Principal Component Analysis for the Opening of Underground Caves in Saline Rocks under Different Temperatures

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Abstract. This study aims to analyze numerical data obtained during the process of opening of caves in saline rocks considering the temperature variations. Over the years, saline caves have been widely used for the safe storage of supercritical CO2, petroleum products and used as final destination of toxic waste such as radioactive waste. The main motivation lies in the possibility of determining the variables from a statistical point of view that most influence the opening process of these cavities. In fact, throughout the development of a cave, the variables involved play a significant role in the success of the operation and also in determining its final behavior, it is important to understand the way that they interact with each other and also with the fluids inside. In this work, numerical simulations of the solution mining process for opening the cave under typical conditions of water injection in a sodium chloride rock (using a finite difference code) are described and performed, after that, the interpretation of the data obtained with the simulations is also done through a multivariate statistical tool (PCA). The simulations show that the temperature and the flow directly influence the cave opening rate, in turn, the statistical analysis of the data shows that the output variables have an almost similar contribution to the opening of this cavern, moreover, it is possible to interpret the total variation of the data using only one component (PC1).

Keywords: Opening of Saline Caves, Process Variables, Data Analysis.

1 Introduction

The dynamics of the oil industry requires the development of concrete and innovative solutions in a timely manner. In order to facilitate the storage of petroleum products and discards in general and even shorten the distance between production - storage, underground caves in saline rocks have been widely used. According to Mirzabozorg et al. [1], rock salt is considered the ideal material for underground storage due to its low permeability, healing capacity and availability. Wang et al. [2] also cite the low cost involved in the process of leaching caves by dissolution using salt rock when compared to other rocks such as granite, mud and basalt. Noorzad et al. [3] highlight the dissolution mining technique as cheaper and more effective for opening underground salt caverns than other conventional excavation techniques. The process of opening and subsequent development of these cavities has different variables, experimental studies were carried out in order to analyze these components, one of the first being that of Durie and Jessen [4] who performed a series of laboratory tests in order to assess the influence from the water injection rate (fresh and salt) to the cave formation rate and the salt removal rate.

In addition to experimental studies, mathematical models were also developed. Still at work by Durie and Jessen [4], a mathematical model was presented that describes the dissolution process as a function of the salinity of the water at any point on the vertical surface of the salt, it was found that under low injection rates, the induced flow does not contribute significantly in the rate of salt removal, more recently there has been an increase in the number of publications on cave construction mainly in the Jintan region of China. Yang et al. [5] presented a mathematical model based on the principle of pressure equilibrium to predict desalination parameters for a salt cave used for CAES (Compressed Air Energy Storage), and also Yang et al. [6] developed a mathematical model to predict cave behavior during leaching into insoluble salt formations. To understand mainly the process of dissolution of the rock, various numerical models were also presented. Saberian [7] developed a 5" tall cylindrical model to study the flow and expansion mechanisms of saline cavities during dissolution, the results combined into a generalized numerical model, where the prediction of cavity dissolution as a function of the time as well as other physical parameters such as speed, radius and dissolution rate. In the last years, Wang et al. [2] presented a proposal for an analytical solution of a differential equation to calculate the dissolution rate of saline rocks subjected to an instantaneous diffusion process, the results showed a fit between the numerical model and the experiment of the salt concentration with respect to time.

This article aims to provide a principal component analysis of numerical data to determine the variables that directly influence the process of opening an underground cave in saline rock by dissolution. For numerical part a finite difference code is used, SALGAS, developed by the Solution Mining Research Institute (SMRI), this software considers only the vertical brine stratification, a finite difference method solves differential equations based on the approximation of derivatives by finite differences. According to Li et al. [8] a finite difference model can provide basic parameters for the construction of rock salt cavities. The results obtained with the simulations are also interpreted from a statistical point of view using a Principal Component Analysis (PCA) in a program named PAST (PAleontological STatistics).

Ferreira [9] highlights in your study multivariate data analysis can reduce data or perform a structural simplification as well as investigate the dependency relationship between variables. Widely used in various fields of science, it encompasses different techniques, the most used being cluster analysis, factor analysis, principal component analysis, multiple regression and logistic regression, each with its own characteristics. In the present study, the variables are studied using Principal Component Analysis (PCA). According Alonso-Gutierrez et al. [10], the PCA technique uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components (PC) that reveal the internal structure of the data in a way that best explains its variance.

