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## **Is the hypothesis of a uniform thermodynamic state still valid in hydrogen underground caverns during fast cycling?**

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### **Abstract**

The rate of injected or withdrawn mass to/from caverns controls the spatial heterogeneities of the temperature and pressure fields. It also controls the magnitude of gas velocity which represents the driving force for the convective heat transfer with the surrounding rock domain. In order to consider as many industrial concerns during cycling as possible (for instance rock creep and gas migration), researchers tend to simplify the cavern thermodynamic problem by neglecting the spatial variations of pressure and temperature which leads to a cavern uniform thermodynamic state. This reduces tremendously the simulation cost, yet it raises up a question about the validity of such assumption during fast cycling. We will be addressing this concern by performing simplified (uniform thermodynamic state) and complete simulations that take into account all the complexities of this computational fluid dynamics problem. A discussion section at the end of this abstract will provide us with a margin of trust with regard to the simplified approaches for seasonal and daily cycling in underground caverns.

### **1. Introduction**

The slow/seasonal cycling in underground caverns stems from the population's seasonal need of energy, where gas is stored in summer and extracted in winter. However, the increase of human energy demands, as well the environmental concerns associated, necessitate the use of viable and clean energy. Hydrogen storage in salt caverns represents a future fuel source. Nevertheless, the use of hydrogen as fuel requires fast utilization of the storage systems to respond to the daily demands of fuel required by the population [1]. Therefore, and due to the considerable simplifications usually adopted in the uniform thermodynamic state modeling, a question always arises about the validity of such simplifications, especially during fast cycling of caverns when spatial variations of temperature and pressure are significant. The miscalculation of these variations leads to a miscalculation of the gas density field in the cavern, and consequently, for a given cavern volume, a misestimation of the stored gas mass.

To address this concern, we made use of an in-house simplifying code (DEMETHER [2]) and a CFD COMSOL license. The goal was to compare the simplified simulation results of DEMETHER, to the complex simulation results of COMSOL, where all complexities of the problem were considered, i.e. full mesh refinement, velocity field, convective heat transfer, and the turbulent flow modeling. The simulation results were correlated for both slow (seasonal) and fast (daily) cycling where one expects better match with regard to the slow cycling and more deviation in the case of fast treatment. In both simulations the cavern was assumed full of hydrogen with no brine or insoluble material, and only thermal conduction with the surrounding rock domain was considered. The abstract ends with a discussion section on the validity of this simplified approach. For a typical spherical cavern of volume 300,000 m<sup>3</sup> created at 910 m depth, severe cycling schemes that led to a mass change in the range of [69% to 29%] of the initial mass, demonstrated almost similar results for slow/seasonal cycling between the simplified and the complete simulations. However, a difference margin of 7% was observed in the compared results during fast/daily treatment.

## 2. General thermodynamics of the cavern

We will start by assuming an underground cavern filled with a mono-component single-phase hydrogen (Fig. 1). The underground storage system can be divided into three domains: (1) the well which extends from the ground surface to the cavern; (2) the cavern itself; and (3) the rock mass that surrounds the cavern and the well.

