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Numerical Simulation of The Operation of Natural Gas Treatment

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ABSTRACT: Natural gas will remain a transitional fuel for many years to come. However, the exploitation of deposits also brings water particles associated with them (with a decrease in their pressure). Therefore, drying natural gas becomes a main activity in providing them as an energy source. In this material, we present a numerical model of the behavior of water in the natural gas mixture and provide data on the use of molecular sieves impregnated with alumina, silica gel, activated carbon, and hygroscopic salts.

KEYWORDS: Moddeling, molecular, water.

INTRODUCTION

Gas-liquid separation is an essential process in many industries, with significant applications in product purification and raw material recovery. This process is vital to preventing operational problems, such as pipe blockage, equipment corrosion, and vibrations, which can lead to plant damage and increased operating costs. Although gas-liquid separation technologies have evolved considerably, their complexity brings innovative solutions and specific challenges [1].

The interaction between droplets and gases, as well as the formation and breakdown of the liquid film, are important aspects of the separation process.

These processes significantly influence the efficiency of separation technologies. In this context, recent research focuses on a deeper understanding of two-phase flow fields, including droplet size distribution, droplet velocity, and phase behavior, to improve the performance of existing technologies.

In addition, combining several separation technologies can expand existing applications and lead to optimized process performance. A better understanding of the relationship between the flow field and separation efficiency can contribute to the standardization of separator design, facilitating the implementation of more efficient solutions in the industry.

In this direction, neural networks have brought promising results for optimizing geometric and operational parameters. Thus, a back-propagation neural network was used to develop a model for predicting a blade demister's separation efficiency and pressure loss.

This model was optimized using a genetic algorithm to improve the system's overall performance.

An Eulerian-Lagrangian model was also used to predict the behavior of droplets in a gas flow, and calculations of particle velocity and trajectory distributions contributed to improving the performance of mist eliminators.

Gas-liquid separation technologies are classified according to the separation mechanisms into several categories, including gravitational sedimentation, inertial collision, filtration separation, centrifugal separation, dynamic separation in "T" configurations, supersonic cyclonic separation, and traditional natural gas dehydration technologies.

Each technology has led to different types of separators, each with its applications, advantages, disadvantages, and a varying level of technological maturity. Despite progress, each technology continues to present specific limitations [2].

A comprehensive review of the most advanced gas-liquid separation methods is presented to meet the growing demand for detailed information on separation technologies.

Each technology's mechanisms and theoretical research are explored, and their applications, advantages, and disadvantages are summarized.

Theoretical models for predicting phase separation are also examined, providing guidelines for selecting and designing suitable separators according to application requirements

METHODOLOGY

Based on the current state of development and challenges encountered, future development directions and research prospects in the field are discussed.

The methods for drying natural gas are as follows [3]:

a. Gravity sedimentation;
b. Inertial collision;
c. Filtration separation;
d. Centrifugal separation;
e. Supersonic separators;
f. Traditional natural gas dehydration technologies.

Gravity sedimentation separates the two phases by their relative motion, generated by the difference in specific gravity between the dispersed and continuous phases.

A specific formula can describe the final sedimentation velocity of a droplet in a gravity separator [4].

$$U=\sqrt{\frac{4\,gd(\rho_l-\rho_g)}{3C_D\,\rho_g}} \qquad (1)$$

where:

- U is the droplet settling velocity;
- d is the droplet diameter;
- ρ_l, ρ_g are the densities of the liquid and gas phases, respectively;
- g is the gravitational acceleration;
- C_D is the drag coefficient, which depends on the state of motion of the droplet and the Reynolds number, correlated with the droplet size.

When the Reynolds number (Re) is less than 0.3, the droplet settling in a gas flow is assumed to occur in a laminar regime, and the drag coefficient (C_D) is given by the formula C_D = 24/Re, according to Stokes' law.

The final settling velocity is:

$$U=\frac{(\rho_l-\rho_g)gd}{\rho_g} \qquad (2)$$

Where μ_g is gas viscosity.

