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Numerical Simulation in Gas Hydrate Formation

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ABSTRACT: The formation of gas hydrates is an undesirable process in the natural gas transportation industry, ensuring the blockage of pipelines and especially the reduction of transport flows and the increase of working pressure. That is why it is necessary to simulate the water adsorption processes using chemicals as well as the mathematical simulation of the processes. The article presents data on the simulation stages and especially the behavior of natural gas with water content in main pipelines.

KEYWORDS: Gas hydrates, modeling, simulation, natural gas transportation

INTRODUCTION

Numerical simulation in the analysis of cryohydrate formation is performed using the numerical simulation program created by the authors of the article (in Python), a well-established software platform widely used in the petrochemical industry. Phyton is a specialized software for the simulation of chemical processes, with applicability in the chemical industry and related processes. This computational tool is used by engineers and researchers from various industrial fields for the design, analysis and optimization of chemical process units. Through Phyton, users can model and simulate one or more stages of chemical processes, including chemical reactions, phase separation, heat and mass transfer, in order to investigate and optimize the behavior of chemical systems in a virtual laboratory environment. To perform the simulation of a plant intended for the treatment of natural gases through the triethyl glycol drying process, specialized numerical simulation software, such as Phyton, is used. This technological approach allows engineers to model and analyze system behavior in detail in a virtual environment, providing a platform for evaluating process efficiency and optimizing operational parameters.

METHODOLOGY

In the triglycol distillation plant (TEG), the rich gas, which carries a significant concentration of unwanted substances, enters the flow at a rate of 24 kmol/h water.

After the first treatment stage, a mixing process between the rich gases and TEG is initiated, with a view to further treatment in a specialized separation plant.

During this stage, a rich gas flow, containing a small amount of water of approximately 0.34 kmol/h, is directed to line 2.

Later, in the separation stage in the separator, another rich gas flow, accompanied by a minor amount of water of approximately 0.016 kmol/h, is directed via line 7.

The water, which contains traces of glycol and, in particular, a significant concentration of rich gases, is processed in two separate distillation columns, where the separation between water and TEG takes place.

In a subsequent step, in the second distillation column, the glycol separation is carried out. The TEG regeneration process involves the use of dry gases to ensure the efficient removal of impurities and to restore the original properties of the TEG for reuse in the treatment process.

This series of complex and interdependent operations demonstrates the rigorous and detailed effort involved in the efficient management and treatment of rich gases within chemical processing plants.

The components used in the natural gas treatment plant by drying with triethyl glycol may include the following:

- nitrogen;
- hydrogen sulfide;
- methane;

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- ethane;
- propane;
- isobutane;
- n-butane;
- isopentane;
- n-pentane;
- n-hexane;
- n-heptane;
- water;
- triethylene glycol.

The chemical characteristics are given in the subchapter: “Characteristics of simulated chemicals”.

The created plant consists of the following equipment:

- distillation column;
- gas separator;
- pump;
- heat exchanger;
- mixer.

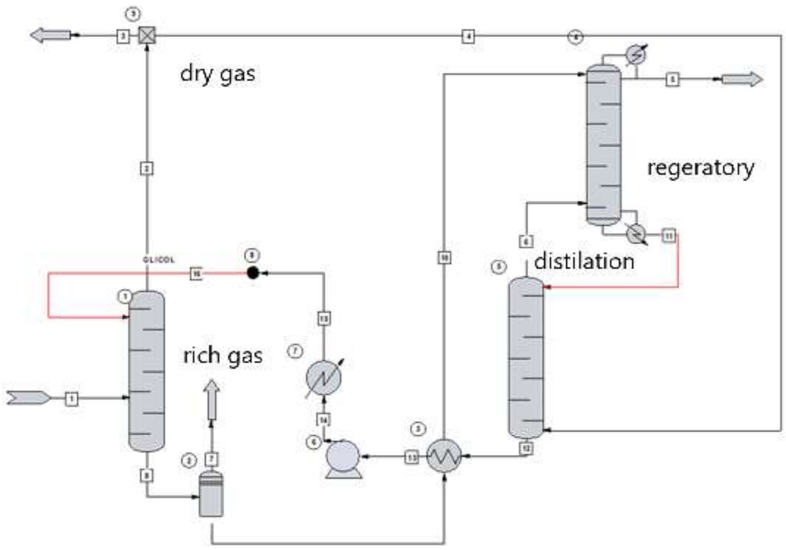

Fig. 1: Deshydratation complex

The developed setup was an essential tool in investigating and determining the gas drying process using triglycol (TEG) with remarkable precision.

