SUPERSONIC SEPARATION: NATURAL GAS CONDITIONING CASE STUDY

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Abstract: Natural Gas (NG) is an important vector in the world energy matrix, playing a fundamental role in the fuels and energy generation in Brazil, therefore the development and application of new technologies to produce gas becomes critical. In this context, supersonic separation has become a viable alternative for gas conditioning because it requires less installation space and consumes less energy in the process, with its geometry as the main driving force. Therefore, the objective of this paper is to describe a supersonic separation case study for natural gas conditioning, from the separation mathematical modeling of water, heavy hydrocarbons and CO_2 from natural gas, using Visual Studio software which can be integrated with Aspen Hysys through the customize option. According to literature data and tests using different NG compositions, the modeling was validated. A CO_2 capture efficiency of ~60 % relative to the input and a purity of 83 % (mol) in the conditioned natural gas stream was achieved.

Keywords: natural gas conditioning, supersonic separator, carbon capture, modeling.

SEPARAÇÃO SUPERSÔNICA: ESTUDO DE CASO DE CONDICIONAMENTO DE GÁS NATURAL

Resumo: O Gás Natural é um importante vetor da matriz energética mundial, portanto torna-se crítico o desenvolvimento e aplicação de novas tecnologias para condicionar o gás produzido. Nesse contexto, a separação supersônica vem se tornando uma alternativa viável para o condicionamento do gás pois necessita menos espaço para instalação e menos energia no processo, tendo como força motriz a sua geometria. Portanto, o objetivo deste trabalho é apresentar um estudo de caso da separação supersônica para o condicionamento do gás natural, a partir da modelagem matemática da separação da água, hidrocarbonetos pesados e do CO_2 do gás natural, utilizando o software Visual Studio que pode ser integrado ao Aspen Hysys através da opção *customize*. A modelagem foi validada de acordo com dados da literatura e testada para diversos perfis de composição do GN. Foi obtida uma eficiência de

aproximadamente 60 % de captura de CO_2 em relação a entrada e obteve-se uma pureza de 83 % (mol) na corrente de gás natural condicionada.

Palavras-chave: condicionamento de gás natural, separador supersônico, captura de carbono, modelagem.

1. INTRODUCTION

Currently, the main transition route to an energy matrix with lower carbon emission levels is through natural gas (NG), but the sustainability and viability of this route depends mainly on the technologies for CO_2 capture and use [1]. The primary process of exploration and production usually generate a NG with impurities such as water, heavy hydrocarbons, carbon dioxide, and hydrogen sulfide. The presence of these contaminants can cause a reduction in the calorific value of the gas and energy loss increase during pipeline transport, as well can cause pipelines and process equipment corrosion [2]. Therefore, due to the demands for NG around the world, there is a growing motivation for developing NG conditioning technologies.

NG conditioning is an important process in the NG production chain, which usually comprises a set of operations that depend on its composition and conditions, such as: (a) H_2S removal; (b) water dew point adjustment – WDPA via dehydration; c) hydrocarbons dew point adjustment and (d) CO_2 removal [1]. However, although these operations guarantee product quality, they demand high energy consumption, especially for CO_2 removal.

The CO_2 removal from NG is one of the most important steps in the natural gas industry, and the most common technologies are absorption, adsorption, membrane permeation and supersonic separation [2]. Table 1 lists the advantages and disadvantages of the main gas separation technologies. The selection of CO_2 separation technology in a Floating Production Storage and Offloading (FPSO), should consider the following characteristics: (a) CO_2 content in untreated and treated gas; (b) treatment capacity; (c) operating costs; (d) investment costs; (e) occupied area; (f) weight of the equipment and mainly, for sustainability reasons, (g) the technology environmental performance [1].

Table 1 - Advantages and disadvantages

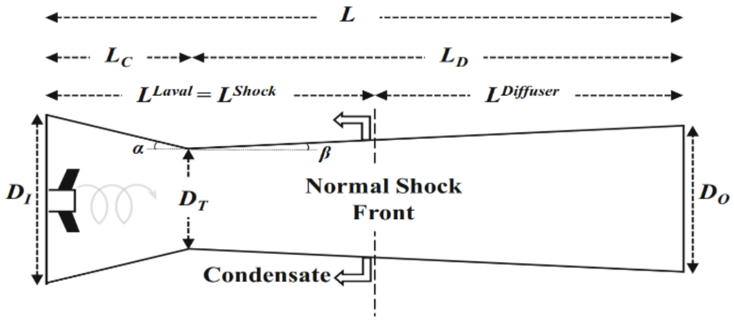
Technology	Advantages	Disadvantages
Absorption	CO_2 absorption high capacity; Flexible capacity; Easy regeneration solvent;	CO_2-rich NG there is a high rate of solvent and heat recirculation for regeneration; CO_2 extracted at low pressure requiring large compression trains for EOR; Low CO_2/CH_4 selectivity, implying high hydrocarbon losses along with the CO_2 product stream;
Adsorption	Suitable to be associated with cryogenic separation;	High investment: High pressure drop requiring large compression trains for EOR; Not applicable for high CO_2 concentration flow;

