within an EU co-funded project (HYPSTER) in which a benchmark study is done. We note that the capabilities of LOCAS, as well as the multiple years of expertise that Brouard Consulting provides, is difficult to replace within the relatively small community of salt solution mining. It is necessary to argue that publishing the code of LOCAS is an unreasonable request as it will negatively impact the key intellectual property of Brouard Consulting. However, we need to share and disseminate use cases and benchmarks studies of LOCAS to prove the software's reliability and correctness (e.g., from project HYPSTER but also possible other studies).

Nobian needs to collaborate closely with Brouard Consulting to identify the sources of instabilities, correct them and rerun the simulation to prove that instabilities had a limited effects on the numerical simulation results.

Finally, in the medium to long term Nobian needs to invest in further diversifying our numerical modeling capacities. This can be done by internalizing some of the activity and/or developing new software solutions in collaboration with public research institutes.

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