2 Numerical Model

The representation of a possible scenario of saline rock dissolution for the formation of an underground cave was possible through the SALGAS software, already mentioned in the previous topic. This finite difference code simulates the dissolution of sodium chloride by water, optionally simulates the hydraulic properties and energy requirements of the mining system. Furthermore, it is also possible to simulate the properties of the fluid bed used to protect the top of the cavern from possible upward dissolution (blanket). This software has been validated through laboratory experiments and from data from caves in saline domes on the US Gulf Coast, developed by Eyerman et al. [11].

For conciseness, the structure of the input data with each of the lines of code will not be shown in this article, this information is all contained in the SalGas' Manual [11]. Aware that SalGas is a software developed for the mining industry for onshore scenarios, the authors developed a hypothetical scenario to simulate the dissolution of saline rock.

2.1 Hypothetical Scenario

In the proposed scenario, water is injected at the bottom of the cave and the brine is extracted from the top of the cave, it is called the direct circulation method, as an input option it can be chosen between two forms of dissolution, direct and reverse, it was chosen in this work by direct mining. The mining module was used together with hydraulic module to simulate the dissolution of the rock by a fluid saturated in 4% NaCl, considering a cave of approximately 300 m, injection temperatures of 40, 60 and 80 °C and injection flows of 120, 360 and 500 m^3/h, over 120 days.

This scenario was based in the example number 1 of SalGas' Manual [11]. From a working flow of 170.34 m^3/h and approximate temperature of 23.9 °C was possible to trace new flow rates by varying the temperature, it was also possible to calculate the pump power and accumulated energy. The diameters of the external and internal piping were respectively 10¾" and 7". The representative design of the proposed scenario with the respective injection and production depths as well as the dimensions of this cavern are illustrated in Fig. 1.

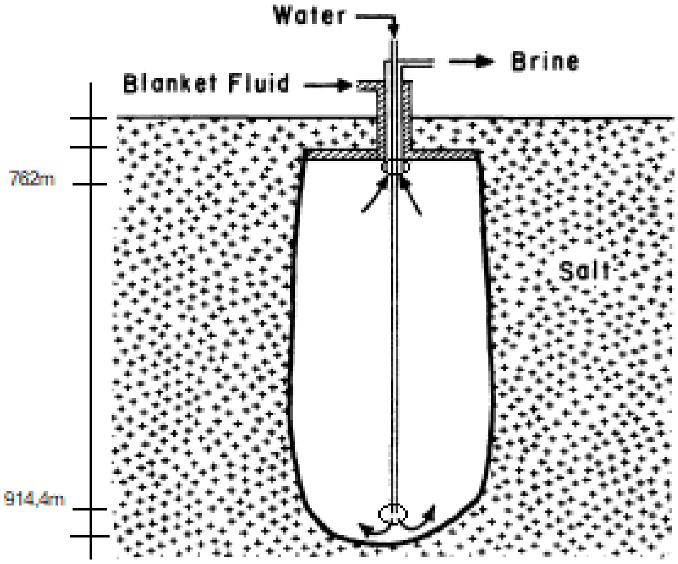

Figure 1. Representation of the direct mining scenario

The initial brine specific gravity and the injection fluid specific gravity are input parameters for SalGas obtained from the Toolbox provided by SMRI. The brine pressure and temperature values are entered and the Toolbox automatically provides the parameters, to determine the brine produced, it is also necessary to inform the fluid saturation which is 4% in NaCl as mentioned before.

According to Saberian [12], it is possible to obtain the dissolution rate of a brine, m_T (cc/cm²/min x 10³), for various temperatures and salinities, as a function of the specific density of the brine, ρ, of the reference temperature, T_0 (° F), and the initial production temperature, T (°F), according to eq. (1):

$$m_T = \ 0.22(1.2019-\rho)^{1.42}\exp\left[0.0119\left(\frac{\rho-1}{1.2019-\rho}\right)^{0.2}\Delta T\right]. \tag{1}$$

SalGas is a software that works with a reference temperature of 23.9 °C and all simulations performed are isotherms fixed for this temperature, for this reason, the input variable is not the dissolution rate but the dissolution factor (DF), which corrects the dissolution rate by compensating between a 23.9 °C isothermal simulation of an "ideal salt", which would generate a brine with the maximum specific density accepted by the software equal to 1.2, and the simulation that actually needs to be done, with temperature and specific densities different from the ideal. Below is the equation 2, where T (°F) is the initial production temperature, T_0 (° F) is the reference temperature and ρ the injection fluid specific gravity :

$$DF = \exp\left[0.0119\left(\frac{\rho-1}{1.2019-\rho}\right)^{0.2}\Delta T\right]. \tag{2}$$

In the simulations performed, the brine production pressure equal to 8.97 MPa (depth of the production point) was considered. The parameters used in these analyzes are presented in Tab. 1. It is noteworthy that the value of the correction factor of the dissolution rate for the temperature of 80°C was obtained by direct extrapolation of the temperature of 60°C for each corresponding flow.

