Instituto Alberto Luiz Coimbra de
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COPPE UFRJ

EVALUATING STRATEGIES FOR MONETIZING THE NATURAL GAS SUPPLY IN BRAZIL - THE ROLE OF STORAGE, LIQUID PROCESSING AND CONVERSION TO HYDROGEN

Ricardo Moreira dos Santos

Tese de Doutorado apresentada ao Programa de Pós-graduação em Planejamento Energético, COPPE, da Universidade Federal do Rio de Janeiro, como parte dos requisitos necessários à obtenção do título de Doutor em Planejamento Energético.

Orientadores: Alexandre Salem Szklo
André Frossard Pereira de Lucena

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TESE SUBMETIDA AO CORPO DOCENTE DO INSTITUTO ALBERTO LUIZ COIMBRA DE PÓS-GRADUAÇÃO E PESQUISA DE ENGENHARIA DA UNIVERSIDADE FEDERAL DO RIO DE JANEIRO COMO PARTE DOS REQUISITOS NECESSÁRIOS PARA A OBTENÇÃO DO GRAU DE DOUTOR EM CIÊNCIAS EM PLANEJAMENTO ENERGÉTICO.

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DEDICATÓRIA

Às professoras
Virgínia Gomes e Sara Kalil,
que me ensinaram, lá no ensino básico,
a beleza de aprender Português e Matemática
e abriram uma imensidão de possibilidades na minha vida

“É necessário conservar o espírito imaculado e aberto;
e a sabedoria, dentro de amplos horizontes.
E é essencial polir tanto a sabedoria quanto o espírito.”

Miyamoto Musashi

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AVALIAÇÃO DE ESTRATÉGIAS PARA MONETIZAÇÃO DA OFERTA DE GÁS NO BRASIL- O PAPEL DA ESTOCAGEM, DO PROCESSAMENTO E DA CONVERSÃO A HIDROGÊNIO.

Ricardo Moreira dos Santos

Setembro/2021

Orientadores: Alexandre Salem Szklo

André Frossard Pereira de Lucena

Programa: Planejamento Energético

A tese define três estratégias de monetização das reservas de gás natural (GN) no Brasil e é dividida em três artigos, dois publicados e um submetido para avaliação. No primeiro artigo, submetido, opções de processamento de GN foram avaliadas comparando a produção de combustíveis ou petroquímicos. Uma unidade de processamento GN foi projetada usando o software "DWSIM" e foi realizado um cálculo de VPL estocástico. Foi realizada uma avaliação de mercado para avaliar as principais barreiras nessa área. O segundo artigo, publicado, avalia a custo-efetividade da estocagem subterrânea de GN para rentabilizar recursos de gás natural *onshore*. Gasodutos foram projetados usando o software Pipeline Studio. O terceiro artigo, publicado, trata da transição energética por meio do uso de H_2 azul produzido por reforma a vapor do metano (SMR). Partindo de previsões de produção de GN avaliou-se a produção potencial de H_2 e elaborou-se uma estratégia para estimular o mercado de H_2 usando as capacidades ociosas de reforma e de transporte de gás natural. Os resultados mostram que as três estratégias podem eventualmente ser associadas e produzir resultados positivos. A produção de líquidos é viável tanto para combustíveis quanto para petroquímicos. O teste de mercado indica desafios para petroquímicos no Brasil, no entanto. A estocagem subterrânea é uma opção viável para o desenvolvimento da indústria de GN, oferece redução de custos e tarifas no projeto de dutos, sendo relevante para a formação de hubs. Finalmente, a produção de hidrogênio azul parece possível quando o CO_2 gerado nas instalações de SMR são usados para estimular a produção de petróleo com recuperação avançada de petróleo. Embora essas estratégias tenham apresentado resultados promissores, as condições institucionais no Brasil mudaram recentemente e devem ser analisadas antes de considerar investimentos.

Abstract of Dissertation presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Doctor of Science (D.Sc.)

EVALUATING STRATEGIES FOR MONETIZING THE NATURAL GAS SUPPLY IN BRAZIL - THE ROLE OF STORAGE, LIQUID PROCESSING AND CONVERSION TO HYDROGEN

Ricardo Moreira dos Santos

September/2021

Advisors: Alexandre Salem Szklo

André Frossard Pereira de Lucena

Department: Energy Planning

This thesis defines three strategies for monetizing natural gas reserves in Brazil and it is divided into three papers, two published and one submitted. In the first paper, submitted, Natural Gas processing options were assessed by comparing fuel or petrochemical options. A natural gas processing unit was designed using the open-source software “DWSIM” and a financial stochastic net present value was calculated. In the end a market crash evaluation was performed based on the main barriers in this field. The second paper, published, evaluates the cost-effectiveness of Underground gas storage facilities as strategy to monetize onshore natural gas resources. Gas pipelines were designed using the software Pipeline Studio by Emerson. The third paper, published, develops a strategy for transitioning from fossil fuels to hydrogen, based on the use of blue hydrogen produced in Steam methane reforming process. A global strategy applying natural gas production forecasts assessed potential hydrogen production and addressed a strategy for stimulating the hydrogen market using idle capacity and natural gas transport capacity. Findings show that the three strategies can be associated and produce positive results. Natural Gas Liquids strategy is feasible for both fuels and petrochemicals. The market crash test indicated sever restrictions for petrochemicals in Brazil, tough. UGS facilities are feasible options for developing the NG industry and offer costs and tariff reduction when designing pipelines and are relevant for hub formation. Finally blue hydrogen production seems possible when CO_2 generated in Steam Methane Reforming facilities are used in Enhanced Oil Recovery. Although these strategies showed promising results, institutional conditions in Brazil have recently changed and need evaluation before considering investments.

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ABIQUIM – Associação Brasileira da Indústria Química

ABEGAS - Associação Brasileira de Distribuidoras de Gás Canalizado

ANP –Agência Nacional do Petróleo, Gás Natural e Biocombustíveis

CX+ - Hydrocarbon with X atoms of carbon. The symbol + indicate “X or more than X atoms”.

CCS – Carbon Capture and Storage

CAPEX - Capital Expenditure

DCF - discounted cash flow

EOR– Enhanced Oil Recovery

EIA – U.S. Energy Information and Administration

GASBOL – Bolivia-Brazil pipeline

GBM - Geometric Brownian motion model

GHG - Greenhouse Gases

GNA – Gás Natural Açu

IEA - International Energy Agency

LPG - liquefied petroleum gas

NG– Natural gas

NGL - Natural gas liquids

M BTU – Millions of BTU

M m^3/d – Millions of cubic meters per day

NPGU – Natural gas processing unit

NPV – Net Present Value

OPEX - Operational expenditure

MME – Ministério de Minas e Energia (Brazil)

PETROBRAS - Petróleo Brasileiro S.A.

PR - Peng-Robinson thermodynamic package

SRK - Soave-Redlich-Kwong thermodynamic package

SMR – Steam Methane Reforming

TAG – Transportadora Associada de Gás S.A.

TBG – Transportadora Brasileira Gasoduto Bolívia-Brasil S.A.

UGS – Underground Gas Storage

USA – United States of America

WTI - West Texas Intermediate

1 Introduction

Monetizing natural gas resources is a challenging subject that intertwines a complex chain of events for producing and trading gas derivates [1] [2] [3] to reach final consumers [4] [5], and that can be hampered when the processing and transporting infrastructure is poorly-developed. Investments in infrastructure are high and revenues from natural gas are usually lower when compared to oil [6] [7], thus not seldom producers opt for flaring or reinjection [8] [9]. Natural gas is a highly cost-intensive industry and presents irreversible fixed costs [10], meaning that hardly can these assets be used for other purposes than originally planned. In addition, delivery contracts are signed for long-term, especially when the expansion of the gas transport network is needed [11], even though the fuel market is uncertain [12]. Such set of issues may result in elevated prices and disengage investors from this market. For this reason, transporters and traders look for protection margins, usually indexing gas prices to oil in sales contracts [10] [13]. A review on the natural gas monetization literature corroborates these statements and shows a number of qualitative studies on natural gas monetization challenges [14] [15] [16] [17] [18].

There are also studies on monetizing stranded or remote gas resources that focus on the process engineering assessment of specific technologies, for example simulating the process associated with gas-to-liquids or liquefaction facilities in remote gas reservoirs [19] [20]. However, these studies do not expand their analysis to evaluate how the technologies they assessed can change the energy planning as a whole, or in a systemic way. In this case, some options deserve special attention.

This study addresses three different approaches of the relevant issue of monetizing natural gas resources: producing natural gas liquids; planning underground gas storage and pipelines; and facing the energy transition challenges departing from the conventional steam methane reforming process. Firstly, natural gas processing by outputting valuable liquids can reduce the break-even price of the gaseous fractions of the raw gas, and establish a diversified market (including petrochemicals and liquid fuels) to this primary source. Additionally, storage can optimize gas pipelines networks and help to deal with seasonal markets related to thermal or electric power supply. Finally, the conversion of natural gas into hydrogen has been seen as a relevant strategy to cope with an energy transition that aims the decarbonization of the energy system.

Those analyses are developed according to different time frames, locations and emphasis. While NGL and H_2 approaches focus on diverting from the conventional energy use of NG, planning a pipeline infrastructure can be associated to any use of natural gas, including its conventional energy use. Moreover, those approaches are based on a broad mix of technological options, from proven technologies such as high-pressure pipelines to technologies yet to be consolidated, such as carbon capture and storage (CCS).

However, the pivotal challenge of developing infrastructure pervades and unites the approaches. Uniting the different perspectives, the use of existing and planning infrastructure is regarded in this study a key factor to define strategies for natural gas monetization. Those strategies can be combined into a larger planning for optimizing the use NG resources. In fact, when included under the same framework, those approaches reveal that decision makers simultaneously face the challenges of producing natural gas, processing it, storing NG products and meet market demands under the current energy transition that aims to decarbonize the economy.

Natural Gas Liquids (NGL)

Natural gas processing yields two basic streams: lean natural gas and natural gas liquids - NGL [21]. A NGL hub requires a concentration of physical assets that connect to supply and demand sources via different transport, storage, and distribution options [22].[1]

Inasmuch as unconventional and deep-water reserves exploitation advances, rich gas production increases [23] [24] and natural gas liquids become more relevant for oil and gas industry [25] [26]. Rich natural gas resources often occur associated with oil in deep waters or shale formations and high calorific gases may damage pipelines and bring interchangeability issues [27].

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[1] It should not be considered coincidence that the Mont Belvieu NGL hub began in the 1950's with underground storage facilities [22].

A variety of process schemes have been developed over the years for obtaining the best processing route, and process simulation is a valuable tool for evaluating technical outputs [28]. Rich gas streams have strong influence in the plant profile [29], and defining schemes for gas processing is worth for decision makers to choose between producing options. Depending on the main objective of the supply chain, and the input raw material, a more complex or simple technology may be applied in gas processing plants [21]. In general, two kinds of liquid products are obtained from natural gas processing beyond the gaseous fraction: fuels and/or petrochemical feedstocks [21].

Establishing bold strategies for producing NGL is a prospective approach to monetize remaining natural gas resources. In this case, it can be relevant to investigate the use of heavy fractions of natural gas as petrochemicals feedstocks. Particularly, petrochemicals, when inserted into long-lasting materials production chain, can store carbon for a long period and become a strategy to change the way gas is used under deep decarbonization scenarios [30] [31]. Notwithstanding, some authors highlight the risk of reaching a carbon lock-in[2] even using natural gas as a petrochemical feedstock [32]. This concern is partly corroborated by Kapsalyamova and Paltsev [33], which indicate that deep decarbonization scenarios would also affect the use of natural gas and oil as fuel and feedstock. However, other authors stress that NGL are valuable products obtained from raw natural gas, and processing it might also prevent flaring [34]. Even conservative projections concerning fossil fuels indicate that NGL should play a relevant role in the future [35].

At the end, for evaluating those different perspectives, economic assessments are needed to support decision makers aiming at selecting between alternative production routes for maximizing the NGL value in the natural gas supply chain [30]. In this case, stochastic analyses can help dealing with uncertainties and the geometric Brownian motion (GBM) [36] is considered an efficient mathematical method for evaluating commodity prices variation, such as natural gas.

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[2] The concept of carbon lock-in evaluates that the existing interlinked infrastructures, technologies, norms, policies, and institutions supports world dependence on fossil resources and creates a strong inertia against most forces aiming to break free from it [359]

Underground gas storage (UGS)

Notwithstanding the importance of NGL, which were mentioned above, the natural gas industry strongly relies on its lighter gaseous stream. Transporting and delivering natural gas to customers is a paramount yet costly task in this industry. Deploying flexible and interconnected networks is essential for improving natural gas market [37], and reaching customers through an adequate infrastructure [38] is an essential asset for natural gas industry [39], mainly for resource-rich developing countries [40] [41]. Once processed, natural gas producers should meet final demands, which requires long-term planning and policy measures that favor physical connections [42].

In this case, underground gas storage (UGS) can be a key feature for reaching these goals [43]. Interestingly, the natural gas demand can be strongly affected by intermittence. For instance, peak shaving is one of the main advantages of UGS facilities. UGS normalize daily supply, meet seasonal demands, define strategic reserves and offer services like parking, capacity trading and interruptible storage [44]. In temperate countries, seasonal variation increases gas demand for heating in the winter, while in tropical regions, seasonal effect is associated with rain shortage in the winter leading to the dispatch of natural fueled-thermal power plants that complement hydropower facilities [45]. In addition, gas-fired thermoelectric plants often operate as peak shaving supplier [46] in electricity generation systems, as they have relatively short-time response to meet demands, being able to address intermittent peaks. Gas-fired plants affect the operation of natural gas networks, since they require immediate gas availability when dispatched [47]. Natural gas pipelines need to meet these sudden demands, and without UGS facilities chances are that gas network expansion will be based on oversized pipelines, or pipelines will be challenged by peaking demands. For instance, Yu et al [43] highlight that UGS is a necessary facility to meet such variations. When a UGS facility is not available, the natural gas carrier will usually rely on regasification installations to deal with liquefied natural gas (LNG) imports [48]. In a natural gas producing country, this is not a desirable condition, since importing NG can displace producing it.

UGS facilities require medium-term planning and investments [49], but once installed, they demand low maintenance costs [50]. However, few studies have already evaluated the gas network expansion planning with UGS [51].Therefore, the natural gas infrastructure long-term planning should consider the coordination of gas pipelines with UGS as a way to optimize the gas network, avoiding idle capacity or oversized grids.

Natural gas to hydrogen conversion (with associated carbon capture)

A contemporary scientific study should not overlook the fact energy use is changing worldwide. The fossil fuels industry may be severely restricted in the next decades by decarbonization targets [52]. Moreover, emerging countries may be penalized for delaying action [53], despite the principle of common but differentiated responsibilities [54].

Sometimes regarded as the fuel of the energy transition by different studies, natural gas may lose this place [55] if carbon emissions are not mitigated [56] [57]. Actually, some authors warn that greenhouse gases (GHG) emissions already reached unacceptably high levels that do not meet the Paris Agreement [58] [59], [60], [61] [62], [63]. Therefore, the fossil fuels phase-out should be steadfast to meet environmental goals and cope with climate change effects [52]. This means that replacing coal by natural gas would not be enough for a low-carbon economy [64]

The idea of converting natural gas into hydrogen and capturing the CO_2 emitted by this process can be an option for both paving the way for a clean economy based on hydrogen and extending the use of natural gas: on the one hand, hydrogen can be key in deep decarbonization scenarios [65] [66] [67] [68] [69]. On the other hand, the state of art of hydrogen technology indicates that the steam methane reforming (SMR) has the lowest cost when compared to other routes, and is already extensively used [70] [71] [72]. Actually, as of today, almost all the produced H_2 comes from fossil fuels [65], being SMR the major source of H_2 [73]. Therefore, although scaling up to a large and sustainable hydrogen production would require a diversity of processes [74], the SMR with carbon capture and storage is a proved and competitive concept [75] [76] [77] [78]. This blue H_2 may be an option to monetize natural gas resources, while bridging towards a low carbon economy [79][3]. It can reduce CO_2 emissions in up to 90%, if applied to

[3] In this analysis we consider Blue H_2 when thermochemical conversion of fossil fuels is compensated with carbon capture and storage techniques.

process and energy CO_2 emission streams [80]. Besides, in the short term, hydrogen transportation and storage can benefit from the use of the existing natural gas infrastructure by blending H_2 volumes in gas pipelines [67], [81]. This is a low-cost strategy for short-term production [69], [82]. Therefore, transitioning from the current intensive use of fossil fuels to renewables and to renewable hydrogen can benefit from the conversion of natural gas to hydrogen.

The *Brazilian Case*

Energy transition may produce wide impacts in emerging countries. In order to avoid losses from the energy transition process, countries that rely on fossil fuel revenues should prepare themselves to both diversify their economy away from fossil fuel resources [83] and optimize the use of these resources from now on.

Actually, under deep decarbonization scenarios [84] [85] the global natural gas market will plummet [86] [87]. This fact raises a dilemma between the green paradox and divestments [88], where the former induces anticipated investments on fossil fuel supply to avoid losses in the future. However, the stronger are the policies to prevent greenhouse gas (GHG) emissions, less encouraged will the investors on fossil fuels be to anticipate production. Hence, the risk of not exploring and extracting remaining resources rises [88]. This can be particularly challenging for petroleum frontier countries, which is the case of Brazil.

Brazil is a continental country relying on large remaining offshore – mostly associated – resources [89]. It also has technically recoverable shale gas resources [90]. Brazil has an insufficient and, until recently, verticalized [23] [91] infrastructure to monetize the gas [92, 93]. It also has a complex but changing regulation [94] [95, 96], and a poorly-developed internal market [97] [98] [99]. The increasingly fragile industrial market accounts for the highest firm demand, while the electric power sector is responsible for large annual variations of gas consumption, being affected by the hydropower dispatch [100]. There are no commercial UGS facilities in Brazil. Thus, when natural gas carriers must cope with seasonality, they mainly rely on regasification installations and liquefied natural gas (LNG) imports. However, this costly and risky strategy [48] is hardly justifiable especially in the case where most of the natural gas production is associated with crude oil (meaning that its production is explained by the crude oil supply). Brazil imports nearly 40 million cubic meters per day (M m^3/d) and reinjects 58 M m^3/d for supplying 90 M m^3/d to internal market; half of these imports come from LNG facilities [101].

Interestingly enough, Brazil already has a relatively high hydrogen production capacity based on SMR (**Table 1**), meaning that, especially in idle-production hydrogen units in oil refineries, there is a starting point for deploying a strategy based on methane-to-hydrogen conversion.

Table 1: H_2 production capacity in Brazil.
Elaborated with data from [102] [103] [104] [105] [106] [107] [108] [87]

Facility type	Capacity kt H_2/y
SMR in petroleum refineries	695
Catalytic reform in petroleum refineries	4
Petrochemistry	70
Na-Cl facilities	46
Fertilizers	549
Methanol	0
Total	**1364**

Objective of the Thesis

The present work has the global objective of proposing and applying combined methods for evaluating strategies to monetize natural gas resources under infrastructure constrains. This main objective of this thesis was divided into three major research questions that led to the preparation of three scientific papers, as discussed below.

a) *Managing rich natural gas resources and heavier fractions*[4]

The first research question investigates feasible strategies for monetizing rich natural gas resources through gas processing. The hypothesis is that natural gas processing is a feasible strategy in Brazil to deal with richer streams and the focus on petrochemicals might present a better economic performance, when compared to the focus on liquid fuels. However, market barriers can hamper this strategy. To address this research question, technical tools (process engineering), financial evaluation (probabilistic discounted cash flow analysis) and a qualitative assessment of market conditions (market failure analysis) are applied.

[4] Journal of Natural Gas Science and Engineering. Submission JNGSE-S-21-01497-2

These simulations considered different natural gas compositions in an open-source process simulation tool. Based on the obtained results (technical and financial analyses), the limitations to the assessed strategies are discussed, according to three pillars: infrastructure, market structure and regulatory framework.

b) Planning the expansion of high-pressure natural gas pipeline networks, with the inclusion of underground storage[5]

The second research question deals with a lacking and ill-connected infrastructure, and tests whether the natural gas transportation network expansion with Underground gas Storage (UGS) leads to the best solution in the case of Brazil. The hypothesis is that UGS can reduce transportation costs by better fitting natural gas supply and demand. To do so, a thermo-hydraulic tool is applied to evaluate bottlenecks in an existing natural gas transport network in Brazil, and propose solutions by expanding the grid with UGS.

c) Blue H_2: paving the way to hydrogen in Brazil by converting natural gas to hydrogen[6]

The third research question evaluates strategies that offer feasible options to emerging countries to both explore fossil resources and cut GHG emissions to avoid large volumes of stranded fossil fuel reserves and foster development. Therefore, a stepwise strategy to enhance the production and use of hydrogen is developed, starting from natural gas resources and installed capacities to produce blue hydrogen aiming at paving the way to an independent H_2 industry. Departing from the assessment of existing capacity for producing hydrogen in Brazil, potential future hydrogen production is calculated based on natural gas forecasts and a strategy that allows a medium-term transition from grey hydrogen to blue hydrogen is proposed. Moreover, carbon emissions generated in the idle capacity of existing SMR plants can stimulate oil production through enhanced oil recovery, thus obtaining extra revenues that can improve the feasibility of carbon pipelines. In the short term, the produced hydrogen is blended with the

[5] Energy and Environment. http://dx.doi.org/10.1177/0958305X211019011

[6] International Journal of Hydrogen Energy. https://doi.org/10.1016/j.ijhydene.2021.05.112

natural gas in existing pipelines. The hypothesis is that the conversion of methane to hydrogen and its injection in existing gas pipelines can be a starting point for the hydrogen industry in Brazil.

Thesis Organization

This thesis is organized into five chapters: the introduction and main conclusion chapters, and 3 chapters that presents papers that address the three research questions mentioned above. **Figure 1** summarizes the whole structure of the thesis.

