Computer models of the salt cavern leaching process - evolution over the last 35 years

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Thirty-five years have passed since the publication of fundamental papers by Durie and Jessen in the SPEJ. It was the very first research effort oriented to construct a computer model of the leaching process. Durie-Jessen formula derived from the results of salt dissolution tests is still in use in some models. Thus, 1964 can be regarded as the beginning of a quick development of modelling software used for salt cavern leaching.

In various countries several centres have evolved since where research on theory and software for leaching simulation is pursued. Computer models are now used more and more for designing caverns in salt-leaching plants. Regular SMRI Meetings have become the main forum for discussion and exchange of research information connected with the new leaching models and their application results. This paper contains three main parts:

Evolution - overview of different approaches to and theories of the leaching process, reflected through simulation software, shown in a historical perspective.

State-of-the-art - the present status of leaching simulation software, i.e. capabilities, similarities and differences of a dozen computer codes currently used all over the world. The software comparison is done based on responses to a questionnaire distributed among the computer code authors.

Future - the authors' opinion about the needs and tendencies which will prevail in future development of the leaching simulation software.

Besides drawing on the literature, the paper is based on the authors' 20-year-long research experience connected with both creating and using the leaching simulation models. Their UBROASYM model is one of those implemented in several countries world-wide.

1. EVOLUTION

1.1. Model prehistory

In the beginning there was Nernst theory: the kinetics of salt dissolution in water is so rapid that the process is controlled by diffusion of newly dissolved ions through a layer of saturated solution being formed along the dissolved salt surface. Although we do not fully subscribe to this theory nowadays, it had been a starting point for early work.

Another milestone was the work by Kulle (1949) whose was the very first attempt to compile a set of mathematical and physical equations describing the leaching process. The oldest research on leaching models was conducted as fundamental, with hardly any prospects of practical applications. The price of salt was too low, and its deposits too common to perceive leaching process optimization (based on a physico-mathematical model) as economically viable. Computers were not efficient enough, with extremely high costs of calculations.

Such a situation continued until the sixties, when salt caverns started to be considered as possible storage space for gas, crude oil and their derivatives. Such caverns have to meet several criteria. This in turn results in the need for more precise monitoring of the cavern leaching process, and thus for computer models.

1.2. Beginnings of computer modelling

Year 1964 can be considered as the beginning because of three papers by Jessen's group: (Durie, Jessen 1964a, 1964b), (Kazemi, Jessen 1964). The first was the most important. It presented both the results of laboratory measurements for various concentrations of the leaching solution, as well as the theoretical relationships derived afterwards. The theory did not match the measurement results and an empirical factor with duly adjusted coefficients was incorporated into the theoretical formula. In this way, a semi-empirical leaching rate formula was obtained. It then became a basis for the American models, which are, with modified parametrization, still present in the majority of currently used models.

Two years later the CAVITY computer program was presented (Sears, Jessen 1966) [2]. It made use of the Durie-Jessen formula as well as of some additional empirical assumptions. In this way, the distribution of concentration was obtained for a cavern leached with water pipe located just below blanket.

The program determined when and how much of the blanket was to be pumped in, for the final cavern shape to be as close to spherical as possible. CAVITY was the very first computer program for modelling the cavern leaching process. Although limited to just one, rather particular, case, it could certainly be applied in the field practice.

Work of Jessen's group concentrated on caverns leached in reverse circulation. However, it is the direct circulation that is much easier for analysis. In that case brine gets mixed thoroughly in the cavern, leading to rather homogeneous concentration in the leached part. European research followed this path. . Röhr (1969) published the very first algorithm describing the direct cavern leaching process, based on the global salt balance. With slight modifications, such algorithms are still implemented.

1.3. First useful programs

Year 1971 is the next breakthrough. That year, at the University of Texas at Austin (USA), Saberian writes his Master Thesis on convective mixing of water with brine.

In Germany, Meister and Kuhr (1972) describe an algorithm similar to Röhr's. In France, Pottier and Esteve (1973) disclose another computer model for direct circulation using quite an original and interesting algorithm describing the movement of cavern wall as parallel displacements of wall segments.. Such approach could well have led to creating an algorithm similar to that used for the UBRO model many years later, if the work had been continued.

All models so far were axially symmetrical, with concentration distribution varying along the vertical axis. Gravitational forces result in either stable stratification of layers with concentration diminishing with height, or in instant mixing of brine in zones of so-called gravitational inversion.