This setup facilitated a detailed analysis of the mechanisms involved in the gas drying process, thus providing a thorough understanding of the interactions between TEG and water vapor.

In the simulation of the water adsorption process by TEG, key process parameters such as adsorption kinetics, phase equilibrium, separation efficiency and factors influencing system performance were examined in depth.

Particular attention was paid to the characterization of the contact interface between TEG and water vapor, as well as how operational conditions such as temperature, pressure and gas composition influence the adsorption capacity and selectivity of the TEG.

Through this detailed simulation, we obtained a deep understanding of the system behavior and TEG performance in the gas drying process, thus providing critical guidance for optimizing and improving the operational efficiency of the plant.

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We have conducted a simulation using the Phyton platform to investigate the process of treating gas with triglycol (TEG). The developed plant comprises a column dedicated to treating gas with TEG, together with two columns specialized in glycol regeneration.

The meticulous analysis performed revealed that, at the specific operating conditions of 35 atm and 30°C, the separation process in the triglycol distillation column proceeds with remarkable efficiency.

The amount of water is removed from the initial flow of 24 kmol/h, reducing to only 0.348 kmol/h.

In the presentation of the plant, we have listed each component included and highlighted the use of chemicals in the gas treatment process.

This complex and rigorous simulation demonstrates our meticulous approach to the design and evaluation of chemical processing plants.

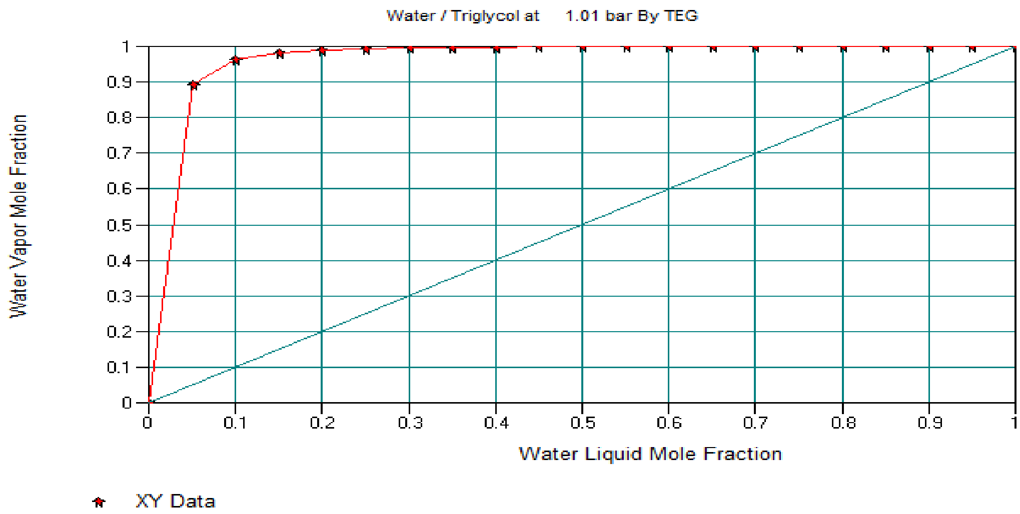

Fig. 2: Variation of water/TEG mixture.