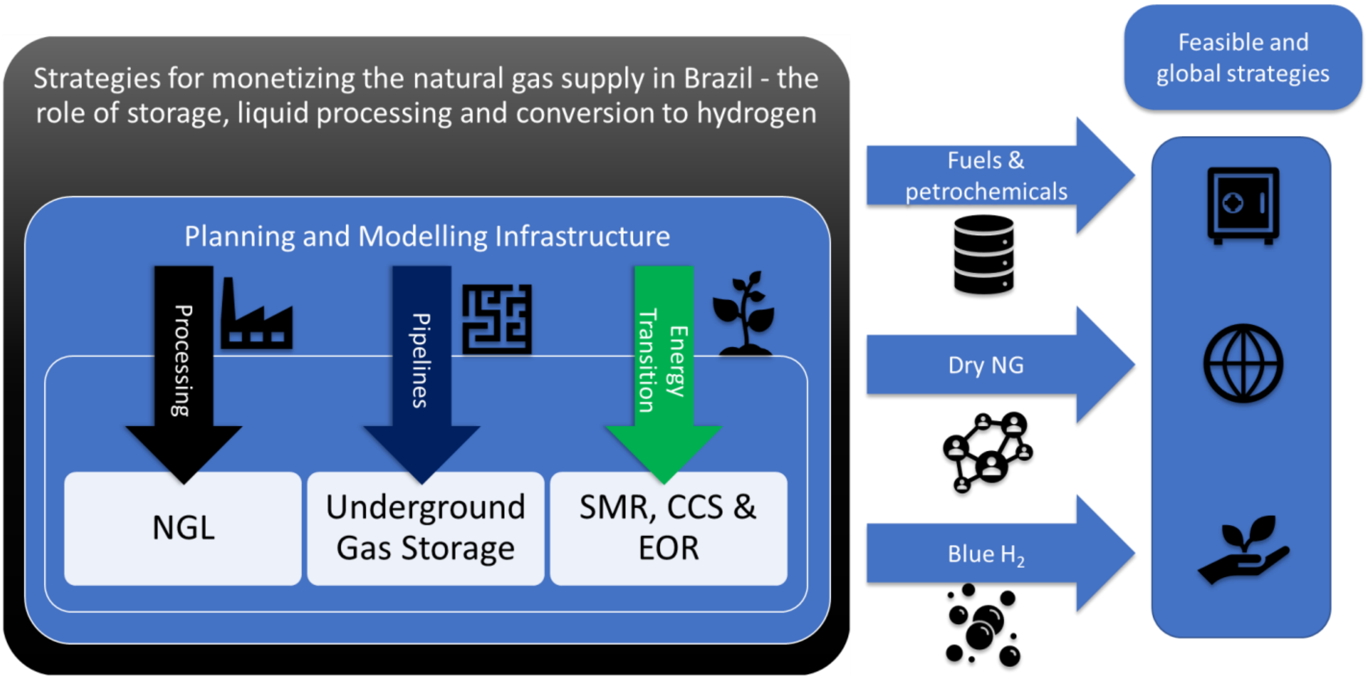

Figure 1: Strategies for monetizing natural gas supply in Brazil

Chapter 2 presents the analysis on liquids production from natural gas resources. The graphical abstract summarizes its structure (**Figure 2**).

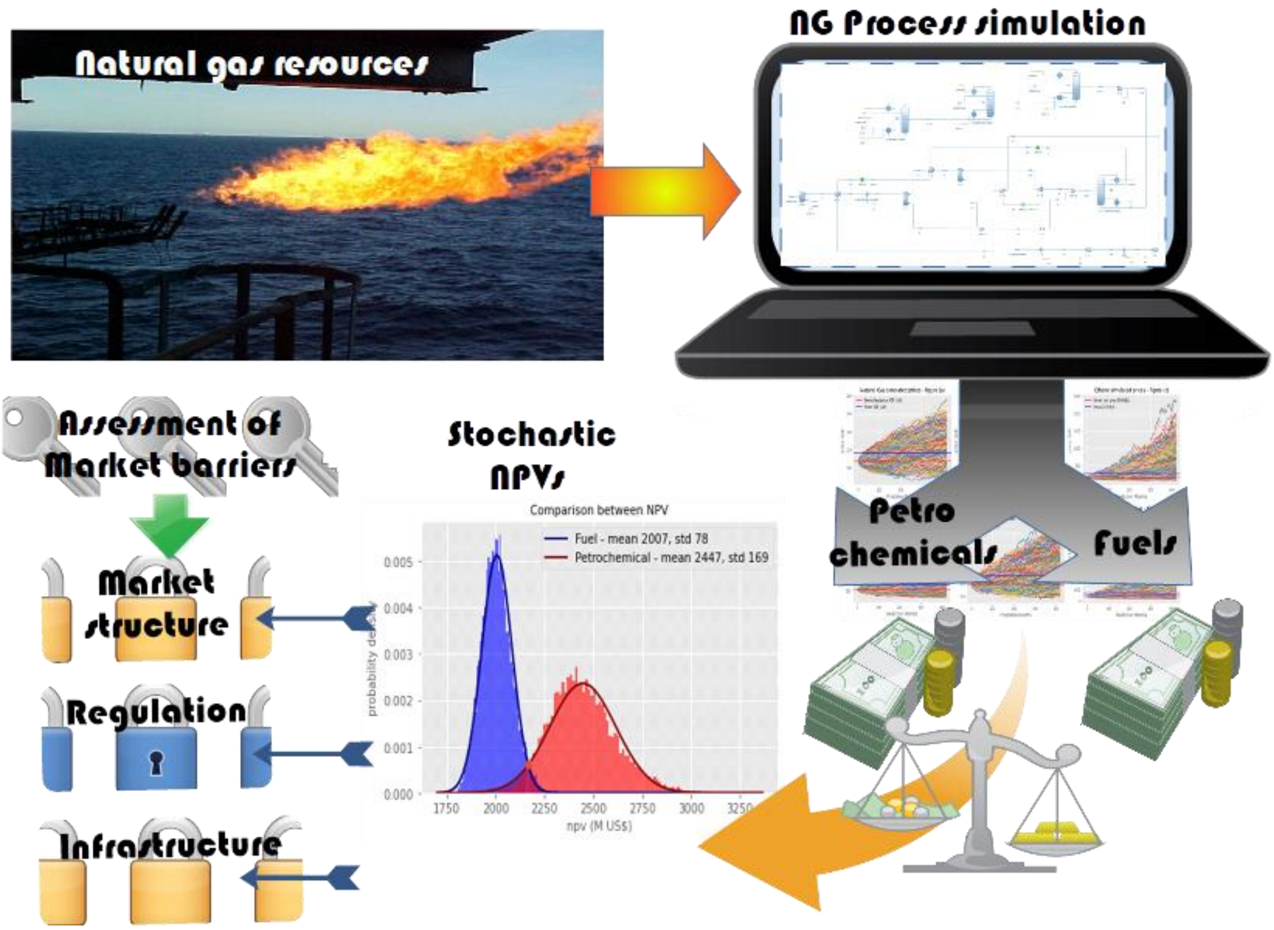

Figure 2: NGL strategy

Chapter 3 aims at evaluating the planning integration of pipeline expansion and underground storage to deal with natural gas intermittent demands, as depicted in the graphical abstract (**Figure 3**).

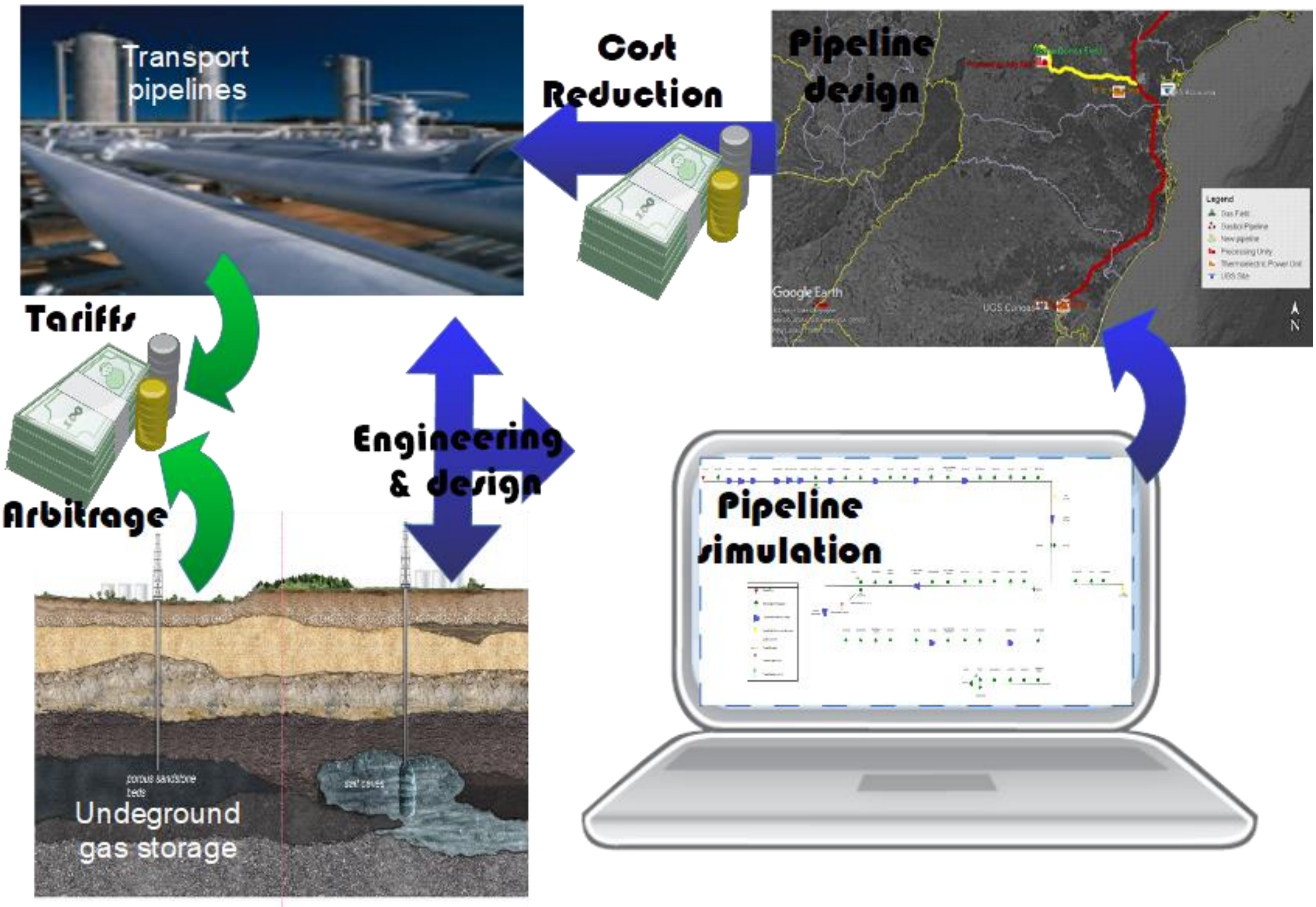

Figure 3: UGS strategy, UGS fig. obtained from [109]

Finally, **Chapter 4** proposes a strategy for developing the hydrogen industry in Brazil. It estimates the Brazilian capacity for delivering H_2 and further establishes a pathway for emerging countries. The graphical abstract summarizes the paper (**Figure 4**).

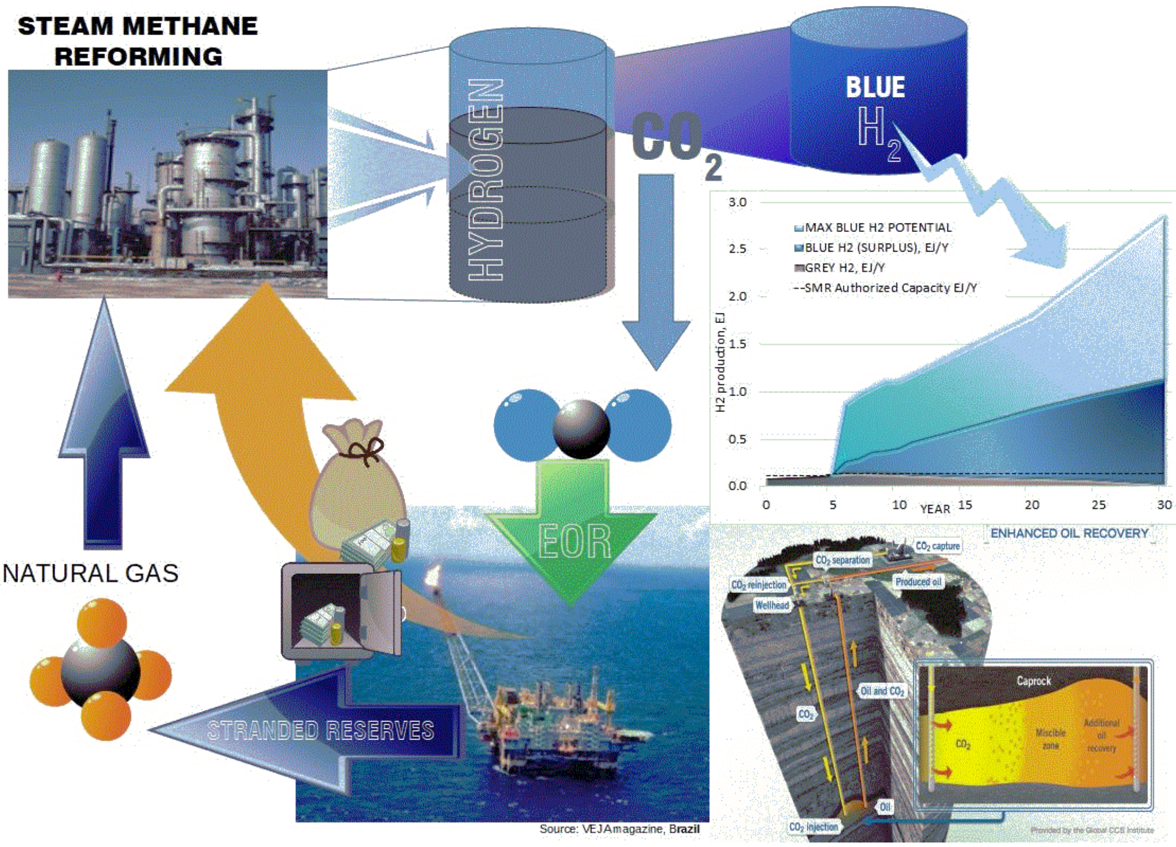

Figure 4: H_2 strategy

The main conclusion chapter addresses the main lessons of this thesis, its limitations and contributions, and indicates further studies on the same subject.

The author opted for keeping the original texts as published. Therefore, readers may eventually find some lack of synchronicity regarding to the thesis publication.

2 *Evaluating strategies for monetizing natural gas liquids from processing plants – liquid fuels versus petrochemicals*

Ricardo Moreira dos Santos
Alexandre Szklo
André F.P. Lucena
Matheus R.P. Carvalho

2.1.1 Abstract

The processing of natural gas resources is a critical step for monetizing them. Its evaluation should deal with the volatility of prices of raw gas and natural gas liquids, the processing technology and the composition of the raw gas. This study combines different approaches – process engineering, probabilistic discounted cash flow (DCF), and market failure analysis – to evaluate the technical aspects, financial results and market barriers of natural gas processing. Two productive strategies are compared: fuels or petrochemicals. Brazil is used as a case study, since the country experienced a ramping production of associated rich gas from pre-salt basins and lacks the required gas processing capacity. Findings indicate that the processing plant designed with turboexpander was able to produce the required scale for the fuel and the petrochemical markets. The Petrochemical Strategy reached a higher average net present value (US$ 2,448 millions) compared to the Fuel Strategy (US$ 2,006 millions) in a 30-years DCF analysis, at a higher standard deviation, however. This highlights the importance of performing the stochastic NPV to deal with price volatilities. The Petrochemical Strategy is also challenged by market failures found in Brazil, while the Fuel Strategy has social and infrastructure advantages in a stablished domestic market.

Keywords: Energy Planning, Natural Gas Liquids, Natural Gas processing, Process Simulation, Petrochemical Feedstocks, Energy Use

2.2 Introduction

Natural gas is seen as an option to replace coal in some energy transition scenarios [110]. It can also provide raw materials for petrochemicals [111]. However, historically natural gas has also been an unwanted by-product of the oil industry [112], whose use depends on large investments and market development [113].

The average natural gas primary supply rose 3.1 % per year between 2010 and 2019, a growth rate higher than the one found for crude oil (1.7%) and coal (1.5%) – [114]. This can be mainly explained by the increasing production of non-conventional gas in the USA ([115]) and the use of gas in power plants mostly replacing coal both for economic and environmental reasons [116]. This increasing supply of natural gas has led some authors to hope that it would be the bridge to the energy transition away from fossil fuels [59], [60], [61], particularly coal, while also prompted relevant studies on natural gas production (e.g. see [117] [118]) and uses (e.g. see [119]).

Rich natural gas (NG) resources often occur associated with oil in conventional or shale formations, and defining the most suitable gas processing route is not a trivial task. Mohakatab et al. [21] define two main schemes for gas processing: one that aims at producing gaseous fuels and another that focuses on Natural Gas Liquids (NGL). Indeed, depending on the main objective of the supply chain, a more or less complex technology may be required by gas processing plants. Designing these plants depends on the desired recovery levels of hydrocarbons, the energy efficiency target and the operational flexibility [21].

In this sense, Getu, Mahadzir and Lee [29] performed a probabilistic study for a gas processing plant and indicated that richer gas streams have strong influence in its profitability. Economic analyses can help decision makers to decide the best approach to monetize gas resources. This can focus on fuels, like ethane-rich natural gas and liquefied petroleum gas (LPG), or petrochemical feedstocks, like lean natural gas, pure ethane and propane. However, fuels such as LPG are the usual choice of natural gas processing facilities, although market changes may require new strategies concerning how natural gas richness is explored [120] [121]. NGL may be a source for adding value to the NG supply chain, especially for richer gas streams [30]. For instance, the shale revolution in USA in the 2010's spurred a two-fold increase on the petrochemicals production based on NGL [115] and new petrochemical projects thrived even during the pandemics of Covid-19. In 2021 there were 126 standalone base petrochemicals units spread throughout the USA territory [122].

This recent history of NGL as feedstock to petrochemicals in the USA indicates a possible strategy to monetize natural gas resources in decarbonization scenarios [35]. Since petrochemicals are a non-carbon emitting use of fossil fuels, at least if dedicated to long-lasting materials, its profitable production should endure even in greenhouse gas emissions restriction scenarios [30]. In addition, Platts [31] estimates that world natural gas use in chemicals and plastic should increase from 4.8 boe/d in 2020 to 15.9 boe/d in 2050, and refined oil in chemicals and plastic production will increase from 17.9 in 2020 to 28.7 boe/d. Besides naphtha, both ethane and propane are relevant petrochemicals feedstocks [123] [124].[7]

Therefore, the general objective of this study is to investigate feasible strategies for monetizing natural gas resources through gas processing, considering the revenue from the NGL products, and combining methods to deal with technical, financial and market failure aspects.

The specific objectives are:

•To estimate the yield of NGL products for two processing routes strategies, Fuels or Petrochemicals, by applying process engineering.

•To compare the financial performance of each route, through a stochastic discounted cash flow that incorporates the price uncertainties.

•To assess market failures for each strategy

Hence, the main contributions of this study are the combination of different methods that allow evaluating natural gas processing strategies for their multiple dimensions. This includes:

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[7] Ethane offers the highest ethene yield for the same process runs when compared to the other feedstocks [345].

•The simulation of the processing of different natural gas inlet streams based on an open-source model.

•A stochastic NPV analysis based also on an open-code robust model.

•A market failure analysis addressing barriers to implement the Fuel or the Petrochemical strategies

Brazil is the case study of the analyses performed in this work. It is an emblematic case, as associated gas from pre-salt basins should account for 63-77% of the Brazil's NG production in the next decades [125] [126]. However, the type of analysis and methodological procedures adopted here can be replicated in other regions/countries. For example, in the Middle East, associated gas reserves are the most common source of natural gas, reaching 70% of the resources in Iraq [25]. Likewise, China and Algeria have faced high-ethane content in shale gas resources and new processes have been developed to meet their needs of processing high-ethane gas [127]. In addition, NGL recovery was proposed associated with NG liquefaction plants in other case studies [128] [129] [130].

In order to evaluate the technical performance of processing plants, this study used the open-source software DWSIM[8]. This allows identifying composition profiles, production levels and processing strategies. For the financial analysis, this study applied Monte Carlo simulations to obtain the probability distribution curves for the net present value (NPV) of two production strategies, according to the uncertainties about the prices of NG and its products. This allows finding the expected value and standard deviation of the NPV for different productive strategies. Finally, the market analysis evaluates the barriers that may undermine the choice of the most feasible options, including market structure, logistics and infrastructure. This market barrier assessment uses the USA as a benchmark. This is due to the fact that the USA experienced a boom in its petrochemical industry during the last two decades, mostly explained by the shale gas production ramp-up [131] [132] [133]. Given that the Brazilian gas production is also

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[8] The acronym DWSIM stands for "Daniel Wagner Simulator", named after its creator and main developer.

increasing rapidly, it is worth evaluating what were the conditions for the promotion of the petrochemical industry in the USA market to assess the extent to which the Brazilian market could follow a similar path.

Therefore, this study contributes to the scientific frontier, which is summarized in

Table 2, both by combining methods based on technical-economic simulations and qualitative assessments, as well as by evaluating an emblematic case, whose results can be useful in other similar contexts.