When Re is between 1,000 and 200,000, the sedimentation of the drops is considered in the turbulent regime, and $C_D \approx 0.44$, according to Newton's law, the final velocity becomes:

$$U=1,74\sqrt{\frac{(\rho_l-\rho_g)gd}{\rho_g}} \qquad (3)$$

For intermediate values of Re, between 0.3 and 1000, C_D is expressed as:

$$C_D=18,5/Re^{0,6} \qquad (4)$$

Equations (2) and (3) show that an increase in the density difference between the two phases, an increase in droplet size, or a decrease in gas viscosity facilitates gas-liquid separation.

Gravity separators, which operate on the principle of gravitational sedimentation, can be classified into two main types: horizontal and vertical, as shown in figure 1.

The primary separation section includes various inlet structures, commonly known as cyclones and baffles, known as “Schoepentoeters.”

In some vertical separators, tangential inlets are used for primary separation. The secondary settling section is central to the gravity separation process between gas and liquid droplets. The flow parameters in this section are critical for determining the structural dimensions of the separator.

The defog section, usually made of materials such as fibers or wire mesh, is positioned immediately before the gas outlet, retaining the smaller droplets that have passed the settling section [5].

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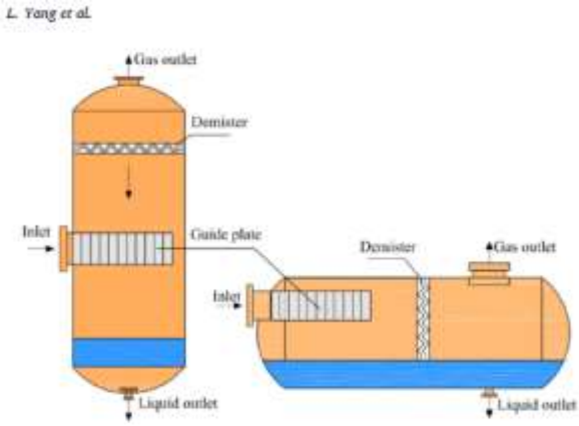


Fig. 1. Gravity separator: horizontal, vertical [3].

The gravity separator has a simple construction with no moving parts, significantly reducing abrasion between the fluid and the tank walls.

This minimizes wear and pressure losses in the system. It is also flexible enough to handle large volume gas-liquid mixtures and easy to operate.

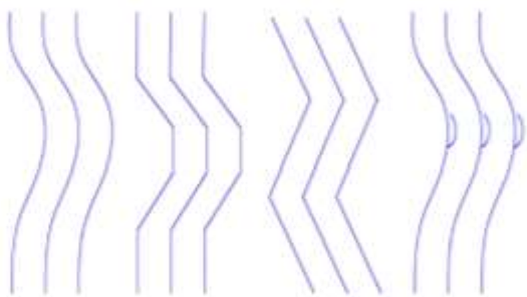
However, due to the large distances the fluids have to travel, and the time required for separation, the gravity separator has a considerable volume and requires a lot of space. It is only suitable for separating large droplets, the critical size usually 100 μm [3].

A separator based on the principle of ***inertial collisions*** is mainly represented by corrugated plate mist eliminators. These are usually composed of two main components: specially designed blades and a cleaning system.

Figure 2. shows the different types of blades used in mist eliminators. In general, blades can have one of the following three shapes: arc, trapezoid, or triangle.

To increase the efficiency of the separation process, additional grooves are often added to the curved areas of these structures, as highlighted in Figure 3.

Corrugated plate mist eliminators can be classified as vertical and parallel depending on the angle between the droplet movement directions and the airflow. In the case of vertical flow eliminators, the gas-containing droplets enter the device horizontally, and the captured droplets are discharged perpendicular to the direction of the gas flow. In contrast, in parallel flow eliminators, the gas-containing droplets enter vertically, and the droplets are discharged in the opposite direction to the gas flow. However, in the case of parallel flow, the gas exerts significant resistance on the falling droplets, which favors their re-entrainment.



a – arc b – trapezoid c – triangle d – rounded ditch

Fig. 2. Types of blades used in mist eliminators [3].