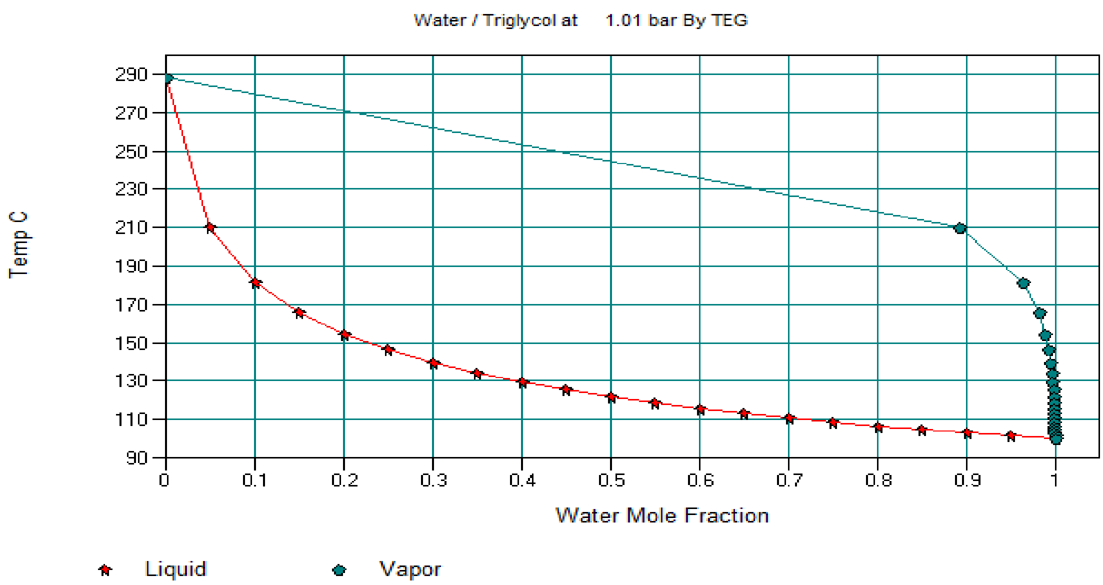

Fig. 3: Variation of water/TEG mixture.

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MODELING AND ANALYSIS

The transport of water through gas pipelines is given by the relationship [1].

$$m\dot{v} = A\Delta p - A\Delta p_l - A\Delta p_r \quad (1)$$

Unde :

- A is the area of the pipe,
- $A\Delta p_l$ represents the local pressure loss,
- $A\Delta p_r$ represents the pressure loss through the valves,
- $A\Delta p$ represents the force applied to the mass of liquid in the pipe.

Applying the relationships:

$$A\Delta p = A(p_0 - p_v) \quad (2)$$

$$\Delta p_r = \rho \frac{Q^2}{k_v^2} \quad (3)$$

$$\Delta p_c = \rho \frac{Q^2}{k_l^2} \quad (4)$$

$$m = LA\rho \quad (5)$$

$$v = \frac{Q}{A} \quad (6)$$

In equation 6, we get:

$$\frac{L}{A}\dot{Q} + \left(\frac{1}{k_v^2} + \frac{1}{k_l^2}\right)Q^2 = \frac{1}{\rho}(p_0 - p_v) \quad (7)$$

For the buffer vessel, the mathematical model will be written taking into account the following assumptions [2,3,5]:

- Thermal phenomena are negligible;
- The vessel is considered with concentrated parameters;
- Through valves *R1* and *R2* the flow is turbulent.

$$\frac{\partial c_j}{\partial t} = div(D_{ef}\, grad c_j) - div(c_j \vec{v}) - r_j \quad (8)$$

Where j=1,2,3,…,n-1.

Taking into account the above assumptions, it can be written:

$$grad\rho = 0$$

$$G = 0 \quad (9)$$

And equation 8 is:

$$\frac{\partial \rho}{\partial t} = -div(\rho \vec{v}) \quad (10)$$

Applying the relationship formula:

$$\int_V div(\rho \vec{v}) dV = \int_\Sigma \vec{n}\rho\vec{v} d\sigma \quad (11)$$

$$\left(\int_\Sigma \vec{n}\rho\vec{v} d\sigma\right)/V = div(\rho\vec{v}) \downarrow_A \quad (12)$$

Where A is a point inside the surface $\sum$ of the vessel.

Solving the integral leads to the result:

$$\int_\Sigma \vec{n}\rho\vec{v} d\sigma = -Q_i + Q_e \quad (13)$$

Where Q_i and Q_e are the mass flow rates entering and leaving the vessel, respectively (kg/s).

$$div(\rho\vec{v}) \downarrow_A = (-Q_i + Q_e)/V \quad (14)$$

$$V\frac{\partial \rho}{\partial t} = Q_i - Q_e \quad (15)$$

We also use the relations of state for perfect gases:

$$PV = NRT \quad (16)$$

$$\rho = \frac{M}{RT}P \quad (17)$$

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Where M is the molecular mass of the gas.
Equation 17 becomes if we also use equations 15and 16:

$$\frac{MV}{RT}\frac{d\rho}{dt} = Q_i - Q_e \qquad (18)$$

Under turbulent flow conditions through $R1$ and $R2$, the equations can be written successively:

$$Q_i = K_{v1}\sqrt{\rho_1(P_1 - P)} = K_{v1}\sqrt{\frac{M}{RT}P_1(P_1 - P)} \qquad (19)$$

$$Q_e = K_{v2}\sqrt{\rho_2(P - P_2)} = K_{v2}\sqrt{\frac{M}{RT}P(P - P_2)} \qquad (20)$$