Table 2: Summary of the compiled literature

Type of Study	Reference	Comment
Process engineering analyses	[128] [129] [130] [134] [29]	References that focus on assessing the impact of NGL processing on the break-even prices of NG and/or on the feasibility of processing facilities.
	[21] [29] [4] [135] [136] [137]	References that evaluate technical options for NG processing, usually highlighting the advantages of a turboexpander
	[138] [139]	References that provide tutorials and data for simulation models used in processing engineering analyses of NGL plants
	[140] [141] [142] [143]	Articles that provide references for DWSIM simulator uses and validation.
Economic evaluation of NG processing and NG markets	[29]	Probabilistic analysis assessing feedstock composition impact on NGL profitability
	[144] [145]	References that provide cost equations for turboexpander processes
	[146] [147] [148] [149]	References that provide NG and NGL price series
	[50][51] [52] [53] [54] [55]	References for the GBM stochastic model that is applied for estimating stock and commodity prices.
	[150] [151] [152]	References for market barrier analysis associated with NGL facilities and the NG industry
Case studies	[25] [127] [39]	Case studies on how to monetize natural gas streams produced in emerging countries in the Middle East, China and Algeria.
	[153] [154] [97] [155] [156] [94]	Studies that evaluate alternatives for monetizing natural gas resources in Brazil; and references on the Brazilian regulatory framework for natural gas and derivates
	[120] [122] [133]	Case studies about the US NG industry
NG and Petrochemicals industry assessments	[121] [30] [131] [132] [157] [158] [159]	Evaluation of how changes in the US natural gas industry affected this country's Petrochemical sector
	[160] [161] [162] [163] [164] [165] [166] [167]	References with data and analyses on the petrochemicals market in Brazil.

To the best of our knowledge, no study has yet evaluated NGL producing plants in emerging countries, applying the combination of methods proposed here and focusing on a petroleum frontier case.

This study proposes an original and universal method for meeting this objective, by associating process engineering analyses with a probabilistic discounted cash flow (DCF).

This paper is organized as follows. The next section ("Materials and Methods") describes the methodological procedure of the study. Then, Section 3 presents and discusses its findings. Section 4 addresses economic barriers and section 5 raises the main lessons of the study.

2.3 Materials and Methods

The natural gas processing technology choice depend on the raw gas composition and the specification of the NGL and dry gas in the main market [135]. Rangel [168] evaluates four technology options for processing natural gas: Joule-Thompson plants, based on isenthalpic expansion in a valve followed by a separator drum; single refrigeration, which separates natural gas streams by dew point values, applying a cooling cycle before natural gas streams separation; refrigerated absorption, which applies condensate recovery in an absorption column and thus obtains propane streams; and turboexpander plants, which are based on isentropic expansion. Turboexpander process is the most efficient technology for natural gas fractioning [21] [4] [135] [136]. It applies a sequence of cooling stages before expansion in the turboexpander that usually has a Joule-Thompson valve as a by-pass resource. Conventional turboexpander process can separate and recover pure streams of ethane (85% recovery from original composition), propane (99%) and C4+ (100 %). Pantoja [138] compares technologies for processing natural gas and concludes that the turboexpander process, associated with acid gas removal with MEA and water adsorption in silica-gel, has the highest NPV.

2.3.1 Technical Analysis

The first step of the study is to emulate the natural gas separation facility based on a consolidated process engineering model. The objective of this technical analysis is to evaluate outputs in turboexpander-based plants according to different input compositions. Production profile will subsequently feed the economic assessment.[9]

2.3.1.1 Production strategies

This study compares two production strategies for the gas processing plants:

- **Fuel Strategy:** it focuses on producing natural gas, LPG and gasoline. This strategy requires less complex fractionation steps, since the obtained outputs are essentially mixtures. Therefore, a debutanizer column is not required and the streams are obtained in the demethanizer (natural gas), deethanizer (LPG) and depropanizer (naphtha). The fractionation is based on the products boiling points [21].
- **Petrochemical Strategy:** it consists of producing (lean) natural gas, ethane, propane, butane and naphtha streams as pure as possible to supply the petrochemical industry. This strategy requires more complex fractionation steps, and low temperatures to separate ethane in the demethanizer. A debutanizer column is required [137].

In Brazil, most of the existing gas processing units focus on producing a relatively rich dry natural gas (with ethane) and LPG [169], while only one facility focuses on maximizing the output of petrochemical feedstocks, like ethane and propane. This study adopted the specifications of products (fuel and feedstocks) from the Brazilian regulation. Nonetheless, a different specification could be applied in

[9] For the purpose of this study, wet natural gas streams mean the streams before processing and dry natural gas means streams after processing. As for the liquid recovery, lean natural gas are NG streams that have less than 6% C2+; rich natural gas streams contain between 6 % and 10% C2+ and extra rich natural gas contains above 10% C2+. For the C3+ content, this study follows the definition of Tahmasebi et al. [346], for which rich streams are those having more than 4% C3+. In this paper, NGL refer to the heavier fraction in a Natural Gas Processing Unit (NPGU), LPG refers to fractions corresponding to C3 and C4, while C5+ refers to natural gasoline/naphtha and fractions containing hydrocarbons with more than 5 atoms of carbon

other case studies. The dry natural gas supplied to the high-pressure pipelines in Brazil is limited by its maximum C2+ composition - see **Table 3**.

Table 3: NG specification in Brazil according to Resolution 16/2008

Characteristics	Unit	Limiting value
High heating value (HHV)	kJ/m^3	35,000 - 43,000
Wobbe Index	kJ/m^3	46,500 – 53,500
Methane (min)	% mol	85.0
Ethane (max)	% mol	12.0
Propane (max)	% mol	6.0
C4+ (max)	% mol	3.0
CO_2 (max)	% mol	3.0
Inert gases (N_2+CO_2, max)	% mol	6.0 – 8.0

The LPG specification in Brazil is limited by the maximum 2% content of pentanes in the C3/C4 mixture and by the maximum 2.5% content of butane and heavier fractions in the C3 stream (**Table 4**).

Table 4: LPG specification in Brazil according to Resolution 825/2020

Characteristics	Unit	Commercial and Special propane	Commercial Butane	Propane and butane mixture
Vapor pressure @ 37,8ºC, max	kPa	1430	480	1430
Propane (min)	% vol	- / 90	-	-
C4+, max	% vol	2,5	-	-
C5+, max	% vol	-	2,0	2,0

Finally, the specifications of naphtha are not established by the Brazilian regulator. Meireles et al [170] classified it as paraffinic (LAN) and naphthenic (HAN) naphtha. The first one (average density 0.6802 g/cm^3) is indicated for producing olefins and should have no more than 78% paraffins. The second one (average density 0.735 g/cm^3) is indicated for producing paraffin and should have no more than 65% paraffins. Vapor pressure (37.8ºC) may vary between 45-69 kPa; minimum specific gravity is 715 kg/m^3(20ºC) (Gasoline A[10] – 688.9-699.8 kg/m^3(20ºC)); maximum aromatic hydrocarbons volume is 35% and olefin 25 % vol.

2.3.1.2 Simulation model

[10] In Brazil there are two kinds of Gasoline (A and C), in which Gasoline C is blended with ethanol [364].

The process simulation was run in DWSIM[11] software version 6.5.2. Building a valid model requires some previous and interactive steps. Streams and systems need to be designed, thermodynamic packages and compositions must be defined and inserted in the model. The simulation steps for developing the model by this study are summarized in **Figure 5**.

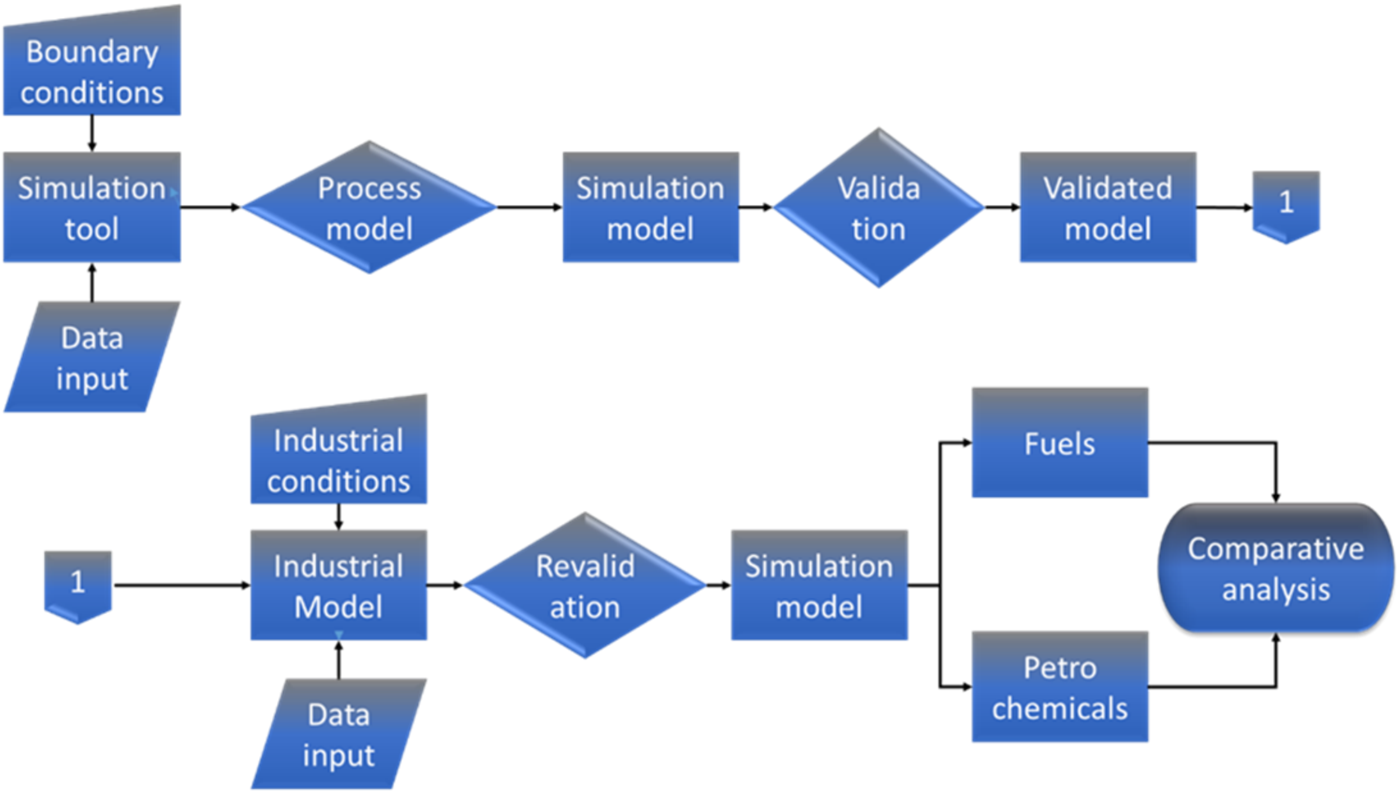

Figure 5: Simulation routine and model construction

Two thermodynamic packages were tested in this study: Peng-Robinson and Soave-Redlich-Kwong, both suitable for polar mixtures in pressures above 10 bar [171] [172] [171]. Once the model was set, a validation step evaluated the results obtained by comparing them to an academic known model. The turboexpander was modelled following Pantoja [138], emulating a compressor mechanically linked to a

[11] DWSIM is a CAPE-OPEN compliant open-source Chemical Process Simulator, run in all platforms like Windows or Linux, performing steady state or dynamic simulations. It comprises advanced property packages like PR, SRK, NRTL, UNIQUAC and has been used by a diversity of academic studies. It is available for download at https://dwsim.inforside.com.br/new/. Testing DWSIM capabilities, Tangsriwong et. al [140] compared DWSIM to commercial Aspen Plus and found differences lower than 5% between them. A diversity of academic papers [141] [142] [143] on DWSIM can be found in https://dwsim.inforside.com.br/wiki/index.php?title=Literature. Since DWSIM is open-source software, its creator does not offer commercial guarantees related to its economic use to profitable activities.

turbine. Validation was performed by comparing the obtained flow rates in selected key points. Those selected points for validation of the model are displayed in **Table 6**:

Table 5: Model validation points [140]

Validation point	Stream Name	Main product	Acceptation criterion
Stream 11	Light Fraction T-01 (Demethanizer)	Natural Gas	5%
Stream 12	Heavy fraction T-01 (Demethanizer)	NGL	5%
Stream 18	Specified Natural Gas	Natural gas	5%
Stream 20	Light Fraction T-02 (Deethanizer)	Ethane	5%
Stream 22	Light Fraction T-03 (Depropanizer)	Propane	5%
Stream 23	Heavy fraction T-03 (Depropanizer)	C4+	5%

However, the model used for validation has some differences from the obtained commercial plant. In this study, the commercial model is based on a real Brazilian facility, the "*Gás Natural Açu*" (GNA) [139] plant, which was designed to process pre-salt gas from Brazil´s Campos Basin. **Table 6** shows the feedstock composition (named here as COMP-0) in this processing plant.

Table 6: GNA composition (COMP-0) [173]

Component	Molar %	Fraction
C1	83. 67	0. 8393
C2	7. 28	0. 0730
C3	3. 65	0. 0366
I-C4	0. 37	0. 0037
N-C4	1. 12	0. 0112
I-C5	0. 31	0. 0031
N-C5	0. 37	0. 0037
C6	0. 17	0. 0017
C7	0. 12	0. 0012
C8	0. 09	0. 0009
C9	0. 04	0. 0004
C10	0. 01	0. 0001
C11	0. 01	0. 0001
CO2	1. 94	0. 0195
N2	0. 54	0. 0054

The GNA plant was designed to process 40 M Sm^3/d (1,643,456 kg/h) [12] of wet natural gas [139], while the academic model run in this study is designed to process 14,500 kg/h [138]. Therefore, a scale-up was performed, followed by a model evaluation.

Then, after the simulation model was validated, it was used for comparing the two strategies mentioned before. Firstly, the strategies were compared for the same composition COMP-0, obtained

[12] Standard conditions= 15,5ºC, 1 atm [139]; Normal conditions = 20,0ºC, 1 atm [169].

from the existing project GNA. From this simulation, production quantities and product compositions were obtained. After this initial run, a new simulation routine was performed with variable inlet gas compositions, ranging from extremely rich to extremely poor gas inlet: COMP-1 (post-salt, Mexilhão non-associated field), which refers to non-associated poor gas. COMP-2 (pre-salt, Sapinhoá and Tupi/Lula fields), which refers to an extra-rich gas. **Table 7** compares these streams to the shale gas field Marcellus, in the USA:

Table 7: Typical NG field compositions, % mol

Composition	**REFERENCE**	**COMP-1**	**COMP-2**
Basin	**Marcellus**	**Santos Post-Salt**	**Santos Pre-salt**
Field	**Shale Gas** [124]	**Mexilhão** [23]	**Tupi (Lula) Sapinhoá** [23]
Associated Gas (AG) / Non-associated Gas (NAG)	AG	NAG	AG
Stream	-	1	1
C1	0.794	0.932	0.700
C2	0.161	0.038	0.113
C3	0.04	0.013	0.074
n-C4/i-C4	-	0.006	0.031
C5+	-	0.005	0.011
Inert	0.005	0.006	0.071

The process plant designed in this study (see **Figure 6**) includes a separator column CS-01 for eliminating eventual impurities in the gas composition, such as nitrogen or acid gas traces. Natural gas is cooled down in a first cooler (E-01) and in a propane chiller (E-02), reaching a temperature of -40ºC prior to a first separation in V-01. Condensate is collected in the bottom, while top stream goes through a new cooling stage (E-03). Cooled stream goes through a second separator V-02. Bottom stream condensate gathers condensate stream from V-01 and goes through a joule-Thompson valve, while top stream goes to turbo-expansion. Joule-Thompson valve is normally closed. Top stream from V-02 and condensate stream after Joule-Thompson valve inlet in first fractioning column T-01 (Demethanizer). Top stream from T-01 is lean natural gas, which is applied to cool down inlet streams in E-01 and E-03, prior to be compressed and exported to transport pipelines. Bottom stream is NGL, which should go through fractionation columns T-02, T-03 and T-04 (deethanizer, depropanizer and debutanizer, respectively).

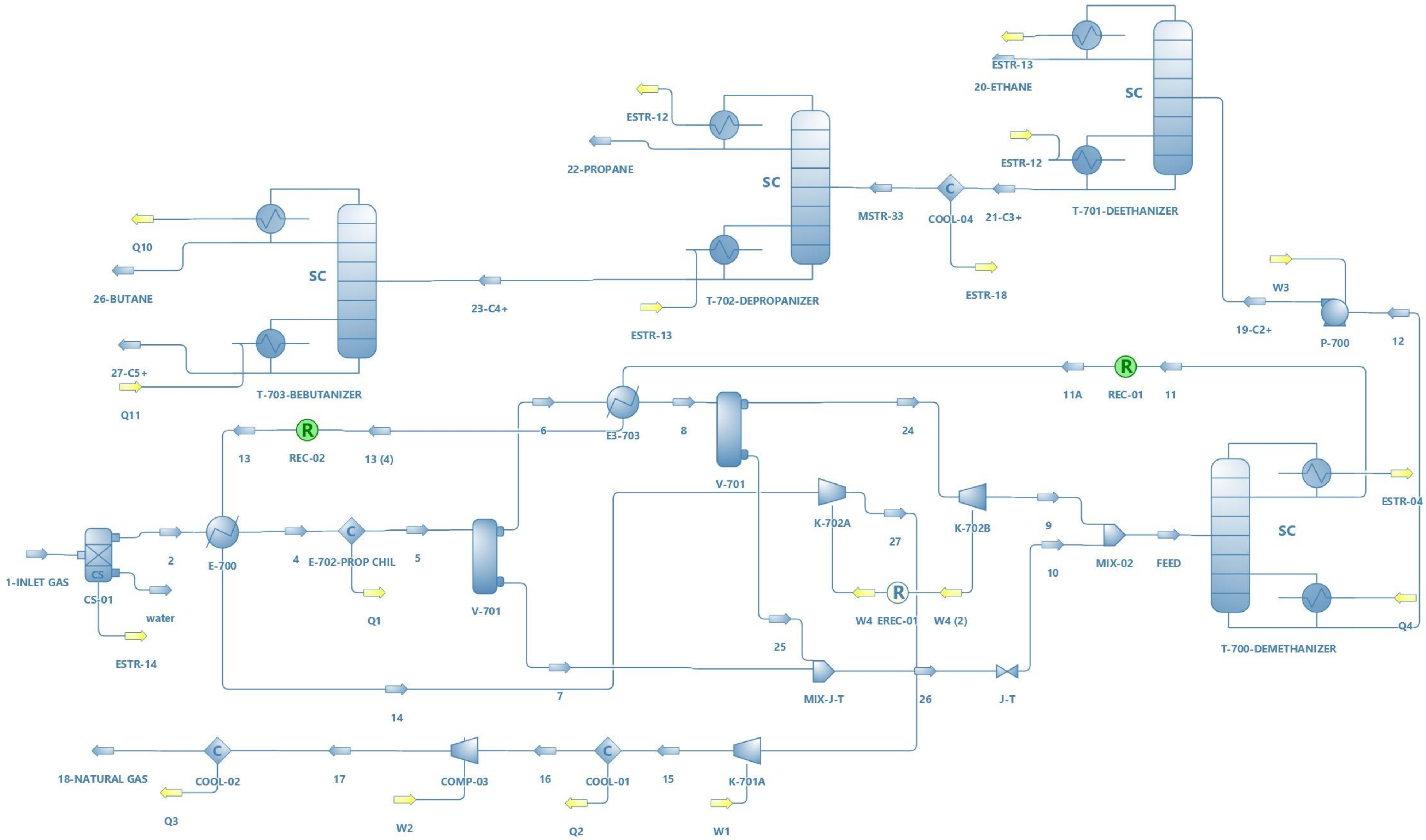

Figure 6: Simulation model of a turboexpander natural gas processing unit built in DWSIM

2.3.2 Financial Analysis

This study applied a probabilistic discounted cash flow (DCF) analysis [174] to evaluate the economic return of the processing plants simulated before. The probabilistic analysis aims to capture the effects of the uncertainties of NG and NGL prices.

2.3.2.1 Costs

Investment costs for turboexpander units were obtained in MME [144], based on Younger's estimates [145] and updated to March 2021, using Chemical Engineering Process Costs Index (CEPCI) [175]. **Equation 1** displays the original investment costs for turboexpander units:

$$\textbf{CAPEX (}10^6\textbf{ US\$, 2019) =168.86 + 34.07*PC (}10^6\textbf{ m}^3\textbf{/d)} \qquad \textbf{Equation 1}$$

Where:

PC = Processing Capacity, in millions cubic meters (Brazilian standard, 20ºC, 1 atm).
CAPEX = Capital Expenditure (overnight)

CEPCI Values for 2020 and March 2021 were respectively 2.9 % and 9.6% higher than 2019, which was 607.5. The plant corrected costs curve becomes (**Equation 2**):

$$\textbf{CAPEX (M US\$, March 2021) =190.44 + 38.42*PC (M m}^3\textbf{/d)} \qquad \textbf{Equation 2}$$

Where:

PC = Processing Capacity, in millions cubic meters (Brazilian standard, 20ºC, 1 atm).
CAPEX = Capital Expenditure (overnight)

As mentioned before, the Fuel Strategy leads to a plant with less fractionation steps. Castro et. al. [134] estimated that fractionation columns represent 7% of the rich turboexpansion CAPEX and so debutanizer column costs were obtained from the total facility cost. Considering four columns, 1.75% of the total Capex was estimated as the debutanizer costs. **Table 8** presents adjusted values for a design capacity of 40 M Sm^3/d (40.7 Nm^3/d).

Table 8: Processing costs (2021)

Technology Turboexpander	**Capacity** **M Nm^3/d**	**Capex** **M US$**	**Opex** **M US$/y**
Fuel Strategy	40.7	1723.4	206.8
Petrochemical Strategy	40.7	1754.1	210.5
Demethanizer column	-	30.7	-

Getu et al. [137] show that operational expenditures are higher in facilities that process rich natural gas when different technologies are compared. This difference is due to the higher costs required to keep low temperatures in the process, mainly in the demethanizer reboiler and in the sale gas compressor. This study considered the annual operational expenditure (OPEX) as 5% of the CAPEX, following MME [144], although Pantoja [138] estimated it as 12%[13]. This value was chosen based on the literature, but also because, in larger plants, some fixed OPEX may be diluted in total OPEX.