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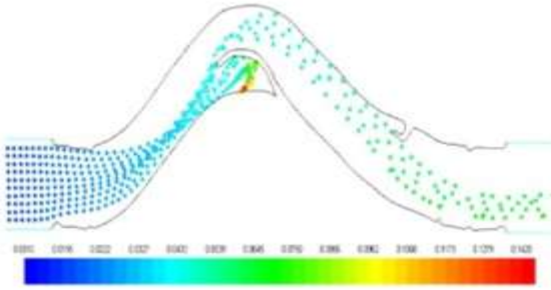

Fig. 3. The trajectory of the droplet released from the injection location into a flow channel [3].

The gas flow containing droplets is deflected along a curvilinear path within the flow passage.

Due to their greater inertia, the droplets cannot follow these sharp turns and strike the surface of the lamella, where they form a liquid film.

As more droplets accumulate, the fluid film thickens, coalesces into a larger stream, and is discharged from the unit by falling.

Meanwhile, the gas passes freely through the eliminator, separating from the entrained droplets and continuing to flow without liquid impurities.

Gas-liquid separation by filtration consists of removing the liquid phase from the gas phase using a filter medium.

The central element of a filter separator is the filter core. Various filter materials are commonly used, of which metal mesh and glass fiber filter offer the best separation performance.

The separation mechanism of these filters is mainly based on three processes: inertial impact, direct interception and diffusion interception, as shown in Figure 4.

Inertial impaction occurs when a gas containing droplets flows through a metal mesh.

The gas changes the direction of its flow lines along the mesh structure, while the larger droplets continue to move straight, under the influence of inertia, due to sufficient momentum.

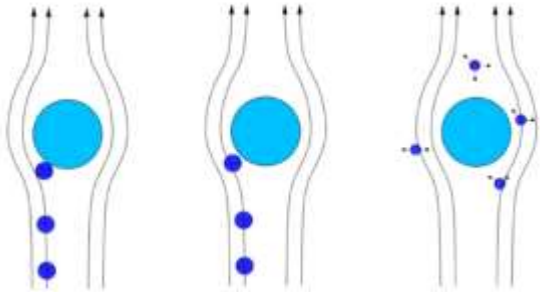

Fig.4. Schematic diagram of the filtration separation mechanism [3].

Finally, the droplets break away from the gas flow line and are separated by impact.

This mechanism can be characterized by the Stokes number, as follows [4]:

$$s_t=\frac{K_M\ \rho_l d^2 u_g}{18\mu_g d_b} \qquad (5)$$

where:

- K_M: Cunningham correction factor;
- ρ_l: density of the liquid phase;

- d: diameter of the droplet;
- u_l: velocity of the gas flow;
- μ_g: viscosity of the gas;
- d_b diameter of the monofilament section.

A higher Stokes number improves the separation performance.

The equation shows that the Stokes number increases as the diameter and density of the drops or the gas velocity increase, but decreases when the viscosity of the gas or the diameter of the monofilament section increase [3].

During direct interception, if the drops are too small and do not have enough momentum, they follow the flow lines of the gas around the monofilament.

They are intercepted only when the distance between the drops and the center of the monofilament becomes smaller than the radius of the droplet.

This mechanism is characterized by the interception parameter Kp.

$$K_P=\frac{d}{d_b} \quad (6)$$

A higher K_p parameter leads to a higher interception efficiency.

Thus, based on the droplet diameter distribution and the separation requirements, a reasonable mesh opening can be determined using this equation.

During diffusion interception, very small droplets, with a diameter of less than 1 µm, undergo Brownian motion, which increases the probability that they will hit the mesh surface and be separated.

However, filter separators are prone to secondary re-entrainment of liquid droplets.

The removal of droplets leads to the deposition of solid particles that can block the mesh and impede the passage of air flow, which increases the pressure loss.

This phenomenon requires periodic cleaning of the mesh, a difficult process in the case of mesh fixed in ducts.

Because of these shortcomings, the operation of filter separators becomes expensive.

Currently, filter separators are mainly used for treating waste gases from diesel hydrogenation, condensate recovery, and purification of raw ammonia gas and natural gas.

The primary mechanism of ***centrifugal separation*** is multiphase separation under the action of centrifugal forces generated by the density differences between the multiphase media.

When a gas-liquid mixture rotates at a high speed, the centrifugal forces become hundreds or even thousands of times greater than gravity, which makes centrifugal separation much more efficient than gravitational sedimentation. Centrifugal separators can effectively separate droplets with sizes of at least a few tens of microns.