Where K_{v1} and K_{v2} are capacity coefficients associated with valves R1 and R2.
Equation 20 becomes:

$$\frac{MV}{RT}\frac{d\rho}{dt} = K_{v1}\sqrt{\frac{M}{RT}P_1(P_1 - P)} - K_{v2}\sqrt{\frac{M}{RT}P(P - P_2)} \qquad (21)$$

If we linearize equation 21 around the point (P10, P0, P20), we obtain:

$$a = \frac{v}{2}\sqrt{\frac{M}{RT}}/E \qquad (22)$$

$$b_1 = K_{v1}\frac{2P_{10} - P_0}{\sqrt{P_{10}^2 - P_{10}P_0}}/E \qquad (23)$$

$$b_2 = K_{v2}\frac{P_0}{\sqrt{P_0^2 - P_{20}P_0}}/E \qquad (24)$$

$$E = K_{v2}\frac{2P_0 - P_{20}}{\sqrt{P_0^2 - P_{20}P_0}} + K_{v1}\frac{P_{10}}{\sqrt{P_{10}^2 - P_{10}P_0}} \qquad (25)$$

The form of the differential equation:

$$a\frac{a\Delta P}{dt} + \Delta P = b_1\Delta P_1 + b_2\Delta P_2 \qquad (26)$$

It presents an important peculiarity, namely that the initial condition is null.

$$\Delta P_1 = P_1 - P_{10}$$
$$\Delta P_2 = P_2 - P_{20}$$
$$\Delta P = P - P_0$$

Genetic algoritms using in gas dehydration

The evolution of life on Earth was a less likely consequence of chemical and physical processes.

Analysis of life forms on Earth shows a very complex development. That is why genetic algorithms, which are based on genetics and evolution, were developed for the study [2,3,4,5].

The basic elements of genetic algorithms are:

- Selection of solutions (depending on the degree of fit);
- Reproduction (for gene crossing);
- Mutation (for random gene changes).

The genetic algorithm identifies increasingly better solutions to problems (as species existing in nature develop and evolve to the environment).

A human being is born through the fertilization of an egg by a sperm.

Before conception, 23 chromosomes are present in both the egg and the sperm. They are numbered with numbers ranging from 1 to 23, a total of 46 chromosomes.

Într-un organism diploid cum este omul, doi cromozomi cu același număr, unul de la ovul iar celălalt de la spermatozoon forms a pair of chromosomes for the developing fetus. Thus, chromosome 1 from the man with chromosome 1 from the woman forms a structure of the shape as in figure 3.4.

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Each pair of chromosomes of the fetus is formed by thousands or millions of genes (gene pairs), taken from both the mother and the father. Each pair or pairs of genes thus formed ensures the formation of specific characteristics of the child, namely: blood type, hair and eye color, etc., characteristics called phenotypes.

Blood type for example can have four possible values: O, A, B and AB.

Each gene for blood type can be one of the following values: 0, 1 or 2 called alleles.

In the human body, the order of genes does not matter (it can be 10 or 01) and some of the genes differ depending on their type (some genes can have 0 and 1, others can have 0, 1, 2, …).

The possible gene pair combinations, called genotypes, and the corresponding phenotypes are given in Table 1.

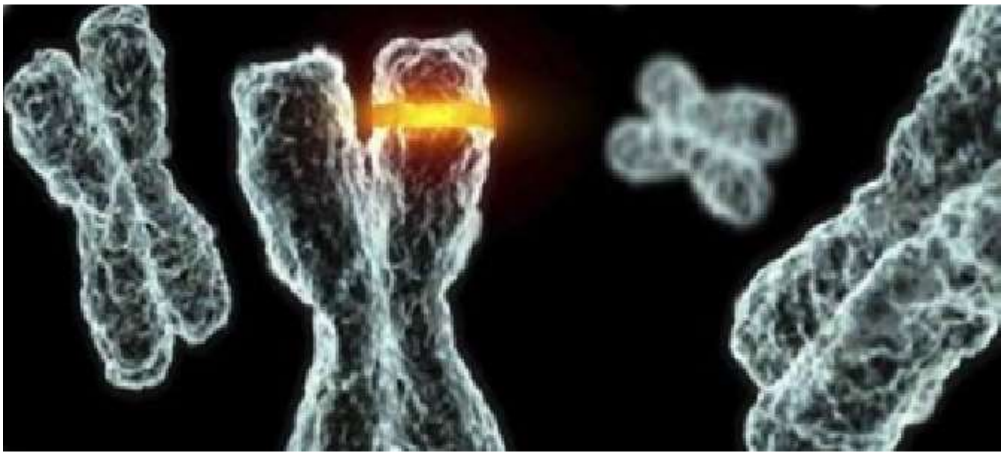

Fig. 4. Cromozomial structures [4]