Finally, in order to perform a sensitivity analysis, CAPEX and OPEX costs were varied by 25%, thus creating a range of 75% to 125% its median value.

2.3.2.2 Prices and other premises

Monthly price series were obtained from EIA [146] for pure chemicals and product mixtures. Natural gas prices (Henry Hub), crude oil (WTI), ethane, propane, butanes and naphtha refer to Mont Belvieu hub, Texas – see **Figure 7**. The monthly prices were used, as this study intends to evaluate strategies for investment, instead of earnings from daily trading.

[13] The author estimated costs for a turboexpander unit: Opex 1026.90 k US$/y and Capex 8620 k US$ in a 14500 kg/h raw gas processing unit.

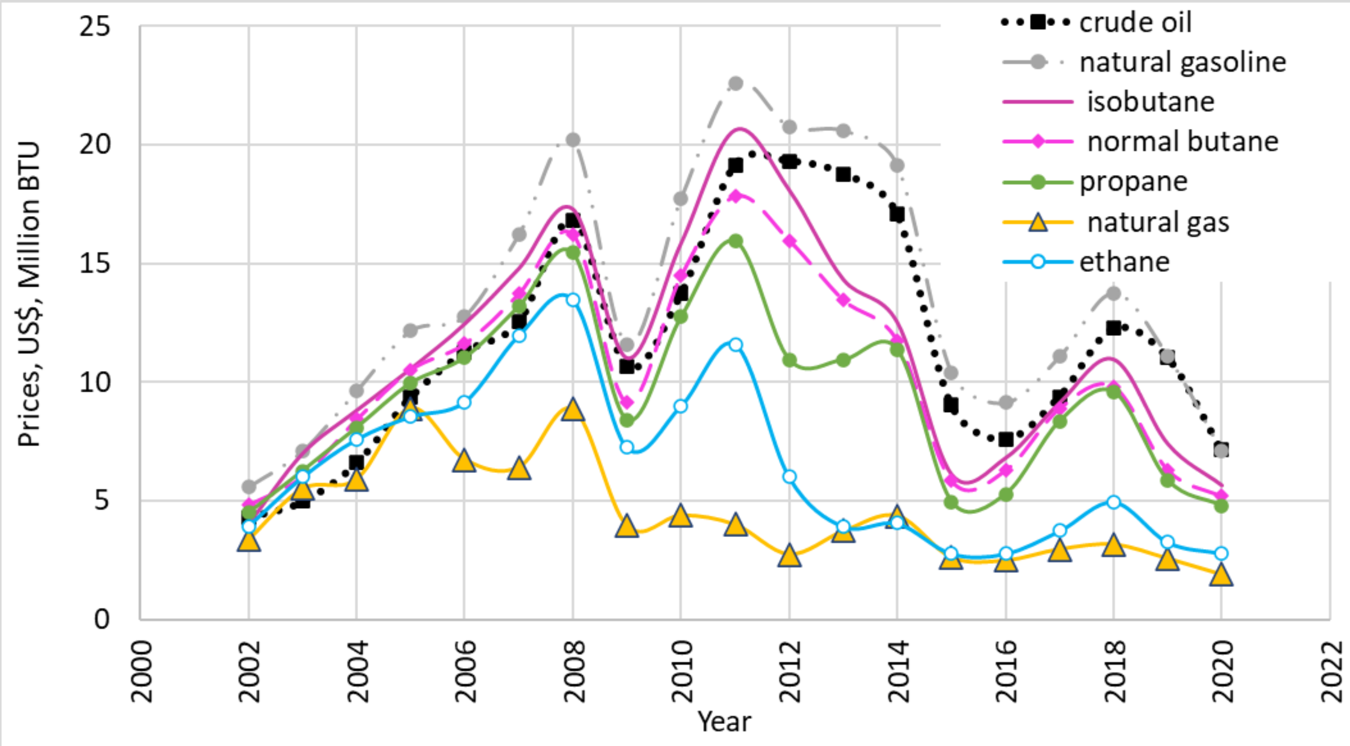

Figure 7: Average prices for hydrocarbon gas liquids, natural gas, and crude oil in the United States [115]

For mixtures like natural gas, LPG or naphtha, a price composition was used. In Brazil, reference prices are calculated by the Petroleum Regulator Agency (ANP), following a proportional formula [176] – see **Equation 3**:

$$\boldsymbol{\pi_m = \sum_{i=1}^{n} p_i x_i} \, , \qquad \textbf{Equation 3}$$

Where:

π_m = Mixture final Price
p_i = component price
x_i = component fraction

The following taxes and discounts were considered (**Table 9**):

Table 9: Taxes and discounts (2021)

Tax/Discount	Rate/year
Income Tax	28%
Interest Rate	7%
Depreciation	3%
CSLL – Tax on profits	9%
PIS/COFINS – Social contribution (tax)	9.25 %
IVA – State (local) tax	12%

As mentioned before, the economic evaluation was based on a probabilistic discounted cash flow (DCF) analysis. In order to simulate possible pathways of price series, a geometric Brownian motion

(GBM) model was used. The GBM model is a continuous-time stochastic model that runs on the premise of a normal distributed and independent prices return [177]. This model is used to stock [178] and commodity price modeling [179] [180] [181] [36]. It has two main terms: the drift, which represents the long-term tendency of the price, and the diffusion, which represents a random shock that the price can suffer in a short period of time. In this context, 10,000 price pathways simulations were realized for the six output products. The GBM formula is shown in **Equation 4**:

$$S_t = S_f e^{\left(\mu - \frac{\sigma^2}{2}\right)t + \sigma B t} \qquad \textbf{Equation 4}$$

Where:

S_f is the last price of the historical series
S_t is the price in time t
μ is the mean of the historical price series
σ is the standard derivation of the historical price series
B is a normal distributed variable with $\mu = 0$ and $\sigma = 1$

The used data consisted of the historical prices from the selected products: natural gas (NG), liquefied petroleum gas (LGP), ethane (C2), propane (C3), butane (C4) and naphtha (C5+) [146]. The data sets have a span of 18 years, from January of 2002 to October of 2020, on a monthly basis. The historical data sets are shown in **Figure 8**.

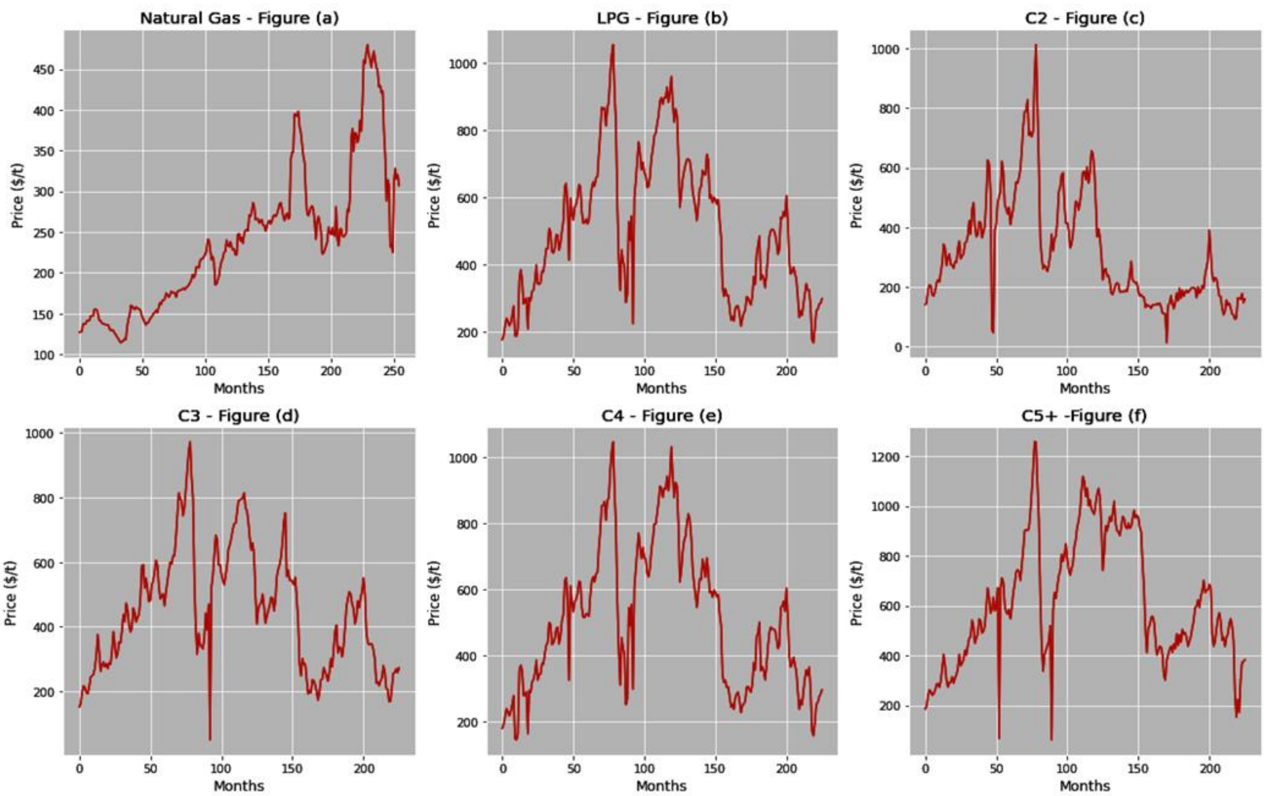

Figure 8: Input data sets [146]

The histograms of these prices are shown in the **Figure 9** below:

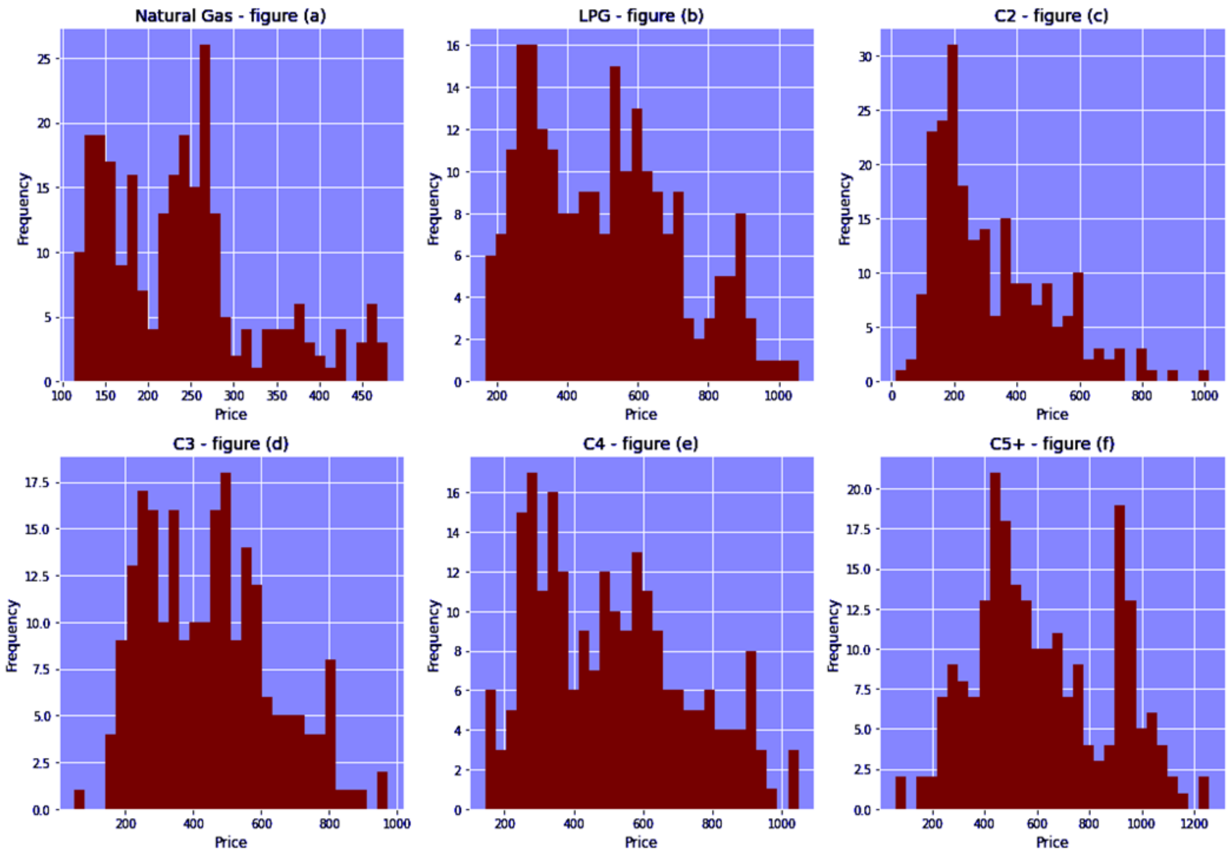

Figure 9: Histograms for price data sets

The net present value (NPV) for each scenario for 30 years was calculated using the stochastics curves from GBM model – see **Equation 5**):

$$\boldsymbol{NPV = \sum_{t=1}^{T} \frac{C_t}{(1-R)^t}} \qquad \textbf{Equation 5}$$

Where:

C_t is the cash flow after taxes
R is the discount rate
t is the number of periods (1, 2, 3…,30)

The probability density function (PDF) was used to verify the simulated variables for the GBM model. The PDF is calculated by **Equation 6**:

$$\boldsymbol{f(x) = \frac{e^{(-\frac{x^2}{2})}}{\sqrt{2\pi}} = \frac{e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})}}{\sigma\sqrt{2\pi}}} \qquad \textbf{Equation 6}$$

To obtain NPV series, the prices were inserted in the GBM and modeled in Python. Information about this programming language can be found in [182][14].

2.4 Results

2.4.1 Model Validation

Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK), thermodynamic packages were tested in the validation stage. Outputs and the comparison to the reference case are shown in **Table 10** and **Table 11**.

Table 10: Model validation on thermodynamic package Soave-Redlich Kwong

Validation point	Stream Name	Mass flow, kg/h Model	Reference	Error
Stream 11	Light Fraction T-01 (Demethanizer)	6789	7009	3.14%
Stream 12	Heavy fraction T-01 (Demethanizer)	5960	5740	3.83%
Stream 18	Specified Natural Gas	6789	7009	3.14%
Stream 20	Light Fraction T-02 (Deethanizer)	1397	1314	6.32%
Stream 22	Light Fraction T-03 (Depropanizer)	4014	3828	4.86%
Stream 23	Heavy fraction T-03 (Depropanizer)	549	598.3	8.25%

Table 11: Model validation on thermodynamic package Peng Robinson

Validation point	Stream Name	Mass flow, kg/h Model	Reference	Error
Stream 11	Light Fraction T-01 (Demethanizer)	6981	7009	0.40%
Stream 12	Heavy fraction T-01 (Demethanizer)	5768	5740	0.49%
Stream 18	Specified Natural Gas	6981	7009	0.40%
Stream 20	Light Fraction T-02 (Deethanizer)	1292	1314	1.69%
Stream 22	Light Fraction T-03 (Depropanizer)	3877	3828	1.28%
Stream 23	Heavy fraction T-03 (Depropanizer)	599	598.3	0.05%

[14] Simulation codes and data may be found on https://github.com/matheuspoggio/Natural-Gas-Processing-Plans-NPV-Analysis.

As noted, the validation for SRK package has a deviation above 5% for deethanizer and depropanizer streams, while the validation for the PR package obtained smaller errors. Therefore, PR model reproduced closely the emulated reference, justifying its choice.

2.4.2 Technical Results

2.4.2.1 Fuel Strategy

This strategy resulted in high flows of LPG for the extra rich gas – **Table 12**. As expected, dry natural gas flows were higher for leaner inlet compositions, while composition (COMP-0) outputs higher quantities of naphtha (C5+).

Table 12: Fuel Strategy - Product flow rates in kt/y

	Nat Gas	**LPG**	**Naphtha**
COMP-0	8,938.76	1,148.02	524.79
COMP-1	10,559.11	290.97	222.33
COMP-2	7,267.49	2,333.56	333.24

Composition COMP-0: A moderate rich stream of natural gas (COMP-0) meets the Brazilian specifications. The plant reached 91% C1, 8 % C2, 1% C3 and traces of C4+; LPG streams are a composition of 65% propane and 35% butanes (**Figure 10**a).

Composition COMP-1: This option reached 95% C1, 3.9 % C2, 1% C3 and traces of C4+. LPG streams are a composition of 37% propane and 62% butanes and small quantities of C5+ (**Figure 10**b). These outputs meet the specification for dry gas transport and LPG in Brazil.

Composition COMP-2: This option reached 85% C1, the minimum limit for natural gas in Brazil's gas networks, 13.7 % C2, 1% C3 and traces of C4+. LPG streams are a composition of 67 % propane and 31% butanes and small quantities of C5+ (**Figure 10**c). In this composition, the ethane content surpasses the allowed specification for gas networks in Brazil.

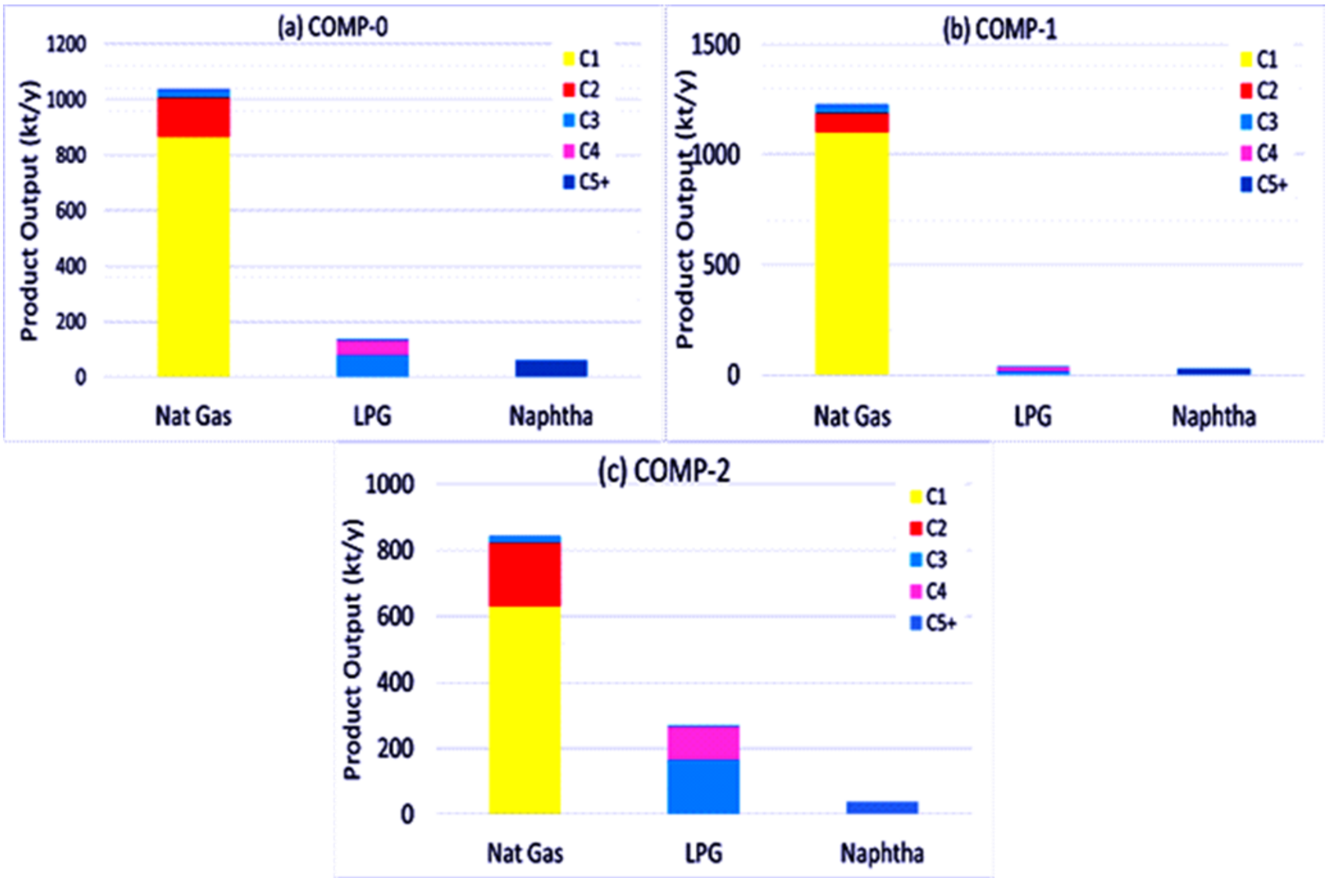

Figure 10: NG and NGL fractions obtained in the Fuel strategy (a) Rich gas; b) Lean gas; c) Extra Rich gas.

2.4.2.2 Petrochemical Strategy

Table 13 shows that the dry natural gas production decreased when processing rich and extra rich gas inlets, while a relevant stream of ethane mass flow becomes available. Similar effect happens for LPG, which split into two streams of propane and butane.

Table 13: Petrochemical Strategy- product flow rates in kt/y

	Nat Gas	Ethane	Propane	Butanes	Naphtha
COMP-0	7,485.74	1,220.92	907.03	466.35	531.07
COMP-1	9,528.24	727.07	369.06	218.34	229.85
COMP-2	5,444.54	1,648.69	1.598.90	856.98	384.75

Each stream composition essentially consists of the main product (**Figure 11**). The dry NG stream is 99 % in C1.