Membrane permeation	Flexible with respect to the CO_2 content of the feed; Simple process; Occupies less space; Easy scaling.	High % CO_2 implies high permeation area and high hydrocarbon losses; Low pressure CO_2 requiring a large compression unit for EOR; Large hydrocarbon loss; For high CO_2 content energy consumption is higher;
Supersonic separation	Unique modularity; More robustness; Avoids the hydrate generation; Short residence time; Occupies less space; Better separation efficiency; Gas and condensate capture;	Little applied in the area of natural gas conditioning;

The supersonic separation consists of expanding the fluid at supersonic speeds through a convergent-divergent nozzle, resulting in a large pressure and temperature drop, promoting condensation of heavier species than NG, such as water and C_3^+ hydrocarbons. Thus, SS technology is composed of hydrocarbon dew point adjustment and gas dehydration, condensing and separating water and heavy hydrocarbons [2]. The supersonic separator refers to a combination of a turbo-expander, with a cyclone separator and a compressor for gas recompression [3], and the equipment efficiency is related to the cooling properties of the convergent-divergent nozzles with the centrifugal separation principles [4].

The supersonic separation mathematical modeling developed was based, mainly, on [1], book with several approach about natural gas processing with supersonic separation and other publications like [5] and, with regard the sound speed calculation, was used the procedure presented by [6]. In addition to these references, were proposed some modifications and optimizations mapped by the SENAI CIMATEC and Petrobras during the developing, validations and tests of the calculation module, based on [7], [8] and [9]. Figure 1 shows a typical Supersonic Separator representation.

Figure 1 – General schematic of an supersonic separator. Source: [1]



Where: D_I is the inlet diameter (m), D_T is the throat diameter (m), D_o is the outlet diameter (m), L_c is the convergent nozzle length (m), L_D is the divergent nozzle length (m), $L_{difusor}$ is the diffuser length (m), L_{shock} is the shock length (m), L is the total length of SS (m), α is the convergent nozzle angle and β is the angle of the diverging nozzle.

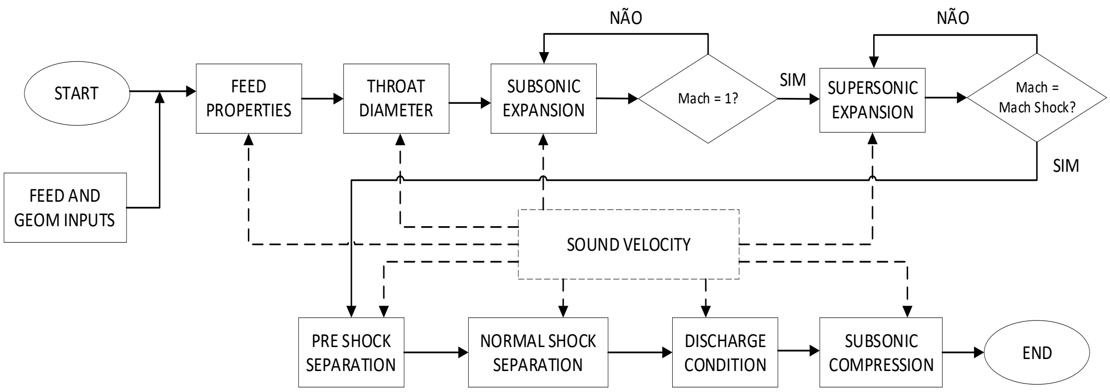
In the supersonic separator, the feeding goes through the converging nozzle, L_C, initiating acceleration/expansion at subsonic speed with Mach < 1 and successive isentropic compressions. Then, the sound speed is reached in the throat with Mach = 1, and goes at the diverging nozzle (L_D) with Mach > 1, characterized by successive isentropic expansions. In the end, there is a CH_4 rich gas stream and a condensate stream.

This paper aims to present the modeling and simulation of supersonic separation for carbon capture from a typical natural gas stream. For the supersonic separation simulation was used a Unit Operation Extension (UOE) in Aspen Hysys™. The UOE is a programming unit in Visual Studio which can be integrated at Aspen Hysys by the customize option. The supersonic separation module was developed in the research project at SENAI CIMATEC with Petrobras.