For example, previous experiments have shown that a cylindrical gas-liquid cyclone can achieve a separation efficiency of 100% for droplets of at least 43 µm. I

n addition, the residence time of gas-liquid mixtures in centrifugal separators is very short (usually a few seconds), and these separators have small dimensions, are lightweight, and have a low cost.

Estimates show that adding a 1 kg load to an oil and gas production platform located at a depth of 3 km can increase the platform's price by $10,000.

Gravity separators and auxiliary systems are very heavy (reaching hundreds or thousands of tons), and centrifugal separators can significantly reduce these costs [3].

In 1989, Stork Product Engineering B.V. of the Netherlands obtained a patent for a ***supersonic vortex separation technology***, called a cyclonic air separator, originally used in air conditioning systems.

In 1997, Royal Dutch Shell began researching supersonic natural gas dehydration technology and established, together with Beacom Ventures capital, the joint venture Twister BV in 2000, which specialized in researching and promoting this technology [4].

Twister BV invented the first generation supersonic separator, known as the Twister Mark I.

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In the supersonic section of the nozzle, a baffle plate was used to induce rotational motion of the gas-liquid flow.

To improve the performance of the Twister supersonic separator, a second vortex tube supersonic separator was created, which optimizes the nozzle design by integrating a central body and an annular nozzle configuration.

The vortex generation was also moved downstream, to the subsonic part of the nozzle entrance.

Extensive testing was carried out at the Gasunie Research Facility in Groningen, the Netherlands, and field tests showed that the Twister Mark II reduced the pressure drop from 33% to 25% and achieved a liquid separation efficiency of over 90%.

Compared to conventional Joule-Thompson expansion, the combination of the Twister with a hydrate separator had an efficiency of 10-20% higher in many cases.

The operating principle of the second supersonic vortex generator is that the saturated wet gas flow first passes through the vortex generator, turning into a turbulent flow.

Then, the rotating airflow expands adiabatically through the Laval nozzle to supersonic speeds, forming a high-speed vortex flow field in which the temperature and pressure of the gas drop sharply.

As the temperature drops rapidly, water vapor and heavy alkane components condense into droplets. Under the action of vortex centrifugal forces, the condensate droplets are thrown onto the pipe wall, while the gas occupies the center of the main flow.

The gas-liquid mixture then passes through the cyclone separator, where the temperature increases and the tangential velocity decreases due to friction.

The liquid and part of the sliding gas are discharged from the separator through the pipe. The dry gas, with water vapor and heavy alkane components removed, enters the diffuser, where the flow velocity is reduced, and the kinetic energy is converted into pressure potential energy. Thus, the pressure is restored to 70–80% of the original value, ultimately achieving dehydration of the natural gas.

In the separation process, the vortex strength plays a crucial role in the separation efficiency. Studies have shown that the Mach number of the gas at the nozzle exit decreased as the vortex strength increased. Intense vortices increase the temperature and static temperature gradient, which affects the expansion characteristics of the Laval nozzle. Therefore, it is necessary to find an optimal balance of vortex strength to ensure both efficient separation and proper temperature distribution [3].

As for larger droplets, they have better condensation rates, but their residence time in the main flow is shorter.

Thus, the droplet inlet radius should be moderate for optimal efficiency.

The critical dimensions of the outer droplets were determined according to the inlet pressure, and the vortex angle and tangential velocity in the nozzle were improved to increase the separator performance.

At the same time, it was found that an appropriate droplet size and a higher mass flow rate accelerated the condensation efficiency of water vapor.

Supersonic separators are appreciated for their high efficiency and their sealed, compact and lightweight structure. They do not require chemical agents or external supports and have been successfully used in various industrial applications, such as natural gas dehydration and liquefaction, liquefied petroleum gas treatments and acid gas removal. They have also been used in seabed mining.

Various studies have demonstrated that supersonic separator technology can significantly contribute to reducing energy consumption and carbon dioxide emissions, thus improving the technical performance and exergy efficiency of industrial processes. Economic analyses have also shown significant financial benefits, such as increased net income and reduced investment compared to traditional natural gas treatment routes [43].

However, the technology has a high pressure loss. In the current context, where there is increasing emphasis on energy saving and emission reduction, the development of a supersonic separator with increased efficiency and the ability to handle a wide range of flow rates is required.