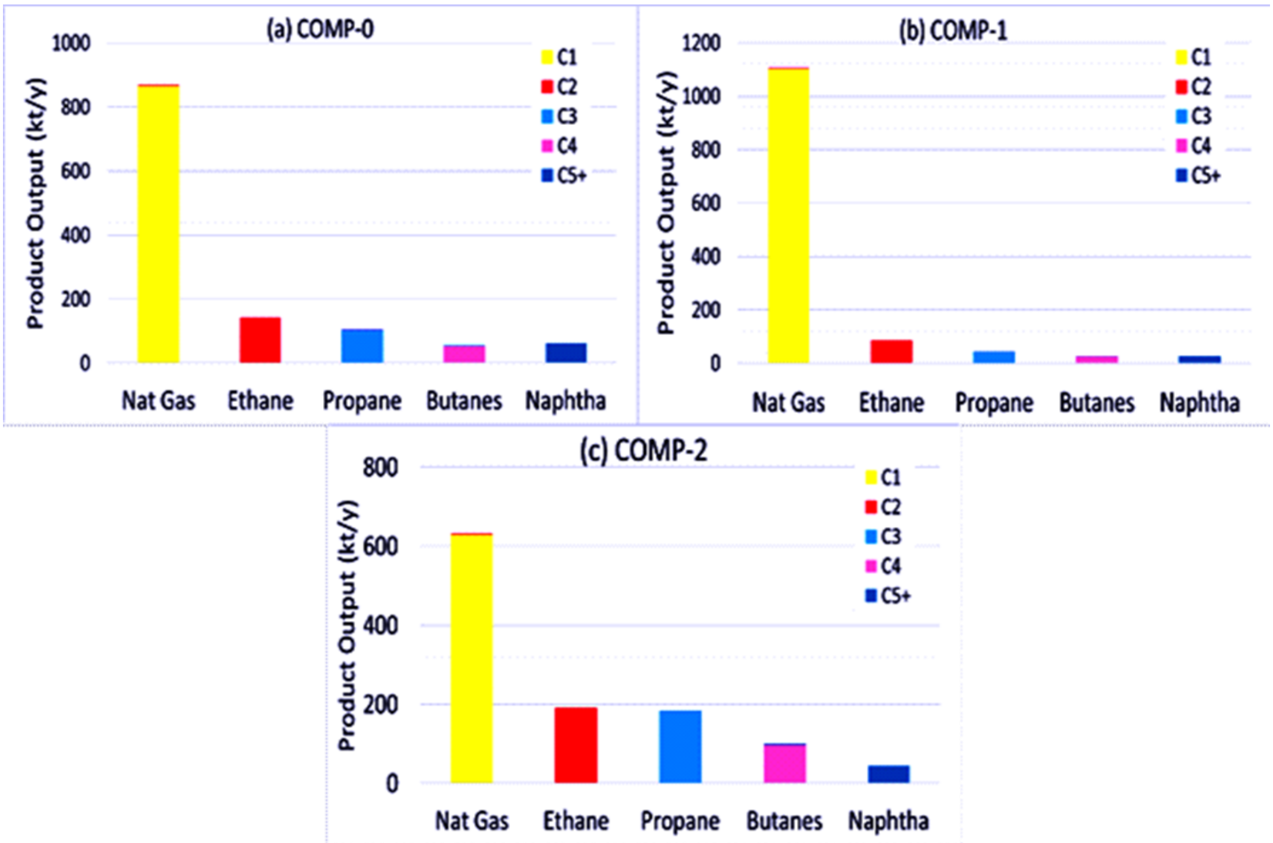

Figure 11: NG and NGL fractions obtained in the Petrochemical strategy (a) Rich gas; b) Lean gas; c) Extra Rich gas.

2.4.3 Financial analysis

Figure 12 (a-f) shows the simulated prices pathways for the six analyzed products. The average prices of NG, LPG, C2, C3, C4 and C5 were, respectively, 316, 326, 261, 364, 329 and 639 US$/t.

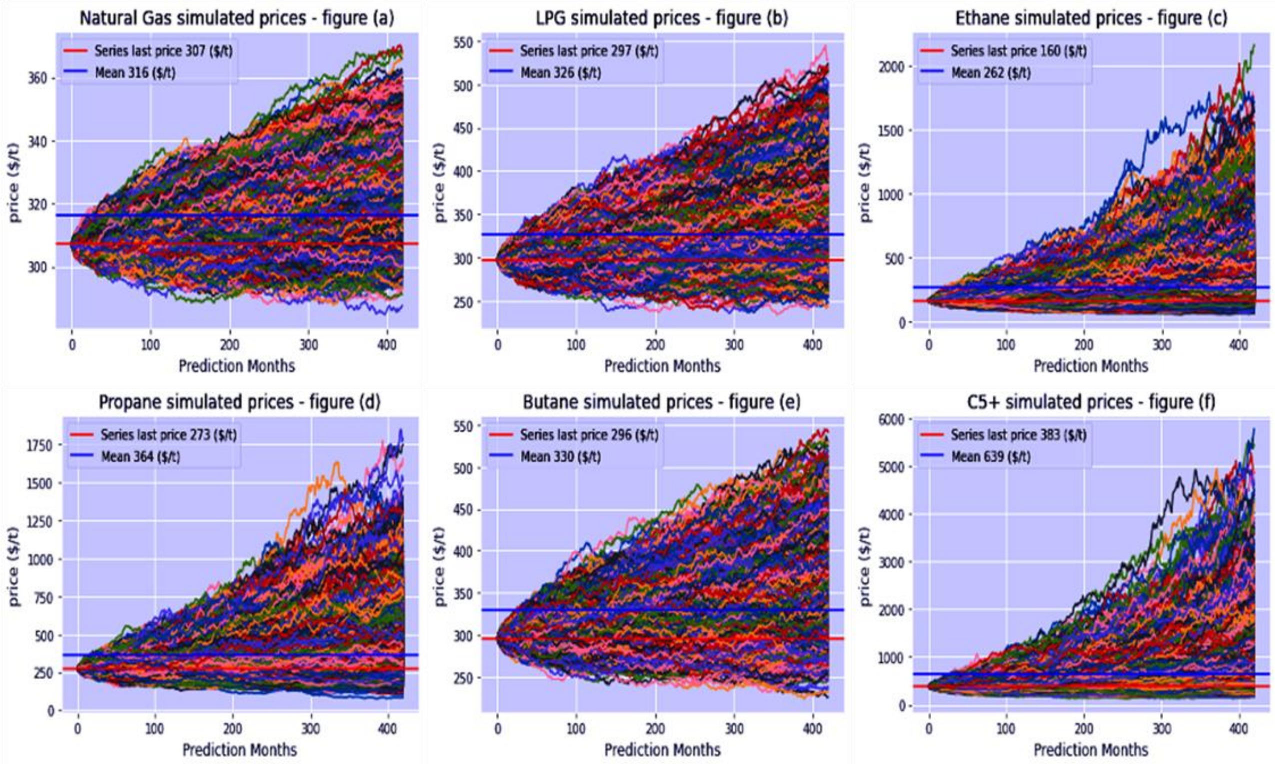

Figure 12: GBM curves for all analyzed products

After 10,000 simulations for monthly prices, the stochastic results for NPV showed a higher NPV expected value for the Petrochemical strategy – see **Figure 13**. While the Petrochemical strategy obtained an average result of MUS$ 2,448, the Fuel strategy obtained an expected NPV of MUS$ 2,006. Comparatively, the Fuel strategy obtained a lower standard deviation (77 MUS$) than the Petrochemical strategy (168 MUS$). The intersection area between the two distributions is equal to 0.065. This is the area where the strategies have the same economic performance. It shows that only the 4.7% worst cases of the Petrochemical strategy yield a lower NPV, when compared to the 98% best cases of the Fuel strategy.

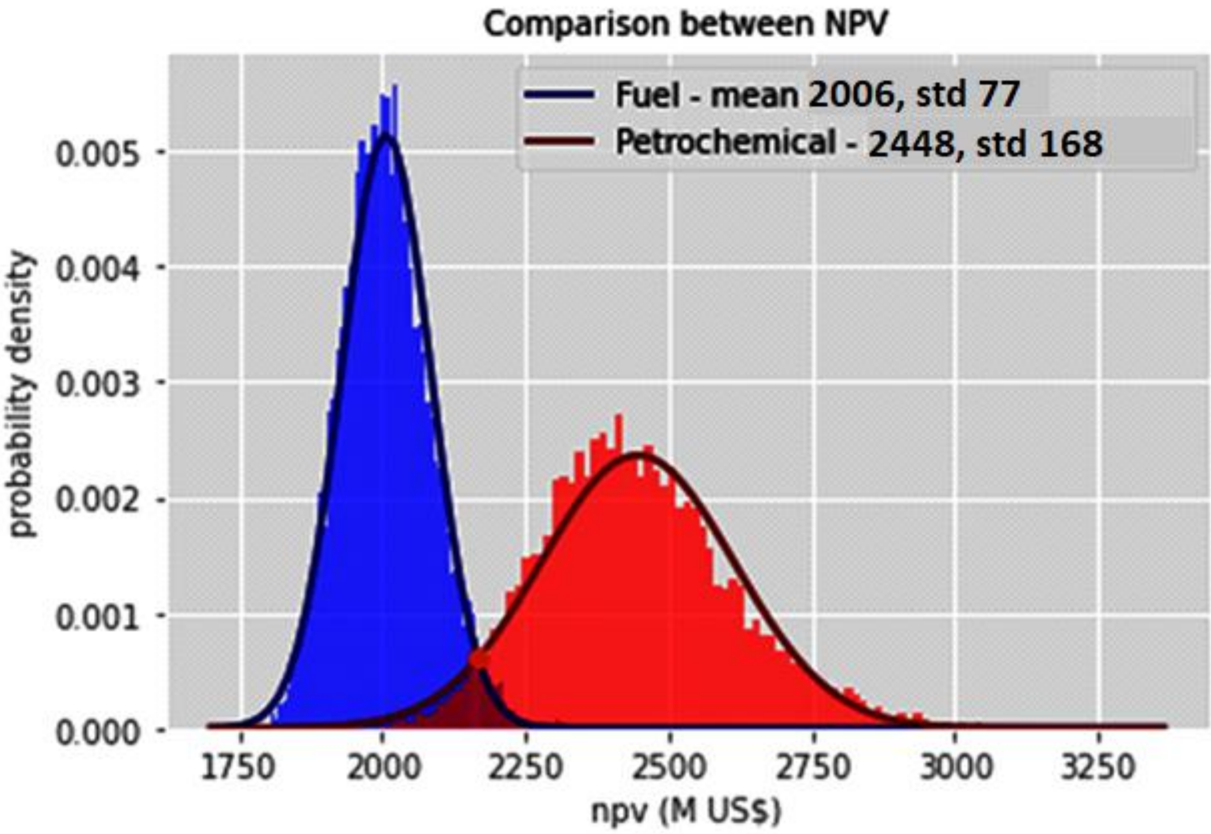

Figure 13: NPV strategies results

Both NPVs are positive, but their distribution functions differ. **Table 14** summarizes the obtained results from the Monte Carlo Simulation.

Table 14 – Summary of stochastic simulation

	Fuel	**Petrochemical**
Min	1727.3	1970.1
Max	2356.4	3306.1
Mean	2006.4	2448.0
STD	76.5	167.7
Median	2001.4	2435.0
Mode	1997.0	2342.0
Coefficient of variation	3.8	6.9
Skew	0.3	0.5
Kurtosis	0.3	0.5
Percentile 95%	(1868.5, 2169.8)	(2155.2, 2808.9)
Confidence Interval 95%	(2005, -1.4)	(2445, -3.2)

Finally, changes in CAPEX and OPEX (sensitivity analysis) did not significantly affect the results. Varying the CAPEX and the OPEX by 75% to 125%, the standard deviation of NPV for the Fuel and Petrochemical strategies remained 77 MUS$ and 168 MUS$, respectively. The expected values for the

125% case were 1762 MUS$ and 2099 MUS$ (12% and 14% below reference values); and for the 75% case were 2250 MUS$ and 2587 MUS$ (12% and 5% over the reference values) for the Fuel and the Petrochemical strategies, respectively. Therefore, the financial choice between the two strategies did not change, what was expected since both options are based on the same type of facility (turboexpander) with a small addition (a splitter) in the case of the Petrochemical strategy.

2.5 Assessment of market barriers

The financial analysis showed a higher NPV for the Petrochemical strategy. However, there are major barriers to newcomers in the Petrochemicals market in Brazil. Azevedo [150] divides entrance barriers into two groups: economic and institutional barriers. While the first group is defined by the non-existence of profits for the newcomers in the market, the second indicate legal prohibitions to newcomers like the patents that legally reserve market. In Brazil, there is no legal prohibition for investors to start in the petrochemicals market. Then, market barriers should be economic. Azevedo [150] indicate that economic barriers may be due to a) product differentiation; b) absolute costs advantage; c) scale economy. Since petrochemicals can be considered commodities, differentiation is not a meaningful barrier. Then, here we focus on the other two barriers.

For the scale barrier, the increase in pre-salt production may open space for scalable production of ethane in steam crackers. Natural gas production should increase by 3 times by 2050 [125] [126] and processing units will be required to trade it. In sum, scale should not be the most relevant barrier to investors in the Brazilian market. In the case of absolute cost advantages, it is worth comparing costs in Brazil to costs in the USA, which is an example of success of the petrochemical industry based on NGL. Costs of capital in Brazil are much higher than in the United States. For instance, nominal interest rates in Brazil in June 2021 were 4.25% p.a. [183], while in USA are 0-0.25% [184]. As for prices, international chemicals producers rely on naphtha, an oil-based and more expensive feedstock [185], while ethane produced from shale gas depend on cheaper natural gas prices. This disparity opened a gap between productions costs and sales prices for the basic chemical's seller [131].

Some other specific market barriers in the natural gas industry are analyzed in the next sections. Almeida [151] highlights four factors that favor natural gas market flexibility: available infrastructure (transport, storage, regasification and liquefaction); diverse commercial modes and agents (spot and future contracts, interruptible contracts); organized markets (hubs); growing international integration. Natural gas transport is a natural monopoly, so infrastructure and logistics play an essential role when planning industrial facilities. In addition, the market structure indicates how actors define investments, negotiate contracts and expand business. Finally, the regulatory framework stablishes the legal rules that can foster the industry or bureaucratic barriers that may curb or delay investments.

2.5.1 Infrastructure and Logistics

Dry natural gas is transported to final consumers through pipelines, compressed or liquefied by trucks or ships. The less expressive modals like compressed gas are used for short distances and quantities, but pipeline networks are always a critical infrastructure for NG transport [39]. Building natural gas pipelines requires years: it must meet environmental requirements, overcome geographical barriers like wet or blocked landscapes, cross rivers, roads and towns and cities, often through highly populated regions [186]. Underground storage facilities offer flexibility to natural gas industry and may be economically feasible, but developing such facilities may take seven up to ten years [49].

One example is the GNA project in Brazil, for which a 100 km-pipeline was required to connect the Açu port to the Cabiúnas processing plant and then to final consumers. Another example is a new port (TEPOR), which is planned to be built in Macaé, in Rio de Janeiro State, where the Cabiúnas plant is located. In both cases new gas processing facilities are projected, but no steam crackers for ethane are considered in association with these facilities. The only ethane cracking unit in Brazil is in Duque de

Caxias, 180 km away from Cabiúnas (connected by pipelines) and 280 km from Açu harbor, which is not connected to the NG network.

Comparatively, the United States has a well-developed natural gas transport infrastructure, with high capillarity and more than 4.8 million km of pipelines and 120 Gm^3 of underground storage capacity [187]. Such infrastructure was an important element that enabled the fast development of petrochemicals in the USA due to the expansion of shale gas supplies with the associated NGL production (**Figure 14**).

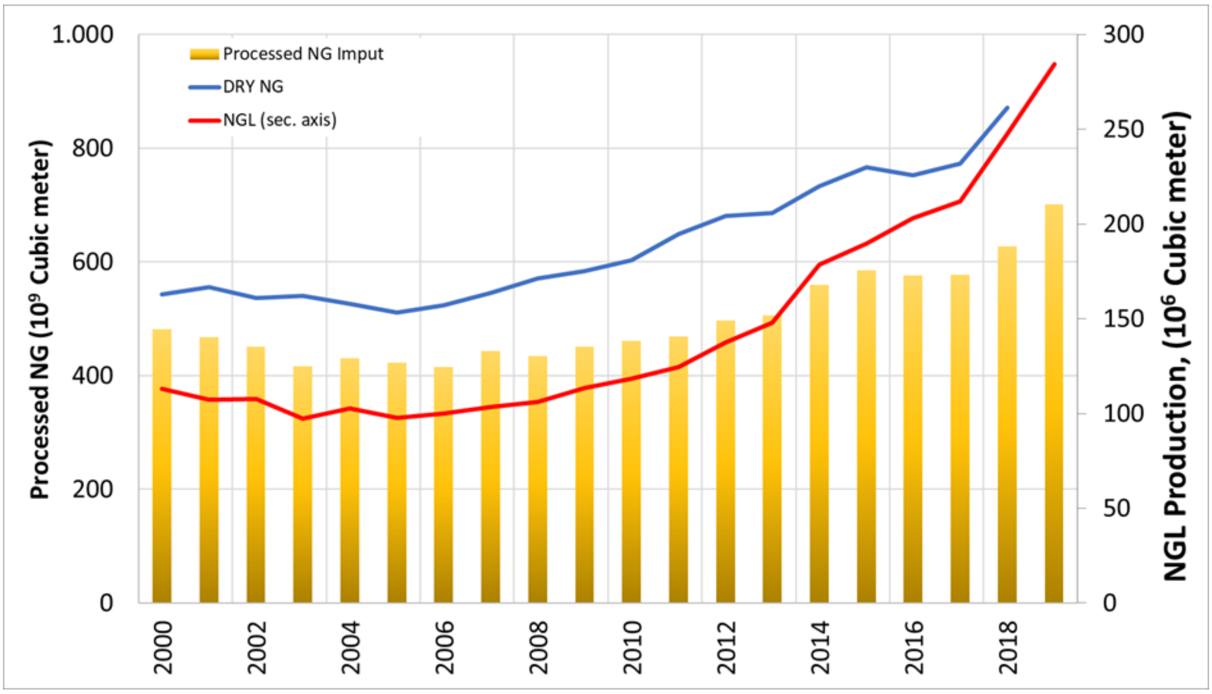

Figure 14: NGL production in the USA [188] [189]

In addition, NGL distribution differ for the Fuel and Petrochemical Strategies. LPG customers are scattered throughout the Brazilian territory [122]. Distribution logistics requires several levels of traders from industrial scale to wholesale and finally retail in a structure that allows fractioning quantities to reach final users. In this way, the LPG transport can reach remote and distant regions [154]. Thus, despite the existing bottlenecks, LPG has been preferred over propane (as a petrochemical raw material), in NG processing plants in Brazil.

In the USA, LPG products are seldom distributed as mixtures. According to EIA [190]: "Virtually all HGL[15] products distributed in the U.S. consumer market with the LPG label is HD-5[16] propane. Propane constitutes most of U.S. marine HGL/LPG imports and exports". HGL transportation (large scale) occurs in pipelines, railroads and trucks to reach final consumers [190]. Comparing to Brazil, where LPG transport occurs mostly by trucks, the use of railroads to transport HGL, mainly over long distances, seem to be a scale advantage for the USA system given the continental dimension of both countries.

In turn, transporting basic petrochemicals, as well as ethane, is not easy, and infrastructure and logistics is a limiting factor. Ethane is a light gas and it is not a simple to trade it [26]. It is unlikely that this gas become an export commodity. Building exclusive and long-distance pipelines for transporting ethane is costly. This explains why steam cracking units are normally intertwined with natural gas infrastructure [185].

Again, in the United States, a relevant existing condition for the petrochemical boom was the concentration of idle capacity of crackers close to the major plays where the shale gas became available. Most of the existing ethane crackers are concentrated in the Gulf region of Texas and Alabama [158] [157]. In sum, in the USA, the existence of idle capacity, favorable infrastructure [132], geographic localization and concentration of ethylene crackers rallied for this petrochemical surge underpinned by the upward shale gas production [158].

Developing petrochemical poles using natural gas faces constraints up and downstream the steam cracker: to establish a petrochemical value chain, processing facilities should yield enough ethane to supply a steam cracker. Downward, the second-generation chemical plants have a lower scale, so a steam cracker needs many buyers to reach its full capacity [158]. This condition was a relevant cost-reduction factor in the USA, since no new units were required when cheap natural gas become available from shale plays [131].

[15] Hydrocarbon Gas liquids

[16] Commercial propane specification for U.S. market

2.5.2 Market structure, contracts and production

The Brazilian refining and natural gas processing industry was in practice a monopoly until recently. Refining was almost fully owned by Petrobras until 2021, when Petrobras confirmed the sale of its first refinery (RLAM) to an international investing fund [191]. In 2020 the first private processing unit (UPGN Caburé) was authorized by the national regulator [192]. Verticalization in the natural gas industry may present advantages, mainly when gas is associated with oil and is a side product. However, verticalization may affect prices transparency, resulting in discriminatory practices [193]. In Brazil, natural gas prices are currently (2021) much higher than Henry Hub prices. In the last two decades, Brazilian and North American prices displayed almost inverted trends (**Figure 15**).