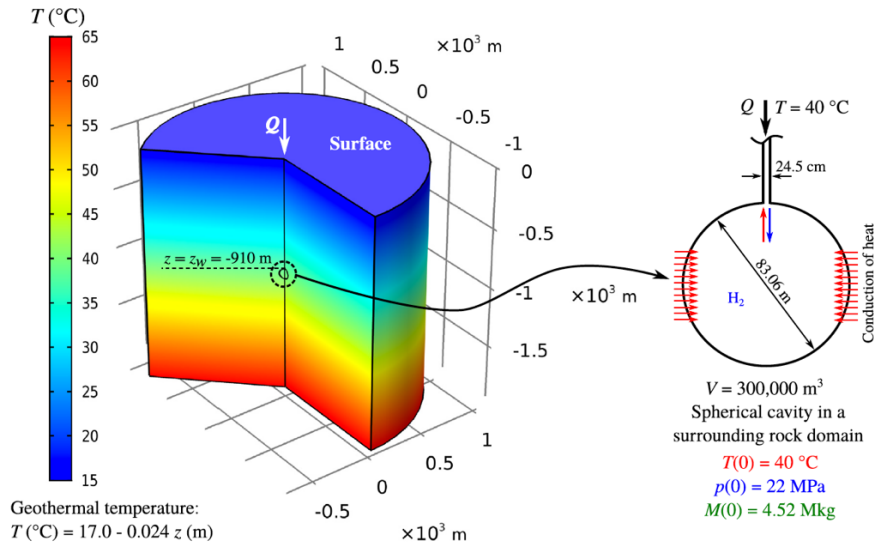


Figure 1: Schematic diagram of the boundary value problem: it represents a spherical cavern created at depth 910 m in a surrounding rock domain. The geothermal gradient gives a cavern volume averaged temperature of 40 °C. The cavern is assumed initially full of ideal hydrogen.

In the complete solution of the cavern thermodynamics, the entire domain of Fig. 1 is simulated using COMSOL. This necessitates the introduction of the mass balance equation, the momentum balance equation, and the energy equation in the cavern and the well domains. Besides, the energy equation needs to be considered in the infinite rock domain to account for power exchange between the rock and the cavern hydrogen.

In the simplified approach, the average value of the velocity field within the cavern volume is assumed negligible. Therefore, the cavern spatial variations of pressure and temperature are neglected in the cavern volume [3]. This allows us to discard the CFD simulations within the cavern volume. The cavern becomes a single point. The well is simulated as a pipe, and the rock domain is discretized in a one-dimensional FEM problem to account for heat transfer.

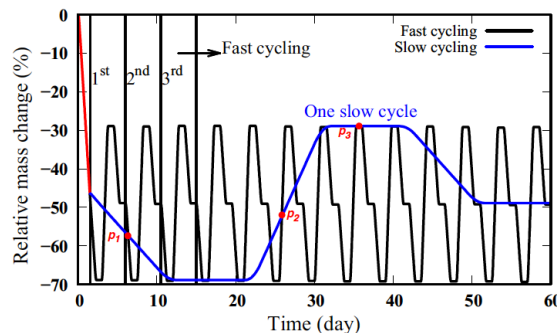


Figure 2: Two cycling schemes to run our cavern: fast/daily cycling that leads to a relative mass change of [69% to 29%] in 4.5 days; and slow/seasonal cycling where cavern experiences the same mass changes yet over a period of 58.5 days.

### 3. Results of the simulations

Figure 3. shows the development of the complete simulations volume averaged and the simplified approach temperature and pressure histories in the cavern during the slow and fast cycling schemes. Since pressure histories are mainly affected by mass changes, simplified and complete pressure histories are too much comparable (Fig. 3(a, c)). However, and with regard to temperature histories, temperature histories show very slight differences in the case of slow cycling (Fig. 3(b)), yet differences are noticeable in the case of fast cycling and they increase with time to stabilize eventually (Fig. 3(d)).