TRADITIONAL NATURAL GAS DEHYDRATION TECHNOLOGIES

Water is the most common impurity in natural gas and can cause several problems.

At low temperatures and high pressures, water can form hydrates that block pipelines and equipment, reducing gas transmission capacity and increasing energy costs.

Also, when water comes into contact with H_2S or CO_2, corrosive acids are formed that can lead to corrosion and damage to pipelines. For this reason, dehydration of natural gas is essential for safe transportation.

There are several methods for dehydration of natural gas:

Low-temperature condensation.

This takes advantage of the fact that water in natural gas decreases as temperature and pressure decrease. Simple equipment, such as a J-T valve or turbo-expander, is used to cool the gas. It is an efficient and economical method for high-pressure gases, but requires additional equipment for deep dehydration and inhibitors to prevent hydrate formation.

Solid adsorption: This method uses porous desiccants (such as molecular sieves) to adsorb water from the gas. Molecular sieves are very efficient and can reduce the dew point to extremely low temperatures (-100°C). However, this method has high costs, high energy consumption, and a high pressure drop.

Solvent Absorption:

In this method, a solvent with a high water absorption capacity, such as triglycol, removes water from the gas. This can reduce the dew point to -30°C, but the regeneration process requires a lot of energy and the equipment is large and expensive. It is more suitable for large natural gas treatment plants.

Each method has advantages and disadvantages, and the choice of the most suitable one depends on the characteristics of the gas and operational needs.

COMPARISON OF ALL GAS-LIQUID SEPARATION TECHNOLOGIES

Many gas-liquid separation technologies and equipment have been used in practical industrial applications. Each technology and equipment for separation has its own advantages and disadvantages, and they can only meet the separation requirements under relatively narrow working conditions.

Filtration separation, supersonic vortex separation and traditional natural gas dehydration technologies are suitable for fine separation, while other methods are more suitable for pre-separation.

Filtration separation has a low treatment capacity and high operating costs, so it is more suitable for small natural gas treatment plants.

Traditional natural gas dehydration is mainly used for cases requiring large-scale gas processing, such as gas gathering stations.

Supersonic vortex separation is a compact, low-cost technology, adaptable to various application environments, and has significant advantages in subsea or downhole production processes.

Inertial collision methods (such as the corrugated plate mist eliminator) are commonly used in the chemical industry and include wet desulfurization.

The flow field in a gravity separator is stable, which makes the separation system easy to control and reliable, making it the most widely used phase separator in oil fields, especially onshore ones.

However, resources in onshore oil fields are limited, and oil and gas exploitation is gradually moving to offshore fields and even deep sea.

In this context, large gravity separators are no longer used. Centrifugal separators and T-junction separators are compact and efficient, and are promising gas-liquid separation technologies for offshore platforms and subsea production systems.

However, these tubular separators have a short residence time and a highly unstable flow. Thus, achieving fast and stable control is difficult, which is the main obstacle to expanding their applications [3].

DRYING OF GASES BY ADSORPTION ON COMPOSITE MATERIALS WITH POROUS MATRIX

A significant part of recent research in the field of gas adsorption is focused on obtaining adsorbent materials with improved adsorption capacity and achieving high heat and mass transfer rates.

Extensive experimental studies on the physicochemical properties and several applications of composite materials used as adsorbents were carried out by Aristov, Liu and Wang and Zhang, respectively [5,6].

All their studies showed that these adsorbents have a higher adsorption capacity than the classical ones and can be regenerated at a low temperature.

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Thus, for the purpose of drying gases by adsorption, composite materials obtained by impregnating porous host matrices with hygroscopic inorganic salts were used.

As host matrices, silica gel in the form of spherical granules and granules of arbitrary shape (angular), activated alumina granules and activated carbon granules were used.

In the case of silica gel, the spherical granules had a diameter of 2.57 mm, and the angular ones, an average diameter of 2.25 mm.

The activated alumina granules and activated carbon had average diameters of 0.15 mm and 0.1 mm, respectively.