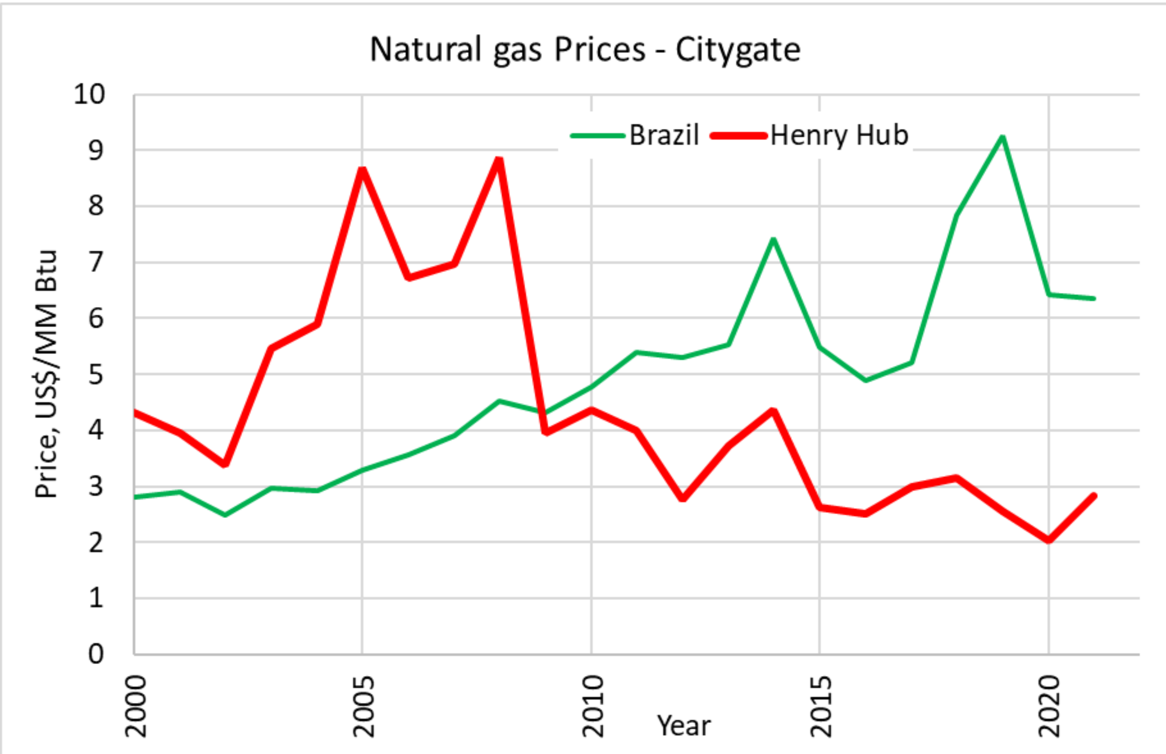

Figure 15: Natural gas Prices – Comparative between Brazil and USA (Gulf of Mexico) – Citygate average. Based on values obtained on [147] [148] [101]

Such high natural gas prices in Brazil are critical for the Fuel and Petrochemical Strategies. In this case, as the specifications of NGL mixtures are relatively easier to match, investing on less costly processing units is a natural choice for a risk-averse investor. This results in an advantage for the Fuel Strategy. Besides, the market structure for LPG in Brazil is well developed. LPG is delivered to a group of 18 distributors (the top 5 control 92% of the market) [169] which count on 70,000 resellers to reach final consumers (**Figure 16**).

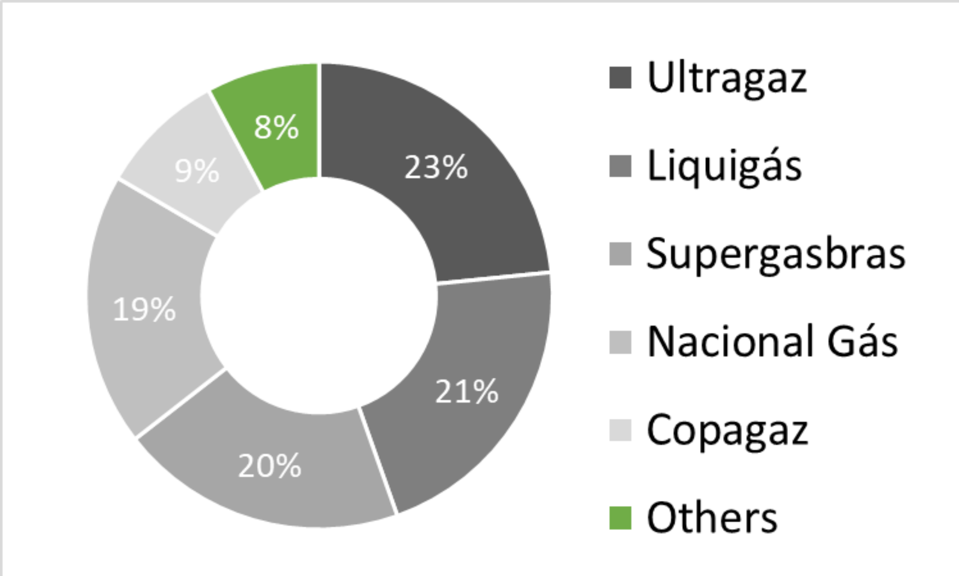

Figure 16: LPG distribution Market in Brazil [169]

In sum, the already developed LPG market structure is an advantage for the Fuel strategy in countries like Brazil. Distribution market is relatively settled. Market structure does not require extra investment to reach consumers [194].

Regarding the Petrochemical Strategy, in Brazil there is only one first-and second-generation petrochemical company, namely Braskem [161]. Therefore, the Brazilian petrochemical market is organized as a monopsony.[17] Moreover, Braskem imports ethene from its own factory in Mexico and buys ethane from Petrobras, in a contract agreed to end in January 2021, extendable for 2 years [162]. A new contract was signed between the two companies for ethane and propane which is valid until 2025 [163]. Braskem buys ethane and propane at Mont Belvieu prices and naphtha at ARA prices, and in 2017 started a project to produce 15% ethene from ethane in Camaçari industrial site (Bahia) [162]. Braskem buys

[17] For instance, Petrobras and Braskem have just signed a supplying agreement of naphtha valid for 5 years, starting on December 2020 [367]. The companies agreed on a 650 kt/y supply for the period 2021-2025 [367], which means that a relatively rich natural gas processing unit would meet close to 1/6 of naphtha demand in one year.

natural gas at Henry Hub prices in Mexico but pays local market prices in Brazil, and sells most of its production to the Brazilian market (exports represent nearly 30% of Braskem's revenues) [162].

Notwithstanding, the current capacity for producing ethane in Brazil is idle, and the country has a deficit in petrochemicals like resins, which is expected to last [164]. In addition, part of national capacity for ethane production is diverted to natural gas streams instead of being oriented for petrochemical use, indicating that increasing petrochemicals feedstocks production in Brazil may face constraints. Some other studies corroborate this stalemate [195] [97] [155], while investments in natural gas processing units focusing on NGL are upcoming in Brazil [139] [196].

Therefore, it is possible to infer that ethane production is not attractive in Brazil due to the high natural gas prices. Buying natural gas at Brazilian prices and selling it at Mont Belvieu prices was 3-4 times less attractive in 2019-2020 then buying NG at Henry hub prices. Since Braskem is a monopolist in selling first generation petrochemicals, and it is a monopsonist in buying feedstocks, high internal NG prices are eventually transferred to third generation market, which has a diversity of players (12 thousand companies [197]).

Comparatively, the market structure in the USA has several producers delivering natural gas to processing units. There are 126 base petrochemicals facilities spread throughout the USA territory [122], and the American fuels and base petrochemicals manufacturers association has 450 members [198]. This competitive structure favor lower prices and competition. Interestingly, before the shale gas revolution, the petrochemical industry in the USA has faced severe constriction, losing place in the American economy and reaching overcapacity by the early 2000's [159]. Due to the shale gas revolution, steam crackers increased operation by 95% in 2010's [185].

On the contrary, the Brazilian petrochemicals market is highly influenced by imports [156] [165]. Brazil has just begun to diversify players, while Petrobras indicate a partial disinvestment plan for refining and processing. Therefore, there are severe constraints to develop strong first and second-generation petrochemical market in Brazil.

2.5.3 Regulatory Framework

The Brazilian natural gas market is not yet fully deregulated. The former Gas Act (11,909/2009) was superseded by Act 14,134/2021 [199], which aimed to provide the legal framework for transitioning from a vertically integrated to a liberalized and competitive market structure. However, Queiroz and Colomer [200] point that the regulatory changes may not be enough to promote the required changes in the Brazilian gas market and suggest further arrangements related to a competitive market development, such as regional regulatory frameworks, incentive policies, openness to new investors and regulatory stability.

Comparatively, in the USA, the natural gas activity is regulated by the Federal Energy Regulatory Commission (FERC) [201]. Transport, storage, distribution and trading activities are unbundled and prices are not controlled. Customers can choose which supplier will delivery gas, so as the interstate transport company. This arrangement grants full flexibility to the natural gas market and prices.

Figure 17 shows Brazilian prices for LPG and gasoline (straight lines, secondary axis in US$/kg) follow international trends (dotted lines, US$/M Btu).

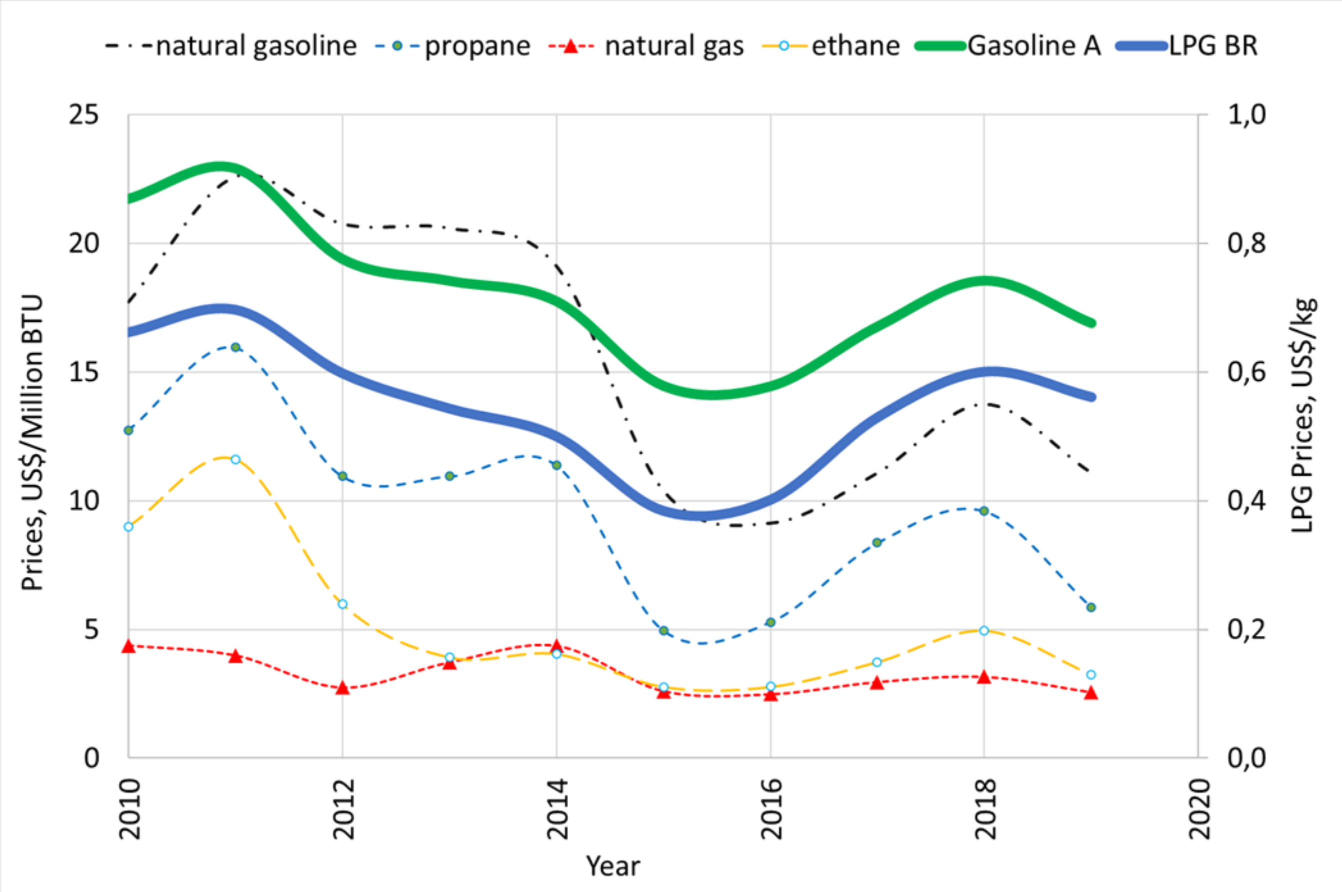

Figure 17: Comparison between international petrochemicals (USA) and Brazilian prices. Based on [115] [169] [202]

As market prices for fuels are set by the petroleum regulator following the international parity, and petrochemicals prices result from a market controlled by one single monopolist and monopsonist company, new entrants may face strong barriers to entrance the Brazil´s petrochemical market. In sum, risk-averse decision makers in Brazil would rather invest in energy products than in petrochemicals, given the already existing fuel market and logistic in Brazil and the market structure in place.

2.6 Discussion

Fuel Strategy

In spite of the results of the financial analysis of this study, the Fuel strategy has some advantages compared to the Petrochemical strategy. Firstly, the Fuel Strategy provide output streams that are mixtures of hydrocarbons. Hence, the required gas processing technology is less expensive. Moreover, LPG is a widely used fuel in Brazil. Replacing firewood in poor regions by LPG is a relevant social policy in emerging countries [203], [204], such as Brazil, where there is an already established market for LPG.

Actually, composition results from COMP-0 meet both gas transport network and LPG regulation. This simulation depicts how NGL are currently traded in Brazil. The operator does not need to find market for the ethane stream, since it goes along with dry NG sales. COMP-1 is a general post-salt composition from a non-associated field (Mexilhão) in Brazil. Compared to COMP-0, it yields high levels of natural gas products for the transportation network. However, this composition might affect NGL market, since it offers low amounts of LPG. Finally, COMP-2 simulations reveal that the extra rich natural gas would require new destination for ethane products, since the produced dry natural gas does not fit the maximum allowed ethane amounts of the Brazilian dry gas specification. Honoré [205] indicates similar concern in the Netherland, due to changes from domestic production (low heating value) to imported NG (high heating value), and points that changing gas facilities would take ten years and require long-term planning. Moreover, COMP-01 supplies a higher amount of butane, which is closer to Brazil's stablished range, while COMP-0 and COMP-2 result in excess of propane. This pre-salt gas composition (COMP-2) may be considered the typical future gas supply in Brazil [125] [126]. Therefore, the processing plant operator needs to find market for the ethane stream.

In addition, it is worth stressing that the Brazilian authorities recently committed to reach carbon neutrality by 2050. In this case, the Fuel strategy can become inconsistent with such commitment. This is particularly true for C5+ fractions, which usually compose the gasoline pool, under the Fuel strategy.

Petrochemical Strategy

Silluria [206] indicates that the conventional steam cracker capacity ranges from 500 kt/y to 1500 kt/y, while ethylene consumers use it in a scale ranging from 50 to 150 kt/y. This means that 4 to 10 ethylene consumers would be required for the smaller cracker size.

The rich gas input (COMP-0) supplies high amounts of ethane. As the reference processing unit (40 M Sm^3/d) is based on five independent modules of 8 M Sm^3/d, for this composition, two of these modules would be enough to supply the smallest feasible cracker presented in Silluria [158]. Besides, the main industrial conventional route for petrochemicals production being steam cracking of ethane (or naphtha) in thermal cracking furnaces [207], co-cracking option can also be considered. Yang and You [124] evaluated producing 1000 kt of ethylene departing from 150t/h (1200 kt/y) ethane and 101.8 t/h propane in a conventional integrated system or 197 t/h of an ethane/propane mix in co-cracking (60%/40% w/w, 952 / 626,4 kt/y), both producing 125 t/h 1000 ethylene and 28.4/87.1 t/h (227.2/ 696.8 kt/y) propylene, respectively. Therefore, for a ratio 60/40 for C2:C3 [124], having ethane as a limiting supply, the high propane volumes in COMP-0 and COMP-2 would supply a total hydrocarbon input of 2034 and 2748 kt/y. For instance, the existing ethane cracker in Brazil (located in Duque de Caxias, in the metropolitan area of Rio de Janeiro city) is sized to produce 520 kt/y ethene [166], consuming 620 kt/y ethane [167]; in addition it produces 75 kt/y propene [166], thus consuming 517 kt/y propane [167].

Finally, even for the leaner composition (COMP-1), the obtained ethane stream can supply the minimum required capacity for an ethane cracker (500 kt/y) found in the literature. For the propane feedstock, if co-cracking is considered in a mass proportion 60/40, an extra capacity of 484 kt/y propane can be absorbed in the lean composition case, resulting in a total hydrocarbon load of 1211 kt/y.

Financial Analysis

The stochastic DCF analysis proved to be worthwhile, as price uncertainties resulted in a higher standard deviation for the Petrochemicals strategy´s NPV. This somehow is an expected result, as the market of non-energetic products tends to be less correlated to the gas market, when compared to the market of fuels (LPG and even C5+ fuels). However, the quantification of this fact is relevant. It shows that, while the process engineering analysis indicates that the gas facility has a proper scale to supply the Brazilian petrochemical market, this could be a risky strategy given the prices for feedstock and products (or in a simplified way, given the price margins faced by the facility). The analysis of market failures raises other challenges to the Petrochemical strategy, due to the market structure of the Brazilian chemical industry.

In general, the use of combined approaches to evaluate gas processing facilities was not found in previous studies, which focus on plant process engineering or even monetization on market aspects, and few on the use of probabilistic analysis. But none has used stochastic NPV series integrated to process simulation studies and a market failure analysis to evaluate possibilities to monetize NGL. The results of this study indicates that, under a deterministic economic perspective, the Petrochemical strategy allows a better monetization of richer gas streams.

2.7 Conclusion

This study compared strategies to monetize NGL fractions focusing on petrochemical feedstocks or fuels. It combined process engineering simulation with probabilistic DCF analysis, followed by a market analysis. The main takeaways from this study are:

- Producing fuels seems to be the less risky strategy for lean natural gas streams. However, in terms of scale, even lean and moderate rich natural gas streams in Brazil can yield amounts of petrochemical feedstocks compatible with steam crackers capacities.
- The Fuel strategy meets the Brazilian specification for the dry gas in the case of lean natural gas inlet, but faces difficulties related to ethane content for richer gas inlet compositions.
- Although the Petrochemical Strategy reaches a higher expected NPV when compared to the Fuel Strategy, it is a riskier option and faces several barriers in Brazil. Particularly, logistic constraints and market concentration undermine the petrochemical strategy as of today.

However, the application of the combined approaches proposed by this study can be improved. Actually, the market barriers were analyzed here in a qualitative way, as usually done in the scientific literature. A further study could use the results of this analysis to re-run the DCF. For example, the market barrier analysis could serve as basis for introducing a discount on the prices of liquid products, associated with the buyer power market in the Brazilian petrochemical industry.

Moreover, the market failures identified by this study can help explaining the risk aversion of investors under non-competitive markets and price control policies for liquid fuels. This is always a threat in emerging countries, including Brazil [208].

Finally, future studies could also focus on a detailed logistics analysis. For instance, LPG has a complex and capillary distribution in Brazil, with many market failures, including a shadow supply market [209], which was not addressed by this study. The detailed logistic associated with basic petrochemicals was not addressed either, which already constrains the Brazilian market. The energy transition risks, which should be more challenging for the Fuel strategy, could also be the subject of additional analyses. Additionally, plastic ban campaigns can affect the Petrochemical strategy and can be incorporated as a transition risk, as well.

3 *Planning natural gas networks and storage in emerging countries – an application to Brazil*

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3.1 Abstract

Some emerging countries, such as Brazil, have large remaining natural gas resources but relatively poor infrastructure to monetize it. When most of the natural gas extraction derives from associated gas, this results in high reinjection rates in production fields combined with fuel imports also to deal with an increasingly variable demand. This study tests the hypothesis that modeling the natural gas transportation network expansion with Underground gas Storage (UGS) is crucial, as UGS can reduce transportation costs by better fitting natural gas supply and demand. Without UGS chances are that network expansion will be based in oversized pipelines, or pipelines often challenged by peaking demands. Therefore, this study emulated an existing natural gas transport network in a thermo-hydraulic model, aiming at diagnosing its bottlenecks mainly caused by demand intermittency, and pointing out infrastructure solutions. Findings indicated the design of UGS associated with new pipelines as a problem-solver for network bottlenecks, under a least-cost approach. This option reduced idleness and lowered gas transmission costs by 60%. In addition, it increased the network operation reliability and created a virtuous cycle, where a better planning reduces the gas tariffs and spur infrastructure expansion by raising the fuel competitiveness.

3.2 Introduction

Developing natural gas industry is a challenging task for emerging countries, which often present insufficient infrastructure and dissimilitude between planned and built networks [41]. This is a costly (high Capex) industry, where planners usually face challenges related to lack of capital to invest, regulatory setbacks, overrun costs, construction delays [210] [211] [212] and demand uncertainties [213]. However, natural gas infrastructure is seen as a strategic asset for countries, playing a central geopolitical role for both importers and exporters [214] [215] [216].

On the one hand, it is worth increasing infrastructure to tackle natural gas production increase, particularly when this gas extraction is associated with crude oil, as is the case in many emerging countries – see, for instance [217]. On the other hand, demand variability may create challenges for operating the natural gas transmission infrastructure – as emphasized by [218], [219] [220].

Our research hypothesis is that modeling gas transportation expansion with UGS from the start is crucial to optimize natural gas transportation networks, severely reducing costs. The implementation of UGS can create a steady demand in pipeline operation, as during high thermal power dispatch periods, UGS can become a supplying point; while during the low thermal power dispatch periods, UGS can become a delivery point. This is paramount, considering the increasing variation of natural gas demand due to power plants intermittent dispatch, and the underdeveloped infrastructure in emerging countries, particularly when natural gas extraction is associated with crude oil exploitation.

For coping with this objective, this study develops a thermo-physical analysis of a real existing natural gas network, and the economic assessment of the impacts of UGS on the gas transmission tariff. The study uses Brazil as a case study, although the methodological procedure can be well transposed to other similar cases, with likely the same main messages.

In the following section, we present a Literature Review, emphasizing the use of UGS in emerging countries and the scientific literature gap in infrastructure planning with UGS, particularly for emerging countries. Then, in Section 3 we discuss the model developed to test our hypothesis, detailing the thermo-hydraulic assumptions and the data collection for inserting into the model. In this study, we run a real gas network case based on the Brazilian natural gas industry example. Finally, in section 4, we show and discuss the obtained results, applying them to test our hypothesis and suggesting further improvements. The last section concludes the paper.