This extrapolation is necessary because the temperature of 80°C proposed in the hypothetical scenario is outside the range for which the SalGas correction factors were implemented, for this reason it is in the red color in the Tab 1.

Table 1. Simulation input parameters

Injection temperature (°C)	**Injection flow (m³/h)**	**Injection pressure (MPa)**	**Initial brine density**	**Injected fluid density**	**dissolution rate correction factor**
40	120	9,05	1,196300	1,023830	1,259618
40	360	9,67	1,196500	1,024130	1,260445
40	500	10,32	1,196800	1,024530	1,261538
60	120	9,05	1,187400	1,014130	1,585764
60	360	9,67	1,187600	1,014530	1,590177
60	500	10,32	1,187900	1,014930	1,594517
80	120	9,05	1,179100	1,002630	1,658297
80	360	9,67	1,179300	1,003030	1,682914
80	500	10,32	1,179600	1,003430	1,705421

2.2 The Multivariate Analyze

The data obtained from the simulations in the SalGas software could also be analyzed using the PAST software, this program performs data analysis using different multivariate tools, for our purpose was used the principal component analysis (PCA). As an initial command, the user pastes the data coming from Excel so that they are arranged in columns and rows forming a table. For brevity, the mathematical equations that govern the PCA technique will not be shown in this paper.

The volume and radius of the cavern in the proposed final time (120 days), the injection temperature, the production flow, the pump power and accumulated energy were considered as input data, in Tab. 2 below their respective values are presented, other variables were not selected, in a new search more variables could be included to obtain greater analysis and results.

Table 2. Simulation output parameters

Injection temperature (°C)	**Production flow (m³/h)**	**Radius (m)**	**Volume (m³)**	**Pump Power (KW)**	**Accumulated Energy (KW-HR)**
40	116.00	7.95	37421.70	660.69	185634
40	348.00	12.04	91937.84	4667.34	1321614
40	483.33	13.60	118039.83	10245.17	2904838
60	116.00	8.47	41966.49	711.40	200589
60	348.00	12.98	106643.62	4822.44	1368760
60	483.33	14.75	138756.56	10412.95	2957507
80	116.00	8.79	45124.26	751.67	212128
80	348.00	13.54	116169.85	4955.18	1407836
80	483.33	15.46	152413.45	10609.82	3014795

In the next topic the main results obtained with both the numerical tool and the statistical analysis are presented. The statistical analysis is still under study and only a small part of its analyzes were considered and addressed in this study.

3 Results

To ensure the quality of the figures, it was decided in this work to reduce the amount of output graphics. In fig. 2 below, it was possible to obtain the final contours of the cave for a period of 120 days considering all injection temperatures and flow rates. For the same temperature, the greater the flow, the greater the radius of the cavern. The maximum value reached for the time of 120 days was approximately 16m radius for a temperature of 80°C and an injection flow rate of 500 m^3/h. Analyzing the same flow value, the radius of the cave increases with increasing temperature, but this seems to have less influence on the final diameter obtained than the flow.