In 1974, a group of German researchers associated with KBB: Nolen, Von Hantleman, Meister, Kleinitz, Hieblinger [3] present a model alternative to all the other approaches. Their 3-D model is cylindrical, and includes hydrodynamics of cavern interior. However, the hydrodynamics proposed there is greatly simplified, applying the laws of flow for a porous medium, and not for an empty cavern. This model was the first one to account for inhomogeneity of the leaching properties of salt. Model results can be verified during cavern leaching, and model parameters adjusted to match the history of the cavern leaching process. However, this advantage was wiped out by the model numerics, allowing only linear leaching rate equation. In addition, describing cavern shape solely using regular blocks distorted natural tendencies of cavern development. The model acted as if the rock salt were able to be leached in the horizontal direction only. The authors also overlooked the fact that turbulent diffusion should constitute a dominating mechanism in the concentration equation, treating turbulence as a marginal phenomenon around pipe openings.

The same year Saberian (1974) completed his Ph.D.Thesis where his model of the leaching process reached its final shape. Röhr (1975) proposed a balance algorithm valid for reverse cycle. Edler and Niquet (1976) developed a model based on similar principles as Röhr's, restricting it to a stationary distribution of concentration. BI Freiberg reported about LOEST model patterned after that of Nolen and co-workers (Kretzschmar, Heidenreich 1978).

The first Polish models developed at CHEMKOP, were also patterned after those known from literature (Sears, Röhr, Nolen) (Kunstman, Urbanczyk 1977). Next model, UNBI, used an algorithm describing cavern shape as a broken line with moving segments (as in Pottier's case) and concentration of cavern brine in balance principles (as in Röhr's case). Contraction of volume and balance of insolubles were incorporated into the model. Both these features were absent in Saberian's model. After few years the leaching rate formula was changed, and the algorithm for leaching without blanket improved. The new version of the model was called UBRO [4].

1.4. The leadership of Saberian

Saberian formulated the principles of water mixing with brine in a cavern as "plume rising". He determined the process parameters in an empirical way. He approximated the cavern using axially symmetrical slices, with radii providing the description of cavern shape. Within a short time, Saberian's model SALT77 sponsored by SMRI dominated the world research (with the exception of Germany and Eastern Europe) for many years, leading to both positive and negative consequences.

In 1981, SANSMIC - a model alternative to that of Saberian appeared in the USA [5]. It was created by Russo at Sandia National Laboratories. Original description of mixing of the plume above water pipe with brine in the cavern was borrowed from flame thermodynamics. Insolubles were considered as well, though they were allowed to settle in the model at cavern floor between the leaching stages only. The model was definitely better than SALT77.

Under the circumstances, SMRI continued to support Saberian's work, but put forward new requirements. To make his model more competitive, Saberian added pressure calculations for leaching pipes. He also included a complex balance for a gaseous pad used as blanket. The new version of the program was called SALGAS. Usefulness of the program is restricted by a large number of factors. The number of model blocks limited to 80 causes the approximation error to be of ca. 10 meters for high caverns. One leaching stage only (with constant injection rate and pipe positioning) can be modelled in a SALGAS run. Therefore, modelling of a leaching process required multiple runs, and results of the previous run served as input data for the next one.

Complete program documentation and source version have been available to the SMRI members [6]. This has made it possible for users to create program mutations on their own. Thus, local program versions crop up in various countries (France, the United Kingdom, Italy). On the one hand, this constituted a major progress since a ready working program can be used as a starting point. On the other hand, this resulted in giving up independent, perhaps worthwhile, research directions, and changing the input to the SALGAS program, impeded by several defects if not errors.

1.5. Attempts at creating a "complete" model

Sharma had the idea of merging the research results of Saberian and Nolen into one general theoretical model of leaching under any 3-D conditions. Sponsored by SMRI, he lost a few years on futile attempts (Sharma 1985). Considering the drawbacks of Nolen's model, one could hardly expect anything else; however, as it seems, Sharma did not even go as far as diagnosing the difficulties correctly.

Work on models with 3D hydrodynamics also continued at CHEMKOP and at BI. Numerical experiments suggested, however, that the concentration distribution obtained in such 3D models may follow from numerical inaccuracies rather than from the model equations. After significant modifications, an axially symmetrical model was constructed by CHEMKOP, with the LOEST equations corrected and cavern shape development taken from UBRO. Several variants of turbulence description in the Navier-Stokes-Reynolds equations were also tested .

Another version of the BI model, called KASOMO, appeared soon afterwards. It had the additional advantage of accounting for temperatures accompanying a leaching process (1988).

1.6. Under DOS

Meanwhile, a new era arrived, namely that of PC's where the existing models started to be implemented. The DOS graphics capabilities, humble at first, were exploited more and more.

In 1987 Kunstman and Urbanczyk succeeded in the first PC implementation of their UBRO model. Since 1991 the program has been available to the SMRI members. In 1989 the KORLOG code was developed, automatically adjusting the UBRO leaching coefficients based on the analysis of sonar measurement results. This still remains the only algorithm of quantitative analysis of sonar measurements for modelling needs. Although the related information has been published several times already (Kunstman, Urbanczyk 1990, 1994) [7], no similar code has been developed as yet.