3.3 Review

Few studies have modeled natural gas transmission infrastructure addressing UGS role in emerging countries [221] [222] [223]. Usually, studies focused on natural gas mature markets in OCDE economies. For instance, [224] indicated that the proper infrastructure can foster the change from an inflexible linear market to a trading region with price convergence and arbitrage. Scholars [225] developed an economic modeling for testing the use of UGS to deal with seasonal gas demand variation. These authors addressed the seasonal variation of heating demands in OCDE countries. Moreover, Verzijlbergh et. al. [47] studied how the intermittent operation mode of thermal power plants can affect natural gas networks, which have to provide immediate gas availability when these electric power facilities are dispatched. For countries based on the complementary operation between hydroelectric plants and thermal power plants, this can lead to gas pipelines idleness during periods of rainfall affluence [226], [227].

Underground Gas Storage (UGS) is considered by Yu et al. [39] a crucial option to meet demand variation and reliability. When a UGS facility is not available, the natural gas carrier must rely on regasification plants and Liquefied Natural Gas (LNG) as a buffer, although, comparatively, UGS usually proves to be an efficient and less expensive option for gas storage and supply-demand regulation [50].

Most of the scientific literature on UGS focused on the geological [228] [229] [230] or technical analysis of UGS [231] [232] [233]. Some studies have also evaluated the UGS economic role [234] or tried to include it into the natural gas network assessment [235]. Nevertheless, usually these studies did not address fluid dynamics or rather presented simplified models [236] .

In turn, detailed studies on natural gas pipelines usually aim to improve the mathematical models representing the pipeline network either to evaluate operation or expansion [43], [237], [238]. However, usually these scientific works did not consider the UGS role for optimizing the network planning and operation, in their modeling exercise from the start. For instance, [239] modeled natural networks and aimed to find bottlenecks, but did not consider applying UGS to solve these bottlenecks, while [240] modeled a network in Poland considering LNG storage and biogas supply, but simply not indicating the UGS option. In South America, [45] used TIMES tool to develop a simplified natural gas network model for the Southern Cone countries but did not focus on UGS. Some studies [241] reviewed the scientific studies on steady-state and transient optimization of natural gas transportation via pipelines (both for gathering, transmission and distribution). These authors indicated that the studies´ aim could be divided into assessing short-term storage through line packing, evaluating gas quality satisfaction to deal with pooling/blending and finding the least cost solution for compressor stations and pipeline diameters, given head losses in pipelines. However, they did not highlight UGS as a possible game-changer to improve the optimization of pipeline expansion, particularly for dealing with variable gas withdraws. Even [242] who designed an artificial neural network to predict the optimum costs for a storage facility did not implement their analysis optimizing the network simultaneously with UGS as one of its facilities (being, hence, a consumer and a supplier node of the network, depending on the operation of it).

Hence, this study aims to fill this scientific gap by proposing a simple but effective methodological procedure modelling to associate the natural gas pipeline network expansion with the UGS option. Then, it applies this modeling to a real case in order to test the main hypothesis of the study, which formulates the likely benefits of associating UGS with the optimization of pipelines investments.

3.4 Materials and Methods

This section firstly details a basic methodological procedure that could be applied by planners intending to expand natural gas transmission networks in any country where this expansion is sought to be needed for different reasons. Then, the section entails the case study.

3.4.1 Network Model

The network modeling was created and simulated in the software *Pipeline Studio (PS)* [18], version 3.4.1.0, module TGNET. This is an engineering computer simulator that performs thermo-hydraulic flow calculation in a designed network. Pipeline Studio uses nodes for each pipeline branch and calculates the pressure loss for these nodes. Then, the software splits the flow through each branch according to its

[18] PS Developer is Energy Solutions, brand which is currently owned by Emerson www.emerson.com.

losses. For the purposes of this study, the tool is reliable and suitable, as it is applied for a single-phase fluid (processed natural gas), and the applied methodology includes a feasibility study.

Pipeline Studio (PS) is a simulation tool well known in the gas industry, allowing multiple approaches to solve gas networks issues [243], [244], [245]. Firstly, [243] run a comparison between TGNET and another simulator for a Coal Bed Methane site, where the authors display major equations and elaborate an accuracy evaluation. Then, [244] developed an analytical solution for transient flow in natural gas pipelines and validated their model comparing its results to Pipeline Studio's TGNET module. Finally, [245] apply Pipeline Studio to evaluate transportation capacity of pipelines branches, aiming at assessing supply reliability of natural gas pipeline networks.

Creating a new model in Pipeline Studio follows basic steps:

- Researching and defining engineering data like pipeline lengths, roughness and thickness for each pipe section, etc.
- Selecting thermodynamic parameters.
- Inserting operational boundary conditions like maximum and minimum pressures and capacities.

A reliable dataset is essential to build an accurate model. Since flow is mostly turbulent and diameter ranges from 8 to 38 inches, for a relatively large network, we applied the Colebrook-White equation, which combines partially turbulent and fully turbulent flow regimes for friction factor and flow rate calculation. In addition, we used the Sarem correlation that corresponds to a polynomial adjustment for the pressure and reduced temperatures established in the figure of Katz for gases and gas mixtures as equation of state for compressibility factor. The correlation developed by Sarem in 1961 applies to both pure substances and mixtures [246] and dismisses gas composition in its formula. Finally, we adopted the LGE equation (Lee, Gonzalez and Eaking) to viscosity calculation in compressible gas flow[19].

Then, when input data is complete for all parameters and correlations of the model, a convergence criterium should be defined, setting the number of interactions in the runs, and city gates delivery priority.

[19] For further details on the correlations used in our study, see the Supplementary Material.

A first run validates the model. When operational data is available from an existing network, it can be used to validate the model outputs.

3.4.1.1 Global Mass Balance

Global Mass balance provides the general supplies and demands in the network. The balance calculation consists of computing and comparing global supplies and demands in the area of influence of the pipeline to verify imbalances in a bottom-up approach. If demand exceeds supply, there is an evidence of gas shortage in the horizon of the study. If supply exceeds demand there may be opportunities for new pipelines

3.4.1.2 City gates (delivery points) distribution

A gas supply surplus in the global balance is not enough to guarantee that all demands are met in the network. Actually, locational aspects are determined by the pipeline infrastructure. Hence, the network balance must be investigated in relation to demands compliance. In an existing network, each delivery point has a consumption behavior and this trend is often repeated along years; thus, acquiring and using historical data is relevant to forecast infrastructure constraints. Based on these data and supply information, a detailed input sheet is obtained to feed simulation model.

3.4.1.3 *Convergence Criteria*

Operational data inserted in the model were obtained from the network operator. Those data were set as limiting factors to control convergence. Often some delivery points need to be reduced or closed (equaled to zero) to obtain a valid convergence. Notwithstanding, the model may mathematically converge and break pressure limits or not fully meet all demands. This convergence is not considered valid, but its results are valuable to evaluate network behavior and identify constraints. A convergence that validates the model occurs when no pressure limits or other settings are broken and all demands are met. This means that the model converges and is valid when all demands are met at set conditions. Hence, when building the model, prior to identify network constraints in projections, comparing the model outputs to operational data is required. In this study, this validation was made by comparing operational data from [247], which composed our case study, to the simulated model outputs.

3.4.1.4 *Simulation steps*

The simulation steps are:

- Validate the model based on operational conditions of an existing infrastructure and compare its results to the obtained values from real operation. No meaningful deviation is expected from original data, since demands and supplies are known. Thus, the model is validated when all supplies and demands are met. It is a simple check that the built model is able to emulate real conditions.
- Network diagnosis. This diagnosis is based on the business-as-usual scenario for the natural gas demand evolution. It does not consider any changes on the existing network. It is a bottlenecks check.
- Finding bottlenecks. New runs evaluate changes in infrastructure, such as compressor stations, pipeline flow reversion, design new gas pipelines or other facilities such as UGS or LNG.

3.4.2 Case Study: Brazilian gas network

Brazil is a potential high-consuming country, whose 1P and 3P natural gas reserves total 364.6 $x10^9$ m^3 and $550.0x10^9$ m^3 respectively [89], and the production is expected to increase up to 253 million m^3/day in 2028 [125]. Brazil was selected as a case study, since it is already expanding the natural gas extraction (mostly associated with crude oil), without a suitable infrastructure in place for providing this source at prices that stimulate its demand. As such, In the last five years (2020-2015), although the natural gas extraction increased by 30%, gas reinjection also increased by 117% and the gas market did not follow the gas extraction decreasing by 30% [101].

In Brazil, gas-fired thermal power plants play a central role in gas demand, as they often operate as peak-shaving suppliers in electricity generation systems, while they have relatively short-time response to meet demands, being able to address intermittent peaks. Unlike temperate countries, where demand for natural gas varies strongly due heating demand between summer and winter, in Brazil, the thermal power dispatch is the main factor behind the gas demand variability [45]. As the Brazilian power system is based on the complementary operation between hydroelectric plants and thermal power plants, this leads to gas pipelines idleness during periods of rainfall affluence

3.4.2.1 *Existing Infrastructure*

The Brazilian gas transmission infrastructure onshore presents 9,409 km of pipelines from 8 to 38 inches[20] [101] and the maximum operating pressure (MAOP) between 20 and 100 kgf/cm^2 [21] [248]. In addition, the country´s natural gas industry has three LNG regasification terminals with total capacity of 41 million m^3/day, an importing pipeline (Bolivia-Brazil, the so-called "Gasbol") of 30.0 million m^3/day, and 14 Natural Gas Processing Units (NGPU) totaling 95.65 million m^3/day[22] of nominal capacity [91].

Brazilian infrastructure for transporting natural gas is relatively new, dating from 1974, and the country´s network covers a relatively small part of its territory (**Figure 18**). The network covers mostly the shore, has few branches, no UGS sites, and relies on three LNG plants and line packing for buffering peak demands.

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[20] Pipelines are usually traded in diameters named in inches (nominal size). The above values range from 0.2032 to 0.9652 m (SI units).

[21] 1961.33 to 9806.65 kPa.

[22] Totaling 1099.5 m^3/s. Due to the large amounts of traded gas whose contracted flows are daily averages, the gas flow is expressed in volume (standardized pressure and temperature) per day.

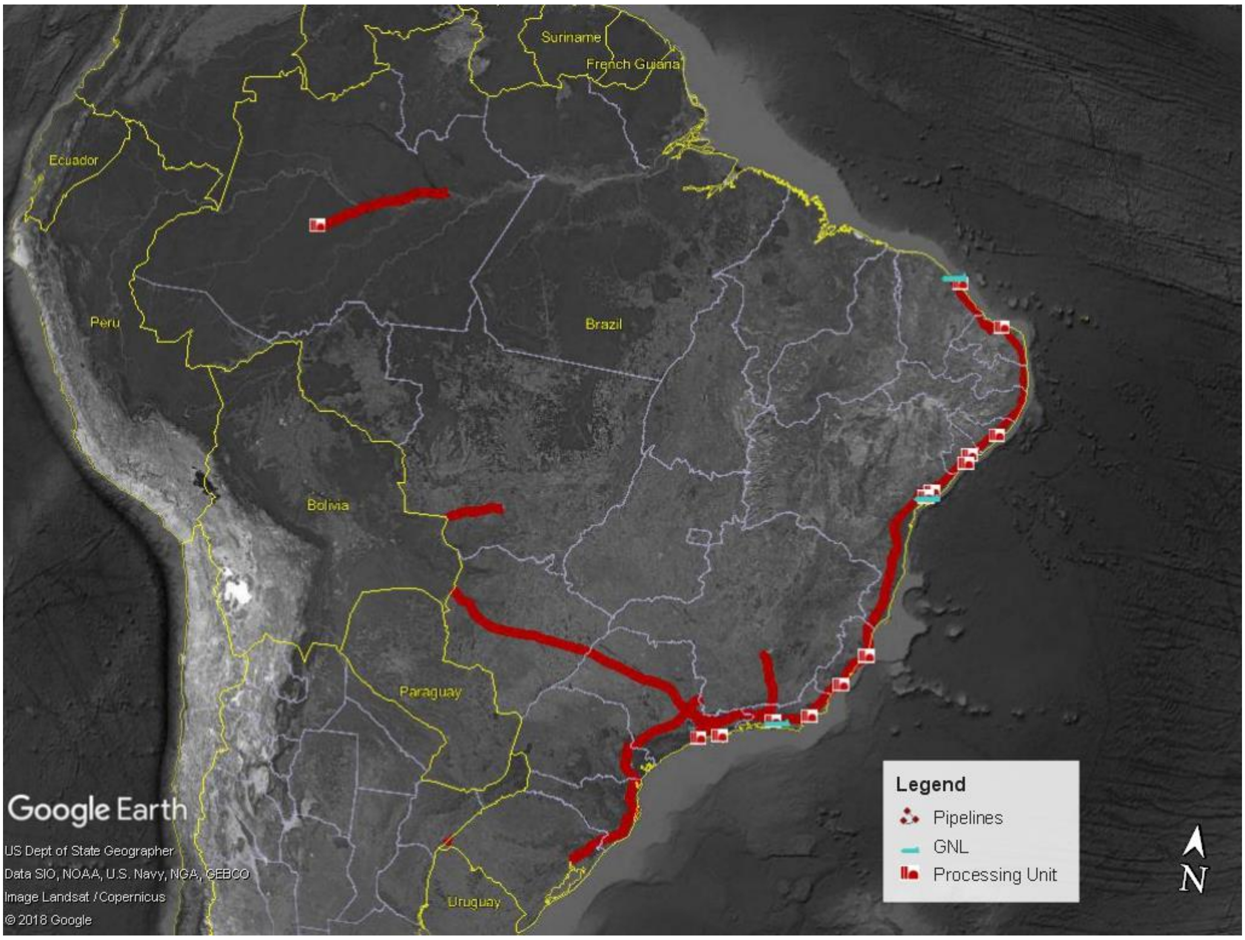

Figure 18: The Brazilian gas transmission network

Gasbol is the transmission pipeline modeled in this study, totaling 3.15×10^6 m (3,150 km) connecting Bolivia and Brazil. Most of it 2.59×10^6 m (2,593 km) lies in Brazil, the minor part 0.56×10^6 m – (557 km) being placed in Bolivia [247]. Gasbol has few supply points, being Bolivia its main source. In addition, there are two connecting points to the northern network. The southern section of Gasbol is "*telescopic*" going from 24-inch (0.6096 m) diameter in *Paulínia* (the northernmost point of the southern section), to 16 inches (0.4064 m) in *Canoas* (final southern delivery point). Gasbol pipeline (**Figure 19**) operates since 1999 (northern branch) and 2000 (southern branch). In 2010 the operator made an upgrade on the southern telescopic branch [247].

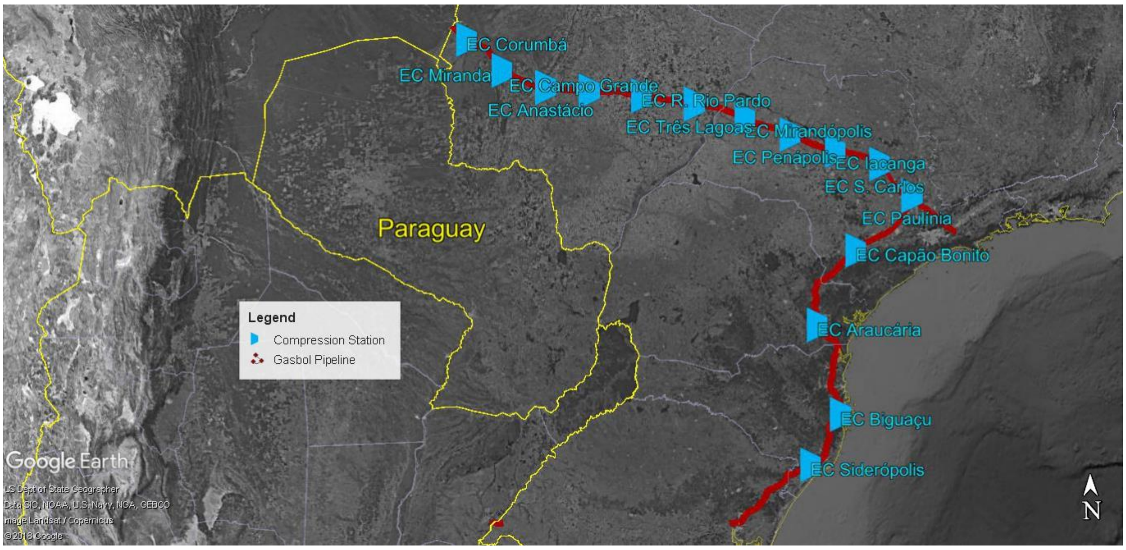

Figure 19: Gasbol pipeline in Brazil

That telescopic section includes two gas-fired thermal power plants, UTE *Araucária* and UTE *Canoas*. Besides, as aforementioned, due to the characteristics of the country´s power system dispatch, seasons when these thermal power plants not operate are common. According to Brazil's regulation, these plants are obliged to contract a natural gas minimum volume. Hence, the natural gas grid is idle when the thermal power plants are not dispatched and the gas available to supply them is negotiated through *interruptible* contracts. Gasbol transmission pipeline crosses 5 states and 136 municipalities in Brazil. The operating conditions of its Brazilian branches are summarized in **Table 15**.

Table 15: Main operational parameters of Gasbol pipeline [247]

Branch	MAOP*, kgf/cm^2 (kPa)	MP**, kgf/cm^2 (kPa)	Diameter, In (m)	Length (km)
Corumbá-Paulínia (north)	100 (9806.65)	35 (3432.34)	32 (0.8128)	717 547
Paulínia-Guararema	75 (7354.99)	35 (3432.34)	24 (0.6096)	153
Paulínia-Canoas (south)			-	-
Paulínia-Araucária	100 (9806.65)	35 (3432.34)	24 (0.6096)	341 130
Araucária-Biguaçu	75 (7354.99)	35 (3432.34)	20 (0.508)	70 200
Biguaçu-Siderópolis	75 (7354.99)	35 (3432.34)	18 (0.4572)	180
Siderópolis - Canoas	75 (7354.99)	24 (2353.6)	16 (0.4064)	65 185

*Maximum Admitted Operating Pressure
**Delivery points minimum pressure

Delivery point minimum pressure is established by contract. As simulation premise, when delivery pressure is lower than minimum, it is understood that the demand has not been met. This condition points out the grid´s bottlenecks. Gasbol displays 15 compression facilities[23] from max pressure output varying from 75 (7354.99) kgf/cm^2 (kPa) to 100 (9806.65) kgf/cm^2 (kPa) [247].

This study considers that all delivery points remain in operation within the period of analysis, as well as compression stations and valves. Since the objective is to guarantee supply in each delivery point, an infrastructure restriction is identified when any point in the network does not fully meet the forecast or operation maximum demand.

3.4.2.2 Natural Gas Processing Units (NGPU)

Produced gas is treated in NGPU before transmitted to final consumers through pipelines. NGPU separates liquids from gas and adequate the major stream to be sent to the network. To calculate the specified (dry) natural gas flow, an average processing factor is calculated, based on the global average ratio between gas input and output from installed facilities production (**Equation 7**):

$$F_p = \frac{V_p}{V_s} \qquad \textbf{Equation 7}$$

Where:

Fp = Processing factor
Vp = Gas input (year basis)
Vs = Dry gas output (year basis)

<u>Gas Demand</u>

Gasbol presents 47 city gates including, thermal power plants and refineries[24]. As for thermal power plants, maximum demand corresponds to the fixed flow to meet their nominal capacity. The same is valid for downstream units (refineries, etc.). For Local Distribution Companies (LDC), including

[23] For further details on the compression stations, see the Supplementary Material.

[24] For further details on the city gates, see the Supplementary Material.

industrial and residential deliveries, a year-based 9.5% increase on delivery was estimated, according to historical regional growth [249].

At this point it is relevant approaching hydrate[25] formation downstream processing units. Hydrate formation is a relevant issue for natural gas pipelines in general and an always present concern for pipeline operators, as emphasized by [250], [251], [252]. Hydrate formation requires three essential conditions: Lowering gas temperature, Elevating gas pressure and sufficient amount of water [253]. There are methods for avoiding hydrate formation conditions, and setting up the water dew point is a frequently used approach [254]. Natural gas should be processed prior to be transported to consumers, and two desiccation processes are used with this purpose: absorption by liquid desiccants and adsorption by solid desiccants [253]. After natural gas is processed and water is removed satisfactorily, additives may be injected in transmission pipelines prior to avoid hydrate formation. Methanol is the most applied hydrate-preventing additive and secant, and water dew point curves may be plotted experimentally, combining temperature, pressure, moisture and additive quantities [255] for analyzing hydrate formation [256]. Therefore, the Pipeline Studio sets used in our study allowed simulating not only environment temperatures but also ground temperatures. Depending on the applied thermodynamic model, gas composition may also be set so flow conditions will be precisely determined [243], [244], [245]. In our study, in the simulations of Brazil´s case study, the allowed water dew point temperature in processed natural gas for transmission (high-pressure) pipelines was set as -45 ºC (228.15 K), according to the country´s National Regulation Office specification [257]. Average temperatures in Brazil are considerably higher than this limit, seldom peaking zero degrees Celsius [258]. In Brazil, Normal (standard) flow temperature according National Regulation Office is 20ºC [169].

The modeling procedure of this study emulated an existing network (depicted in **Figure 20**) to evaluate its operation and propose improvements by adding UGS to manage bottlenecks.

[25] Hydrates are solid and crystalline compounds formed from water and mainly small molecules such as methane, ethane, propane, carbon dioxide and hydrogen sulfide.