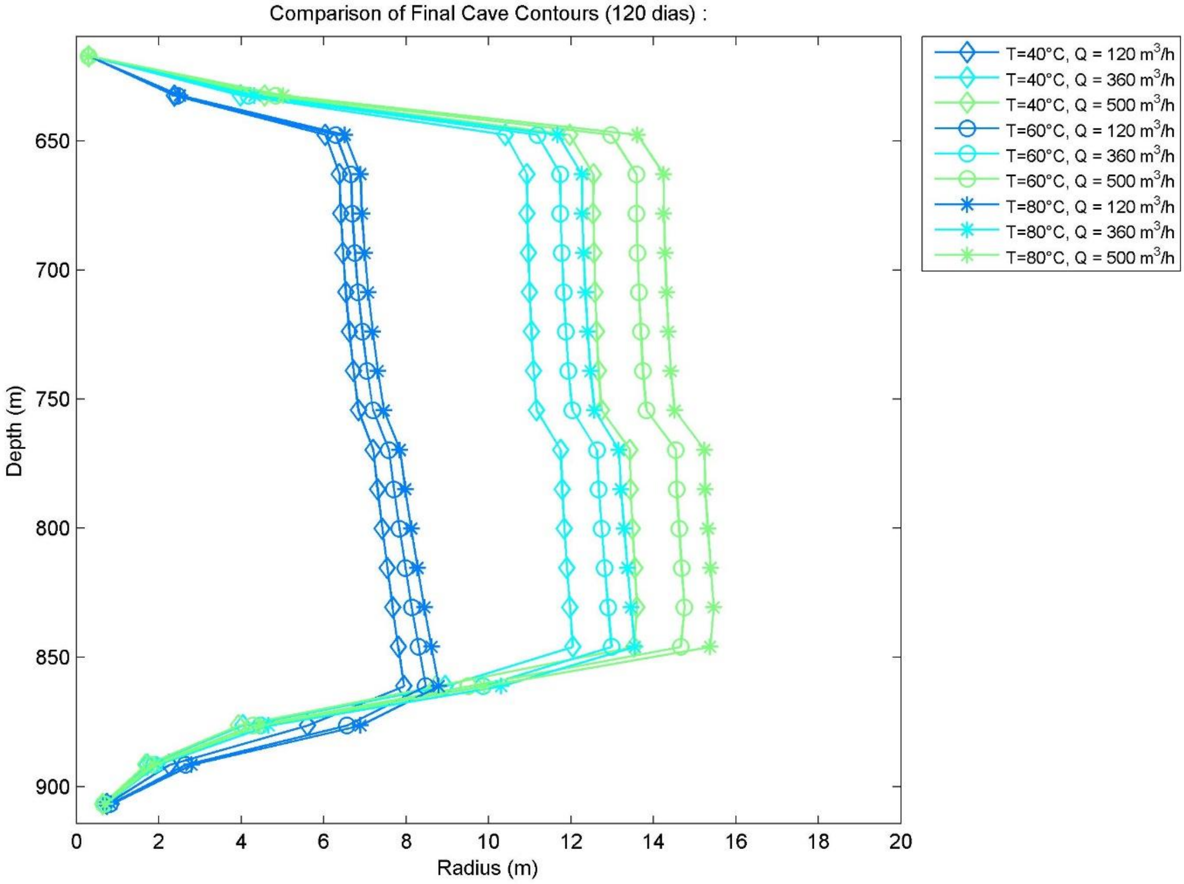

Figure 2. Final contour of the cave considering all flow rates and temperatures

In addition to the final geometry, the authors also considered it important to evaluate the final volume of the cave for a period of 120 days.

In Fig. 3, the final contours of the cavern were obtained considering all injection temperatures and flow rates. Analyzing the influence of temperature, it is observed that for the same temperature, the higher the flow, the greater the volume of the cavern. The maximum value reached for the time of 120 days was approximately 1.5 x 10^5 m^3 of volume for a temperature of 80°C and an injection flow rate of 500 m^3/h.

The Tab. 3 shows that, in terms of variance, the first component comprises approximately 97% of the data, the second component represents an infinitesimal portion of the data, whereas the third, fourth and fifth are practically insignificant for the analysis of the total variation of the data.

Finally, in Fig. 4 an analysis of the output variables from the perspective of multivariate analysis. In terms of first component (PC1), all variables contribute almost in a similar way to the opening process of this cave, being radius with volume and pump power with accumulated energy strictly related, on the other hand, radius and volume are opposite parameters to pump power and accumulated energy.