THE EFFECT OF DRYING GASES ON THEIR PHYSICO-CHEMICAL PROPERTIES

Following the controlled analysis of the gases that were treated, we created a numerical model based on artificial intelligence, which provides us with:

a. The higher calorific value as a function of pressure (X1-bar), standard volume V (X2-Sm^3), temperature T (X3, ºC) and gas composition (X4-methane, X5-ethane, X6-propane, X7-butane, pentane X8, X9-hexane-mol, %);

The equation obtained is of the form:

Y=0,0959493303+2,85616E-07 X1+7,11779E-10 X2+4,66504E-06 X3+0,103961843 X4+ 0,169664444 X5+0,568081755 X6+ 0,069168677 X7+0,416031709 X8+0,494161811 X9,

b. Very important is the determination of the standard density as a function of pressure (X1-bar), standard volume V (X2-Sm3), temperature T (X3, ºC) and gas composition (X4-methane, X5-ethane, X6-propane, X7-butane, X8-pentane, X9-hexane-mol, %);

In this case the error of the relationship is quite large but it is useful in engineering calculations.

Y=-6,74265-0,00062 X1+6,71E-08 X2-0,00032 X3+0,072654 X4- -0,57208 X5+12,54585 X6+ 8,914667 X7 + 1,104452 X8 -5,28813 X9

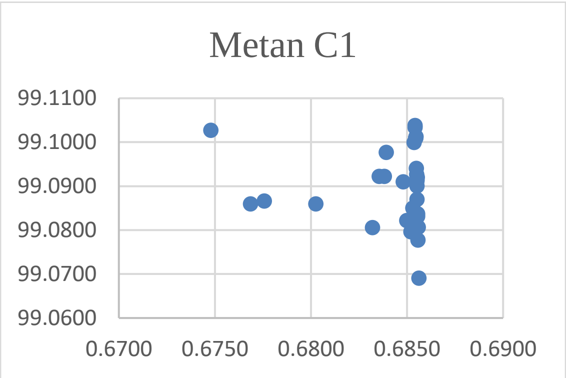

Fig.5. Density variation (kg/Sm^3) depending on methane content (mol, %).

CONCLUSIONS

Efficient and compact separators: For the future, research in the field of gas-liquid separation must focus on the development of compact, energy-efficient, stable and easy-to-operate separators. Theoretical and experimental studies, together with numerical simulations, will be essential in advancing this technology.

Complex separation mechanisms: Although theoretical and experimental research in the field has advanced considerably, the mechanisms of droplet collision, breakup and diffusion are influenced by uncertain factors, such as gas flow and droplet interactions. A thorough understanding of these processes will facilitate the development of accurate and efficient models of droplet breakup and coalescence.

Improved prediction models: Currently, empirical formula-based models are used to simulate gas-liquid separation, but these generate significant errors. A more detailed approach, which includes internal flow fields and phase distributions, is needed to improve predictions and optimize separator performance.

Drying process optimization: The use of neural networks and mathematical computation to determine the parameters of a natural gas drying station allows for accurate results, reducing the time required for analysis and operational costs.

These approaches facilitate the centralization and accessibility of data, contributing to the optimization of the drying process.

The importance of flow field level research: The measurement of macroeconomic parameters, such as flow rate and separation efficiency, is important, but detailed flow field level research, including droplet sizes and phase and velocity distributions, is also needed to validate and improve existing numerical models.

Sensitivity of separators to operational parameters: Gas-liquid separators are sensitive to operational parameters, and effective control strategies are required to ensure fast and stable control of the separators. An optimized approach to the overall separation system will contribute significantly to improving process performance.

Innovative Adsorption Materials: Composite materials impregnated with hygroscopic inorganic salts have demonstrated superior moisture removal capacity from natural gas compared to classical adsorbents. This represents a promising direction for improving the efficiency of the natural gas treatment process.

Accuracy of mathematical models: The mathematical models developed to estimate the properties of the treated gases provided high accuracy, such as the relationship for the higher calorific value of natural gas, which demonstrated an excellent correlation between the analyzed variables (R^2 of 0.9998).

Development of energy-efficient separators: Future research should focus on improving gas-liquid separators to reduce uncertainties related to the collision and coalescence phenomena of liquid droplets. A better understanding of these mechanisms will lead to the development of more efficient and accurate solutions for gas-liquid separation.

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