Table 1. Types of blood group combinations [4]

Genom	fenom
00	O
10 sau 11	A
20 sau 22	B
21	AB4

If the mother's gene is 0 and the father's is 1, the child's genotype becomes 10, so the phenotype will be blood type A.

When the child grows a single chromosome (from each pair), it is selected for the egg or sperm, this is how a phenotype is inherited from an individual to the child.

Occasionally, some genes change their value, causing mutations (due to chemical, physical or biological effects).

Within any biological species, those individuals that are better adapted to the environment and existing living conditions have a greater chance of survival, the less developed disappearing (the theory of natural selection or evolution).

The genetic algorithm begins by defining the representation of solutions for a problem that needs to be studied.

By solution is meant that value that can be the correct solution to the problem, the way of representing the solution being in the form of character strings.

The representation of chromosomes is necessary to describe each individual in the population. The representation scheme determines the structure of the problem as well as the genetic operators used.

Each individual or chromosome is formed by a sequence of genes represented by a certain alphabet (binary digits, symbols, floating point numbers, matrices, etc.)

It is used to compare solutions and determine which is the best.

There are variants and extensions of the genetic algorithm procedure.

That is why a classic example will be presented.

Basic stages

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Step 0 – population initialization;

A random solution is generated.

Step 1 – reproduction.

The degree of matching and the corresponding probability for all solutions of the population are determined.

The fitness and corresponding probability for all solutions in the population are determined.

A mating center is created. Solutions weighted by their fitness are randomly selected. Solutions with a higher fitness degree thus have a higher probability of being chosen than less fit solutions, and therefore a higher chance of surviving in the new generation.

So the concept of evolution based on natural selection is emphasized.

Step 2. Crossover.

Two solutions are randomly selected from the set of possible solutions at a given time. A crossover probability is chosen, set at 0.7. Then it is randomly determined whether crossovers occur and if they do, two offspring are formed that are exact copies of the two solutions.

Internal points (crossover points) of the solutions are randomly selected and then the portions after that point are swapped between them.

This procedure is repeated on the population obtained in step 1, until the size of the new population reaches the initial size of the population, randomly choosing one pair at a time.

So each solution can represent a set of values for the chosen parameters, parts of each solution can contain relevant or important elements.

The genetic algorithm uses this information by reproducing useful notions and crossing them between stronger individuals.

Step 3. Random mutations

With the help of a small mutation probability of the order of 0.001. Then, small portions of the solution representation are selected randomly, and they are artificially modified.

In this step, the way in which mutations occur is modeled, by applying the genetic algorithm at a given time, the entire population tends to be similar (as a result of applying the working iterations).

Also, at the end of the iterations there is no longer a significant shift towards the extreme.

The procedure presented above consisting of step 0 followed by step 1,2,3 until the termination condition is met forms a single stage, but applying the genetic algorithm requires multiple runs of the algorithm until the optimal solution is defined.

Table 2. Cross-breeding of individuals [4]

Solution	Before crossing crossing points	Next generation solutions
Number 1	◊◊◊◊◊□□□□□	◊◊◊◊◊▫▫▫▫▫
Number 2	▪▪▪▪▫▫▫▫▫	▪▪▪▪□□□□□

CONCLUSION

The genetic algorithm represents an abstract model of natural genetics and the evolutionary process described previously.

Genetic algorithms include concepts taken from the genetics of living species, namely: chromosomes, genes, mutations, evolution, reproductive processes).

The application of a genetic algorithm involves the following steps:

a. Random generation of solutions to the problem – chromosomes;

b. Development of iterations that include selecting the best solution and performing reproduction operations;

c. Performing mutations on the solutions.

Solving iterations will lead to the identification of increasingly favorable solutions, as well as within the natural process of evolution.

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