1. METHODOLOGY

In this section, the supersonic separator calculation modules are described, such as sound velocity, inlet properties, throat diameter, modules for subsonic and supersonic expansions, separation and shock modules, calculation of discharge conditions, and subsonic compression. In the customize option, is possible to use a HYSYS functions to calculate a supersonic separation, like an isothermal and isentropic flashes, and process stream thermodynamic properties. For the simulation was adopted Peng Robinson thermodynamic model because it is the most indicated model due to the hydrocarbons presence. The mathematical modeling general flowchart of the supersonic separator is shown in Figure 2.

Figure 2 - SS mathematical modeling general flowchart. Source: SENAI CIMATEC (2022).



With the feed stream input data - pressure, temperature, molar flow and components mole fraction of natural gas, and some data of the equipment geometry - inlet and outlet diameter and convergent and divergent sections length, and the Shock Mach number, is possible to apply the sound speed calculation module, which is used in the inlet stream properties and throat diameter, in the subsonic and supersonic expansions calculation modules, in the pre- and post-shock separations modules and in the discharge conditions and subsonic compression. The sound speed calculation module receives data as pressure, temperature, molar flow rate, composition, density and entropy and uses the central derivative method and isentropic flash to determine the gas density at different pressure, and then is possible to calculate the sound speed (Equations 1 and 2).

$$EEP = \frac{(DEN_1 - DEN_2)}{2dP} \quad (1)$$

$$C = \frac{1}{\sqrt{EEP}} \quad (2)$$

The input stream and geometry data are inserted in **feed properties** module by the user to determine the sound speed, mass flow rate, fluid speed, kinetic and total stream energies and Mach number at supersonic separator inlet. Then, from the feed properties determination, the SS **throat diameter** is calculated using the secant method. With the throat diameter, the **subsonic and supersonic expansion** module are calculated. In both module N iterations are executed and each is associated with the longitudinal position calculation (x) of the supersonic separator length, which in turn is associated with a Mach number of the fluid and specific diameter of the SS. The **subsonic expansion** is completed when the calculated Mach number is equal to 1 and the calculated diameter coincides with the already determined throat diameter. The **supersonic expansion** refers to the region between the throat and the shock position, when the calculated Mach number is equal to the Mach number at shock (input data provided by the user). At this point, the gas properties in the shock (temperature, pressure, velocity, diameter, and position) are determined. In **Pre-Shock and Normal Shock Separation** modules, the stream conditions before and after shock are determined, when is verified the gas and condensed phases separation. With the current conditions after shock, the **discharge conditions** are determined and, finally, is calculated the **subsonic compression**, which comprises compression successive in the region between the separation and the final length of the separator.

2. RESULTS AND DISCUSSION

From mathematical modeling implemented in Visual Studio in association with Aspen HYSYS, supersonic separation was validated using cases reported by [7], [8] and [9]. Based on the geometry data provided in the literature, a case study was developed with a natural gas composition supplied by a Brazilian oil and gas company. From this initial input, the simulation was done according for the values of T, P, Mach number, L_c, L_d, D_i and D_o, to drive convergence or optimize the modeling. Thus, Table 2 presents the data collected from the literature and the data determined in the convergence and optimization of the supersonic separator simulation. Then, the SS geometry data obtained by simulation were: Convergent Angle (º): 10.91, Divergent Angle (º): 1.06, Mach Nº (inlet): 0.2851, Throat Area (m^2): 0.006, Shock Pressure (bar): 14.00; and Shock Temperature (ºC): 75.61.

Table 2 – Geometry parameters from literature and simulated.

Parameters	Arina [7]	Wen et al. [8]	Arinelli et al. [9]	Wen et al. [10]	This work
D_i (m)	0.01784	0.13	0.13	0.12	0.13
D_s (m)	0.01382	0.13	0.13	0.09	0.13
L_c (m)	0.05	0.10956	0.10956	0.14980	0.1095

L_d (m)	0.05	0.56481	1.14423	0.52430	1.1442
Mach *shock*	1.50	2.02	2.00	2.00	1.80

Table 3 shows the inlet current conditions for the supersonic separation simulation, as well as the gas and condensate conditions obtained from the simulation.

Table 3 – Inlet and outlet stream conditions.