In 1990 appeared the INVDIR (Chaudan 1990) [8]. It was developed at Gaz de France for a PC and based on the Saberian's model. It had insolubles added, with the mixing algorithm simplified, the number of blocks increased and an algorithm for correcting the calculations of wall angles introduced. Indeed, a corrective algorithm was necessary, as in all the western models, cavern shape was determined through the approximation block radii only (Van Vliet 1990). Appearance of these models constituted a challenge for Saberian, who also implemented his program on an IBM PC the same year (1990).

In 1994 Kunstman, Urbanczyk presented Ubro-Asym model, a new version of UBRO, free from the limitations of axial symmetry [7]. Soon afterwards the Russians let the world know of their work for the first time (Kublanov 1995). The VNIIG developed RAZMYV, a model of leaching in a general 3-D case. However, no information is available as to its algorithm, in particular, how cavern shape is approximated and turbulence described. Most probably, RAZMYV model duplicates here the Nolen model.

Meanwhile, SANSMIC in its DOS version was implemented on a PC. Since 1995 the program has been available to the SMRI members. SOFREGAZ US began to create its further modifications for their own use. In 1996 Guarascio describes the CAVITA model which is an Italian mutation of Saberian's model, also duly enriched with multi-stage capabilities and insolubles (Guarascio 1996) [9]. Also in 1996, the first model similar to UbroAsym is created; namely PROSACAV developed by Edler from UGS Mittenwalde. The same year, Klafki from BI Freiberg describes a version of KASOMO under DOS for a PC and under UNIX.

1.7. Under WINDOWS

Poor usefulness of the SALGAS model leads to user reactions. While keeping the old model algorithm, Chen from RE/SPEC writes a new interface for the WINDOWS operating system, employing its graphical capabilities. At the same time, the majority of model deficiencies are corrected (number of blocks, multi-stage calculations in one run). (Chen et al. 1994).

This was another challenge, this time concerning the exploitation of possibilities offered by the WINDOWS operating system. The first was CHEMKOP, which in 1996 implemented its UbroAsym algorithm under WINDOWS95, significantly expanding the graphic interface and the procedure of user-friendly data entry. Besides the UbroAsym model, the integrated WinUbro package included the KORLOG algorithm of sonar measurement analysis, generalized to the asymmetrical case. Very soon Groenefeld from KBB presented CAVSIM, Nolen's model implemented under WINDOWS95.

The WinUbro package is purchased by a number of companies from Poland, Germany, the USA, the Netherlands, and Slovakia. New, customized versions of the model for Windows98 & Windows NT, including 16 sectors option and pressure calculations, adapted to the varying needs of customers, are generated.

2. CURRENT SITUATION: CODE FEATURES

The main scientific advantage resulting from the 35 years of the leaching models is a definitive selection of theoretical description of the leaching and the choice of factors really influencing the process.

During the 35 years described here, several computer programs have been developed all over the world, implementing various models of the leaching process. In the Table we describe a range of models selected for their practical use and for being well-known world-wide. The data have been obtained mostly from the program authors or users.

3. THE STORY IS NOT OVER

3.1. Controlling cavern leaching processes with the help of computer models

At first, computer modelling was applied in designing new caverns. For caverns which had already entered the leaching stage, the real leaching process was rarely modelled. At the most, the real and the predicted concentration plots or the sonar-measured and the predicted cavern shapes were compared. Such comparisons, however, rarely lead to conclusions concerning model correctness or applicability because leaching technology slightly differs from that designed.

At many leaching sites, injection rate and produced brine concentration are recorded in a computer. These data can be used to correct model coefficients automatically and, consequently, to update the leaching prediction periodically.

In 1997, CHEMKOP staff developed another WinUbro version including the option of a leaching process scenario recorded in a computer. Such a scenario, containing data on injection rate and pipe location during the real leaching process, makes it possible to adjust model coefficients repeatedly without the need to introduce leaching data anew. Co-operation of the model with the KORLOG segment differentiating model coefficients on the basis of sonar measurements is facilitated as well.

3.2. New challenge - horizontal models

Software mentioned above describes caverns created traditionally by leaching around a selected zone of a vertical borehole. However, in thin salt beds this technology cannot be used to leach regular caverns of substantial volumes. This has led to the idea of horizontal caverns and for appropriate models .

A breakthrough occurred in 1995, when three papers on horizontal cavern models were presented during the SMRI meeting in San Antonio [10].

The HORSMIC model (Russo) was developed at Sandia National Laboratories. Unfortunately, this horizontal model is quite disappointing. The problems of leaching a uniform tunnel cavern are solved through an idea of diffused water supply along the whole length of the borehole, so as to achieve homogeneous concentration in the whole profile. This is to be obtained through proper water pipe perforation.