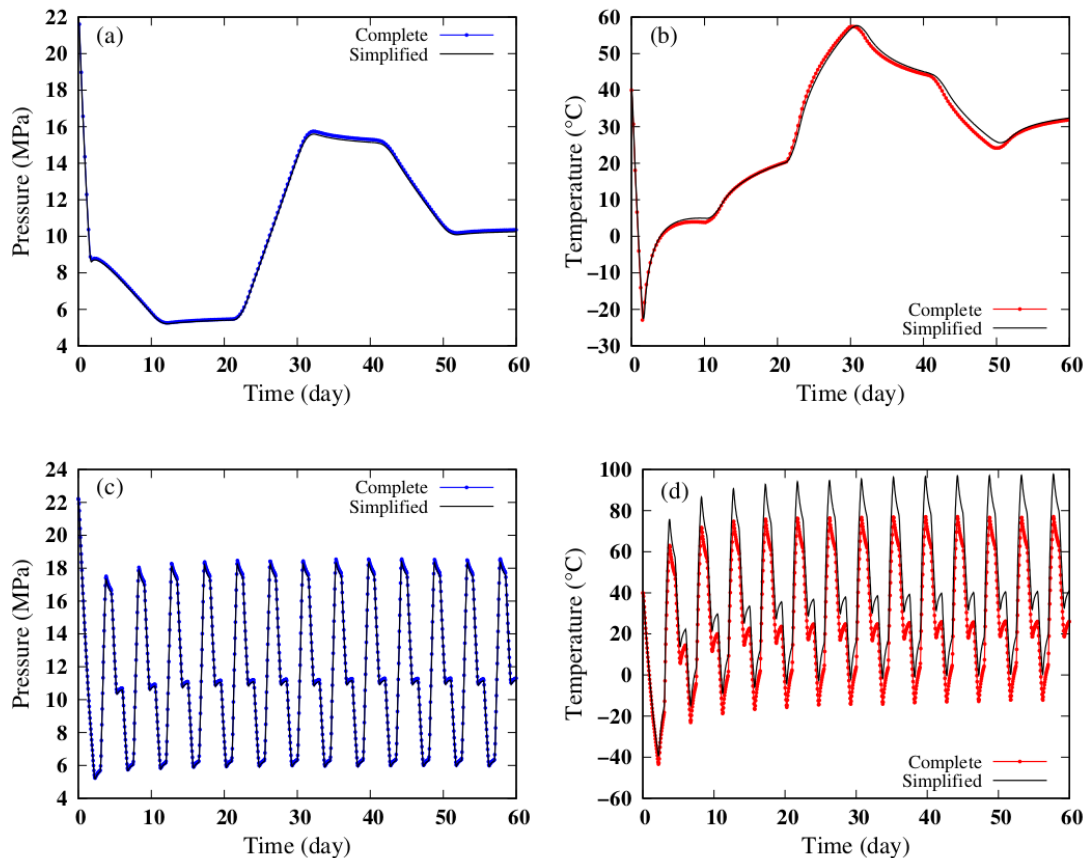


Figure 3: Development of cavern pressure and volume averaged temperature: comparison between slow/seasonal (a, b) and fast/daily (c, d) cycling of the simplified and the complete approaches.

### 4. Discussion and conclusion

The objective of this research was to know to which level the simplified uniform thermodynamic state simulations of gas storage in underground caverns (used generally) could be valid, by comparing it to complete simulations that would address all the complexities of the problem, i.e. mesh refinement, gas velocity field, turbulent flow model, and convective heat transfer. Figure 4 shows the absolute value of the relative Kelvin temperature difference between complete and simplified simulations of Fig. 3(b, d). In the case of slow cycling, relative differences are quite small and do not exceed 1%. However, these differences increase over time in the case of fast cycling, yet they tend to reach a maximum plateau of 7%. The increase over time is related to temperature exchange with the rock mass, where the gas velocity by the cavern wall drives the convective heat transfer.

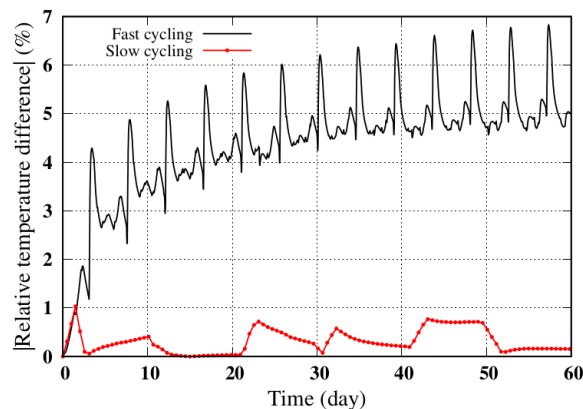


Figure 4: Relative Kelvin temperature difference: comparison between complete and simplified simulations for fast and slow cycling of Fig. 3(b, d).

It is understood that a trade-off between accuracy and the calculation time is to be made. It is, until this time, still unfeasible to run complex complete simulations over the entire cavern lifetime, i.e. 30 years and maybe more. Yet, the simplified approaches can give out results in a few days. In the case of seasonal utilization of underground caverns, the simplified simulations are quite efficient in terms of results and the calculation cost. In addition to that, such simplified approaches allow researchers to concentrate on/address other problems that are of significant importance to the industry, of which we might cite the thermo-hydro-mechanical behavior of the rock mass during cycling, real gas behavior, interactions between the cavity species (gas, brine, and insoluble material), multi-phase simulations, and gas diffusion/loss into the rock mass. Still, while modern humanity demands on energy increase, the simplified approaches, to a certain level, will impose a definite level of inaccuracy that might be unacceptable. The miscalculation of the cavern thermodynamic variables development will lead to misestimation of the stored gas mass, as an example.

### References

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