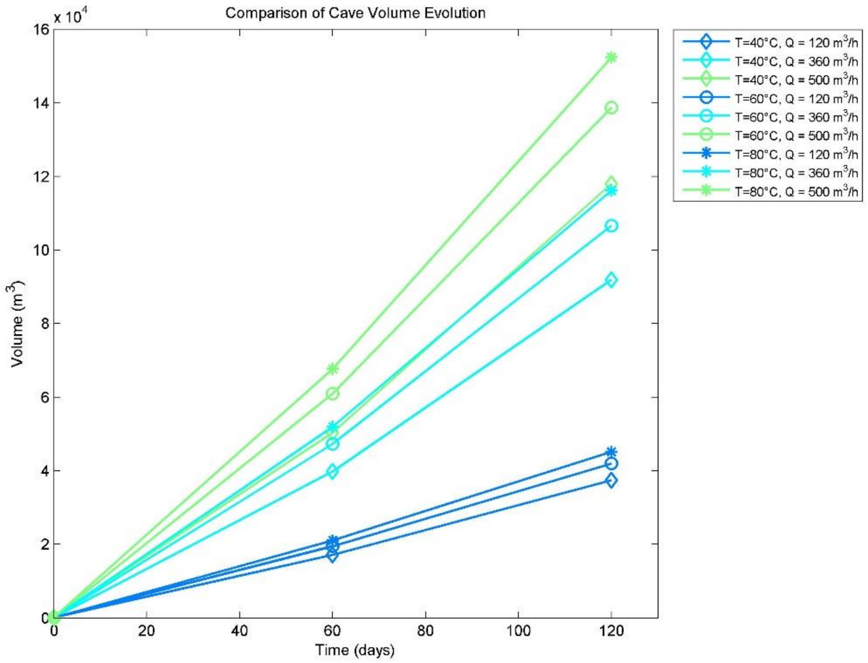

Figure 3. Final volume of the cave considering all flow rates and temperatures

Table 3. Variance in terms of components

PC	Eigenvalue	% Variance
1	4.8415800	96.832000
2	0.1358730	2.717500
3	0.0218025	0.436050
4	0.0007427	0.014855
5	0.0000000	0.000001

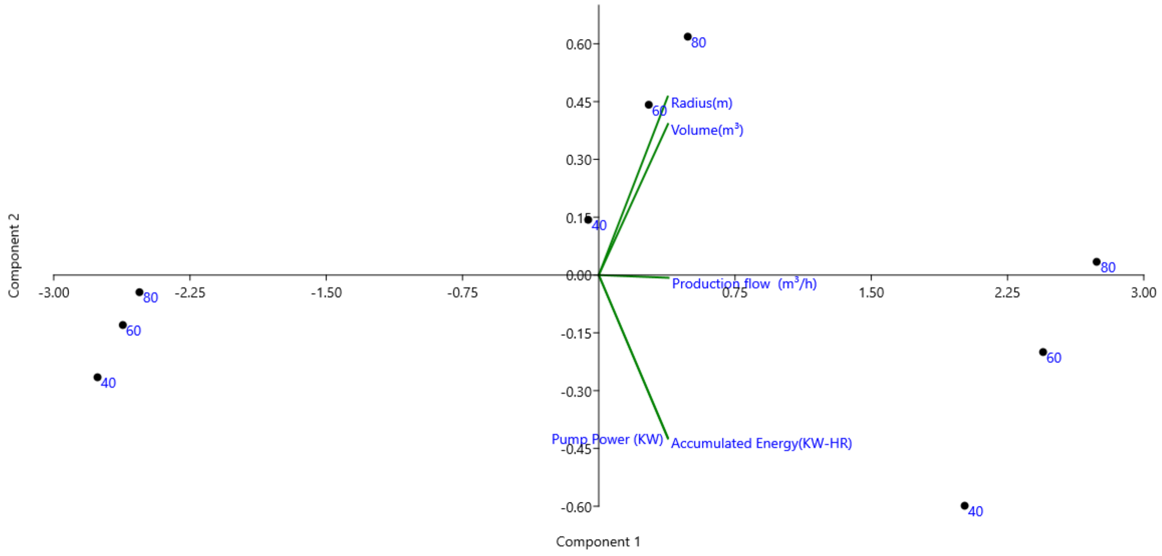

Figure 4. Output variables correlated in x and y coordinates

4 Conclusions

The use of a finite difference code to study the process of opening an underground cave in saline rock by dissolution was investigated. The simulations carried out with the software considering different temperatures and injection flows and a period of 120 days for the formation of the cave found that for a direct mining scenario, the largest radius reached and also the largest volume were obtained for the temperature 80°C and injection flow rate of 500 m^3/h, that is, the higher the injection flow rate, the greater the radius and volume of the cavern. Similar behavior is verified in relation to the influence of the injection temperature, the higher the temperature, the greater the volume and radius of the cavern. The principal component analysis showed that the output variables are directly related, being volume with radius and pump power and accumulated energy closely linked, in addition 97% of the data are in terms of the first component, which reinforces that the first and second components (PC1 and PC2) are the most considered in a matter of variance.

Despite the success with the simulations and the good response surfaces generated, it is important to emphasize that for high temperatures, pressures and flows it is necessary to carry out an experimental validation to obtain more realistic parameters such as the dissolution rate of the rock. In this sense, carrying out experiments to validate such conclusions is a bet to improve this work in the future. Another important point is that to better understand how the analysis of principal components works, more variables and simulations are needed, this work was just an introduction to the subject.

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