The model of Saberian is a general one using a system of cylindrical co-ordinates with its axis along the axis of the leached borehole. Most probably, such a model works well in the initial stage of the leaching process only. Afterwards, when cavern floor is covered with insolubles, floor leaching terminates, while a semi-circular zone, not predicted by this model, develops above the water inlet.

HORSALT model (Kunstman, Urbanczyk) uses a Cartesian system of coordinates, and an auxiliary cylindrical frame with its axis perpendicular to the borehole axis and directed upwards at water inlet.

Software name	Developed by	Source	Algorithm of wall movement	Mixing algorithm	Leaching coefficient	Insolubles	Operation mode	Graphic interface
SALGAS	Saberian USA SMRI-sponsored	Fortran	associated with cavern blocks	plume rising	varying with depth	no insolubles	batch	none
CAVSIM	Nolen and others KBB Germany	Fortran	associated with cavern blocks	resulting from 3-D hydrody-namics	varying with depth	insolubles fall down immediate ly	interactive	full Win95
SANSMIC	Russo, SANDIA USA	Fortran	associated with cavern blocks	plume rising	homo-geneous	insolubles fall down after some time	batch	none
INVDIR	Gas de France	Fortran	associated with cavern blocks	complete gravitation equilibrium	homo-geneous	insolubles fall down immedia-tely	batch	simple DOS
UBRO	Kunstman, Urbanczyk CHEMKOP Poland	Fortran	indepen-dent of cavern blocks	complete gravitation equilibrium	varying with depth modified in time	insolubles fall down immedia-tely	interactive	simple DOS
KASOMO	Heindenreich Riegel, BI Freiberg Germany	Fortran	associated with cavern blocks	resulting from 3-D hydrody-namics	varying with depth	insolubles fall down immedia-tely	batch	none
VISUAL Salgas	RE/SPEC USA	Visual Basic	associated with cavern blocks	plume rising	varying with depth	no insolubles	combined	Win3.1
CAVITA	Mining Italiana Italy	C++	associated with cavern blocks	plume rising	varying with depth	insolubles fall down after some time	batch	simple DOS
UBRO ASYM	Kunstman, Urbanczyk CHEMKOP Poland	Fortran	indepen-dent of internal blocks	complete gravitation equilibrium	varying with depth modified in time	insolubles fall down immedia-tely	interactive	simple DOS
WinUbro	Kunstman, Urbanczyk CHEMKOP Poland	C++	indepen-dent of internal blocks	complete gravitation equilibrium	varying with depth modified in time	insolubles fall down immedia-tely	interactive	full Win95
RAZMYV	Kublanov and others VNIIG, Russia	Pascal, Delphi	associated with cavern blocks	resulting from 3-D hydrody-namics	varying with depth	insolubles fall down immedia-tely	batch	none
PROSA CAV	Edler UGS, Mittenwalde Germany	Pascal	indepen-dent of internal blocks	complete gravitation equilibrium	varying with depth modified in time	insolubles fall down after some time	both	none

The algorithm of cavern wall development is similar to that in UBRO, although it is used independently for each subsequent cavern cross-section. The most rapid development of cavern roof occurs above the water inlet, while the cavern may expand beyond the points of water injection and brine production.

Saberian's model and the HORSALT model were developed partially in collaboration with Gaz de France who have been drawing on this experience while working on their own model. A field experiment on a semi-technical scale was conducted there to provide model testing data. Because of the high cost of these studies, their results have not been published. From the information disclosed so far it follows that leaching is strong in the vertical direction, while mixing in the horizontal direction is weak.

3.3. Anticipated future trends

The authors present here their own opinions which are based on their long-term experience in modelling the leaching processes. These predictions may be summarized as follows:

A model with complete 3D-hydrodynamics is still to be developed. This is not an easy problem, and probably not the most pressing one.

A more vital issue is to provide a better description of change in salt properties (e.g. sloped layers of salt more easily leached, or oblique non-leachable inserts). This would require a change in the approximation principles in order to fully account for all 3 dimensions, as well as a change in the principles of a mathematical description of cavern walls.

Growing computer capabilities will result in the fact that the only models to count in the future will be those with enhanced graphics and automatic connection to the leaching databases [11].

Full use of sonar data achieved by connecting the measurements with the leaching models in easy way, will become a required standard.

Even in the future, complete controlling of the leaching process by a computer model is unrealistic and unnecessary. The salt deposit in which a cavern is being leached is a creation of Nature, and as such it may deviate from all the studies and models in an unpredictable way. Thus, a computer model will always constitute just a tool in the hands of experienced leaching engineers, and it is they who will have to make decisions on the basis of continually improving data provided by the models.

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