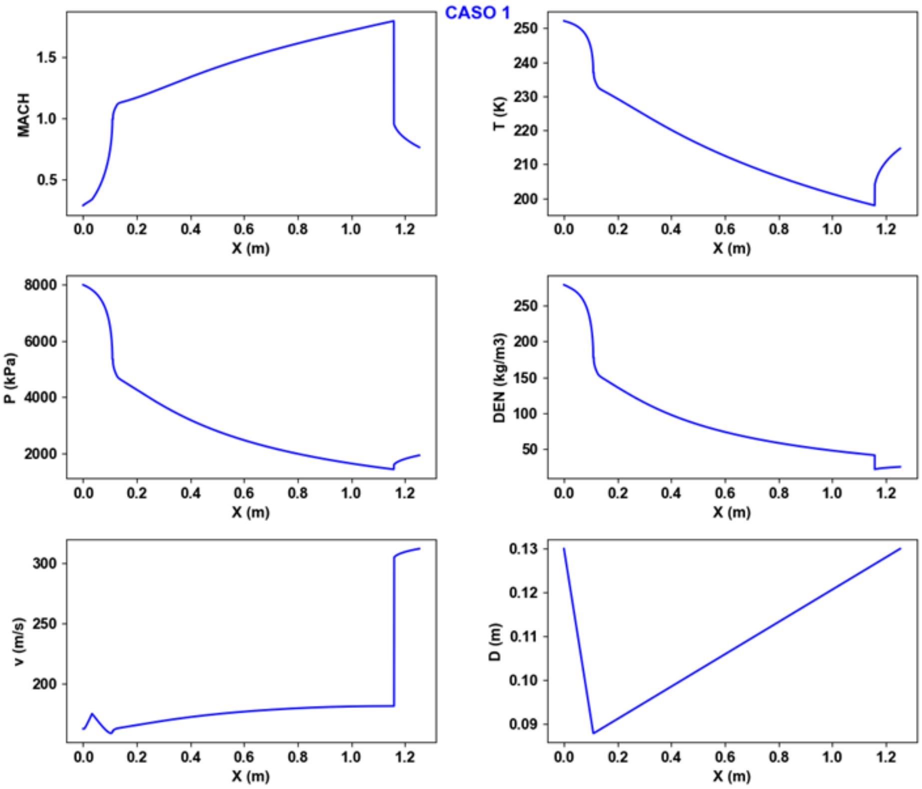
Streams	**T (ºC)**	**P (bar)**	**Flow rate (kmol/h)**	**Molar composition (%)**
Inlet	-21.00	80.00	23,000.00	58.58 CH_4; 20.24 CO_2; 2.16 H_2O; 0.017 H_2S; 0.50 N_2; 3.85 C_2H_6; 0.40 C_3H_8; 2.55 Heavy HC's
Gas	-59.70	18.67	14,270.00	82.14 CH_4; 13.06 CO_2; 0.00002 H_2O; 0.01 H_2S; 0.32 N_2; 8.72 C_2H_6; 5.58 C_3H_8; 0.036 Heavy HC's
Condensate	-59.23	18.67	8,728.00	20.06 CH_4; 31.99 CO_2; 5.70 H_2O; 0.04 H_2S; 0.02 N_2; 16.68 C_2H_6; 14.05 C_3H_8; 11.46 Heavy HC's

Figure 3 shows the behavior of Mach number, temperature, pressure, density, velocity, and diameter along the supersonic separator according to iterations developed in the mathematical modeling of the SS, using the inlet data presented in Table 3.

From the Mach number plot, it is possible to observe that the SS throat diameter (Mach = 1) is located approximately 0.1m from the inlet, which is the length of the SS converging section. This region (convergent section) is characterized by subsonic expansion, where there is mainly a decrease in fluid temperature and pressure.

The divergent section, where the supersonic expansion occurs, is represented by the region between 0.1 and 1.15 m. In this section there is a significant increase in Mach number, an abrupt reduction in temperature and pressure, and Mach number between 1 and 1.8 (Shock Mach). The location where the shock occurs, 1.15 m.

Figure 3 - Supersonic separator performance. Source: SENAI CIMATEC (2022).



From the results obtained, was found that a good separation of the components occurred. The gas phase concentrated mainly methane (82.14%) and the condensed phase concentrated CO_2, water, heavy hydrocarbons, some methane, and other impurities. The CO_2 capture rate achieved by SS in the condensed phase was approximately 60% relative to the CO_2 content present in the inlet stream. However, when analyzing the purity of the generated streams in relation to the gas (CH_4) and the condensate (CO_2) and possible uses for them, may be necessary to adopt purification processes or another SS. Regarding the energy demand for separation, SS has advantages because it only requires electrical energy for input gas compression.

4. CONCLUSION

A Supersonic Separation is an innovative technology that is still maturing. From the energy point of view, this technology has a significant advantage because the driving force is the equipment geometry. The opportunity to use SS to conditioning NG represents a differential, because involves both CO_2 capture and the removal of water and heavy hydrocarbons. Other opportunities for the application of SS should be analyzed in future works, highlighting the potential for this technology application.

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