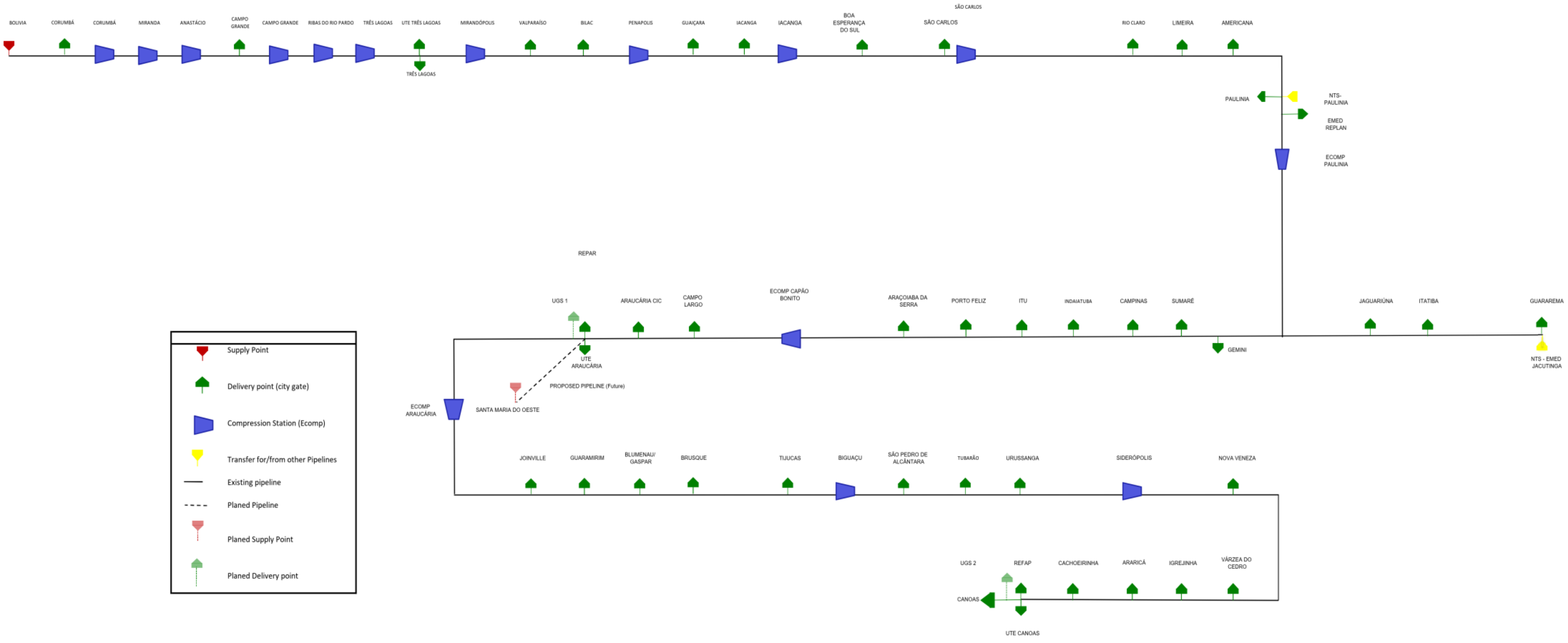

Figure 20: Network model created in pipeline studio.

3.4.2.3 *Potential gas supply expansion*

Accumulations of non-associated onshore gas are likely in the following Brazilian sedimentary basins. Barra Bonita Field in Paraná basin (Figure 21) estimated gas volume in place is around 500 x10^6 m^3 and 1.12 billion barrels of oil [90] [259].

This study proposes to connect a transmission pipeline from *Barra Bonita* field to Gasbol. Santa Maria do Oeste, a town in the State of Paraná, was the reference for supply point and the closest existing compression station (Ecomp), Araucária (344 x 10^3m) is the delivery. Pipeline tracing was estimated using software Google Earth [260] from a corridor already expropriated, such as a road. This approach is adequate for preliminary analyses [261]. **Figure 21** shows the defined route of the new pipeline named here as Santa Maria do Oeste-Araucária (SMO-Araucária).

Figure 21: SMO-Araucária pipeline and possible locations for UGS sites: Araucária (PR) and Canoas

Forecast supply and demand series were prepared based on available data from 2014 (year 0) to 2024 (year 10).

3.5 Results

3.5.1 Model Validation

Validation was based on operational data [247]. The validation criterion is that all demands must be met when the model converge and the flow error should be under 1%. For validating purposes, only flow results are required, once delivery pressure is set for minimum values and the convergence criteria acceptation means that required pressures were reached. The same criteria apply for maximum pressures in supplies and valves positions (on/off; control valves openings, etc.). For the 47 evaluated delivery points, results indicated error values varying between 0.000% to 0.377 %, (**Figure 22**)[26], and for most of them (44 city gates), errors were under 0.02%, which validates that the built model can reproduce historical data, and further emulating deliveries and supplies. This also corroborates the choice made for the PVT and friction factor correlations in the tool. Since most of high-pressure pipelines connecting supply nodes to citygates present partially turbulent and fully turbulent flow regimes, we can expect that with minor or even no changes our procedure could be applied to other cases.

[26] For further details see the Supplementary Material.

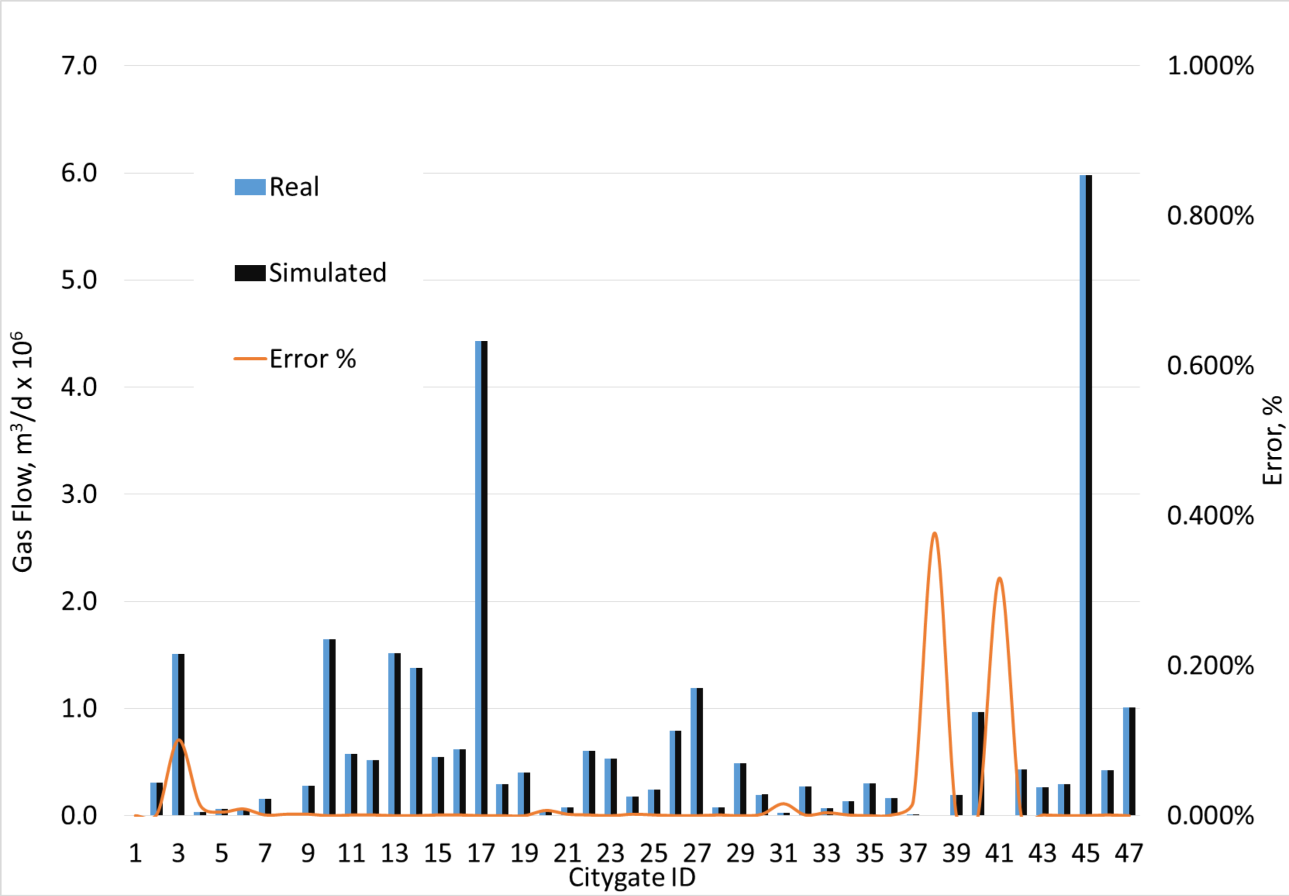

Figure 22: Simulation model validation results

3.5.2 Network Diagnosis

The network diagnosis aims at finding where a bottleneck appears in the pipeline infrastructure. Actually, findings confirmed Araucária delivery point as a severe constraint node, where operation pressure reduces from 100 to 75 kgf/cm^2 (9806.65 to 7354.99 kPa) and pipeline diameter decreases from 24 in to 20 in (0.6096 to 0.5080 m). In this case, a growing-demand scenario of 9.5% per year (LDC) would create a bottleneck in the network. Four years after the base year, the gas carrier would need to reduce its deliveries to meet contracted demands, mostly to reach its extreme south deliveries. In addition, the gas balance indicates an increasing risk of failing deliveries if thermal power plants are required to operate simultaneously at maximum capacity.

Moreover, six years after the base year, the mass balance indicates the need to restrict supply to power plants (*Canoas, William Arjona*) and Três Lagoas. A conventional possible solution for capacity expansion and meeting these demands would be duplicating the section between city gates *Igrejinha* and *Canoas* in year 5, plus a compression facility in *Várzea do Cedro*. Finally, in year 10 there would be an average deficit of $20x10^6$ m^3/d (231.5 m^3/s) in the network, considering forecast demands and supplies. Our study forecasts that a growing demand scenario in year 10 leads to the closure of all thermal power plants, including those in Gasbol's northern branch, combined with the fact that the pipeline would not have capacity to meet demands of UFN III fertilizer plant and REPAR oil refinery. Otherwise, it would not be possible to guarantee gas supply to LDC delivery point Canoas in extreme South. LDC consumers include industries and households that are seen in the Brazilian regulation as priority gas users, since power plants may eventually be replaced by other power facilities. A conventional but expensive solution to meet the demands would be duplicate the southern branch of Gasbol from *Paulínia* to *Canoas*.

3.5.2.1 Expanding gas supply: SMO-Araucária Pipeline sizing

The present study fixed as premise to deliver at least 86.8 m^3/s (7.5 $x10^6$ m^3/d) of gas at minimum pressure of 3432.3 kPa (35 kgf/cm^2) and MAOP of 9806.65 kPa (100 kgf/cm^2), which represent the contract limits for most pipelines in Brazil. Pressure losses limits were set according to a rule of thumb [246]. This rule avoids computational efforts at extreme conditions. Therefore, losses lower than 15 Pa/m (kPa/km) and higher than 25 Pa/m (kPa/km) were considered excessive.

Findings indicated the use of 20 in (inches) or 24 in pipelines. Those 18 in runs showed pressure losses above the recommended for most situations, and pipelines with diameters above 26 in exceeded the required flow rates. Pipeline diameters of 26 and 28 inches delivered more than 70% the required flow, which indicates that costs would likely to be excessive. Thus, maximum diameter of 24 inches was enough for attending minimum flow requirements, indicating a feasible and economic option. Therefore, the selected pipeline was the one that met the maximum and minimum conditions of gas delivery, when integrated to the existing network given the demand projections.

Simulation connecting the new pipeline to the network, associated with Gasbol back pressures, showed insufficient flow rates and very high head losses for 20 in diameter. Moreover, the selected diameter was 24 in for a pipeline without a compression station. Possible future compression stations depend on more accurate ramp-up[27] information. From year 5, when the operation of the pipeline SMO-Araucaria was projected to start-up, part of the imported supply of Bolivia would be displaced by the natural gas supplied from SMO, being able to attend Gasbol Southernmost branch. In addition, the startup of this new pipeline avoids the needed capacity expansion in the network that was previously identified, in most of the branch between Paulínia and Araucária. This also allows the imported gas from Bolivia to be redirected to other regions.

Therefore, our analysis indicated that a new gas supply source close to the identified bottleneck site, when connected to this site, improved the gas transportation network without the need for investing in capacity expansion in most of the branches of the original pipeline. This means that after identifying bottlenecks in gas pipeline networks, it is worth evaluating if these bottlenecks can be easily solved by new gas supply sources than by expansions in the branches of the original networks. It remains to be seen, though, if the addition of the UGS option still enhances this solution.

3.5.2.2 UGS facilities

Connecting a UGS to a network, in short, involved three steps:

1) Developing a storage project, that involves studies on the local geology, reservoir conditions and technical characteristics required to make it possible to store gas.

2) Filing the storage facility. During this period the UGS site becomes a demanding point in the network. Natural gas must be supplied to the site to fill the reservoir.

3) Becoming a supplying point. When the reservoir is full, UGS becomes a supplier and its working volume maintenance must occur in periods of low gas demand. In this study, the filling periods were forecast between years 5 and 6.

Concerning to locations, two possible sites were evaluated for their role in the network:

27Ramp-up determines the expected growth of demands over time and can determine the option of smaller pipe diameters associated with compression stations at a more accurate stage of design ([246]).

- UGS CANOAS (extreme south): Since the thermal power plant (UTE Canoas) has to be supplied in its average dispatch (as a premise), in the simulated filling period, UGS Canoas stores 445 x10^3m3/d. Yet, this stored volume is insufficient to meet the demands of the region. In year 6 there would be no sufficient gas for simultaneous filling UGS, and supplying local distributors, Canoas thermal power plant and REFAP refinery.
- UGS ARAUCÁRIA: location in Araucária allowed a larger UGS facility than in Canoas. In Years 5 and 6 system may accumulate about 840 and 710 x10^3 m3/d, respectively. Nonetheless, faced with the projected growth of 9.5% in local distributors demand, the infrastructure restriction for the southernmost branch of Gasbol continues. In this way, the need for expansion of the pipeline to meet the demands of this region would remain. Therefore, an additional improvement was applied. In this case, UGS Araucária allowed the decrease of the new gas pipeline SMO-Araucária to the diameter of 20 inches. A feasibility study was run to evaluate the project.

Therefore, the solely implementation of a UGS in the identified bottleneck site (or close to it) did not solve the infrastructure restriction. However, by combining this option with the gas supply expansion, we were able not only to solve the mentioned restriction, but also to do that using a smaller, hence lower cost, new pipeline (20 inches compared to 24 inches). This means that our procedure step-by-step (from bottleneck diagnosis to expansion planning with UGS) was able to find an effective solution. It remains to be proved the economic efficiency of our finding.

3.5.3 Feasibility Study

The feasibility study adopted year 0 as the base date. The National Construction Index (INCC) was used for construction cost data escalation and the IGP-M (General Market Price Index) for gas prices adjustments [262]. This study considered capital opportunity cost of 11.75% per year [263], plus the risk factor of 2.87% [264], which is the estimated risk for investments in infrastructure in Brazil in the base year. The exchange rate was based on average daily values in year 0. No leverage or depreciation was considered for any alternative. Taxes totaled 34% to income and 12% to added value [265]. Prices are not usually open in supply contracts in force in Brazil. Therefore, estimate values were applied (**Table 16**)

Table 16: Brazilian Specified Natural Gas prices estimate (US$/ 10^6 BTU)/ US$/GJ

Non associated gas - onshore fields	1.13/1.07
Associated gas - onshore fields	0.56/0.53
Non-conventional gas (low permeability reservoirs) - onshore fields	6.00/5.69

Source [266]

Investments costs in NGPU were based on Caraguatatuba plant, US$ 185.06 x 10^6 [267], processing 86.8 m^3/s (7.5 x10^6 m^3/d) of natural gas. Annual operating cost was estimated as 4% of Capex. Pipeline average cost was calculated in US$ per meter and per nominal diameter (US$/m.in). Data indicates that there is significant cost variation in relation to pipeline extension (**Table 17**), as some pipelines require more complex construction techniques, such as tunnels and directional wells. For the purpose of this study, average values were used.

Table 17: Gas pipelines investments made in Brazil

Gas pipeline	Length (103m)	Diameter (in)	Investment (106 US$)	US$/m.in*	US$/m.in (Nov/2014)
GASFOR II	83	20	123.82	74.59	74.59
GASAN II	38	22	54.84	65.60	83.40
GASPAL II	60	22	106.80	80.91	102.87
GASDUC III	179	38	979.08	143.94	197.06
GASCAC	949	28	1370.71	51.58	70.62
Itaboraí-Guapimirim	11	24	44.76	169.56	169.56
Average Value					**116.35**

Source: [267]

*US$ per each meter (length) and inch (pipe diameter).

Schedules were estimated as following: Project conception, 1 year [96]; bidding, 6 months; basic and executive project [268], 1 year and 6 months, respectively; construction and start-up, 1 year and 7 months for a 300 km pipeline [269], respectively. Considering that the previous periods do not overlap, the total project reaches 4 years and 7 months. Hence, this study considered a simplified period of 5 years for the construction of the pipeline from its conception to start. The data of the feasibility analysis is summarized in **Table 18**, following the results presented before in this paper.

Table 18: Gas pipeline SMO-Araucária

Length (10^3m)	344
Diameter (in)	24
Processed Gas flow UPGN (10^3 m^3/d)	7044.4
Design Pressure (kgf/cm^2)	100.0
Unitary cost (US$/m.in)	116.35
CAPEX (10^6 US$)	960.58
OPEX (10^6 US$)/yr.	38.42
Development time (years)	5
Disbursement (%)	10-10-20-40-20

Transmission tariff (**Table 19**) was based on the data from [270], updated by IGP-M.

Table 19: Tariff and Net revenue for SMO-Araucária pipeline

Updated tariff (US$/BTUx$10^6$) / (US$/GJ)	3.17/3.00
Net revenue (10^6 US$)/yr.	304.16

Investment in UGS was based on the amount of gas in the network available to be stored [49]. This value was used to define UGS maximum size. Average CAPEX is estimated at US$ 0.70 per m^3 of working gas. The average OPEX of 0.6 US$ per m^3 of gas withdrawn was applied [49]. UGS total revenue is calculated considering that gas injection into the reservoir takes half of its available operation time. Therefore, revenue corresponds to the withdrawal operation for 182.5 days. **Table 20** summarizes economic results for UGS Araucária.

Table 20: Output of UGS Araucária.

Operation	
Stored volume ($x10^6$ m^3)	565.8
Minimum withdraw 1% ($x10^6$ m^3/d)	2.8
Maximum withdraw 5% ($x10^6$ m^3/d)	14.1
Costs	
CAPEX ($x10^6$ US$)	198.00
OPEX ($x10^6$ US$)/yr.	24.28
Development time (years)	7
Disbursement (%)	2-3-5-15-25-35-15
Revenue	
LNG average price (US$/BTU$x10^6$) / (US$/GJ)	11.4/10.05
Domestic gas price (US$/BTU$x10^6$) / (US$/GJ)	8.6/ 8.15
Storage tariff (US$/ BTU$x10^6$) / (US$/GJ)	3.2/3.03
Minimum revenue ($x10^6$ US$/yr.)	92.58
Average revenue ($x10^6$US$/yr.)	277.75
Maximum revenue ($x10^6$ US$/yr.)	462.87

Net present value (NPV) calculation considers revenues from average withdrawal of $8.5x10^6$ m^3/d. Exempted from taxes, it corresponds to US$ 776.80 $x10^6$. NPV plus taxes equals US$ 201.63$x10^6$. This proves that the proposed UGS reaches positive NPV. Being based on a gas integrated gas planning (pipeline and UGS), this facility can be attractive to private investors.

3.5.4 Tariff Calculation

Another way to evaluate the feasibility of the same project is to find the required tariff to pay the investment opportunity cost. The reference tariff used in this study to evaluate the proposed investments feasibility is the average tariff of US$ 2.66/ 10^6BTU, updated by prices index IGP-M to US$ 3.17/10^6BTU (Table 21). Therefore, tariff values lower than US$ 3.17/ 10^6BTU would be feasible. Three options were assessed: 1) pipeline SMO-Araucaria (no investments in gas processing facility); 2) pipeline SMO-Araucaria (investing in a gas processing facility); 3) pipeline SMO-Araucaria (investing in a gas processing facility) associated with UGS.

As can be seen in **Table 21**, only the last option would be feasible, highlighting the advantage of associating UGS with the proposed new gas pipeline. Moreover, it is worth noting that the tariff of this option is around 60% of the current tariff in Brazil during the same period, meaning that it could boost the gas market in the region, by lowering prices, and even justify the new source of gas in Parana Basin, by guaranteeing the demand.

Table 21: Gas transmission tariffs for the gas pipeline SMO-Araucária (US$/106BTU)/ (US$/GJ)

Pipeline SMO-Araucaria	3.65/3.46
Pipeline SMO-Araucária + gas processing	4.30/4.08
Pipeline SMO-Araucária + gas processing + UGS	1.77/1.68

Therefore, although the impressive gas transmission tariff reduction found in this study clearly refers to the case studied, we can safely stress that, firstly, our step-by-step procedure was able to find a proper solution for both solving bottlenecks and lowering gas transmission cost, and secondly UGS must be assessed when planners evaluate the expansion of existing networks, instead of being implemented after this expansion.

3.6 Conclusion

Our study proposed and applied a simple method for evaluating existing networks to find and solve potential bottlenecks associated with a growing and variable gas demand. Clearly, solutions that point to new pipelines indicate that these planned pipelines should be designed integrated to the existing network where they are inserted. Performing simulation runs allow the comparison between single and integrated solutions, as well as offer options for investigating supply and demand variations. Some macroeconomic expectations are essential to evaluate future supply and demand balances, but locational issues are only revealed when all network maximum conditions, such as maximum pressure and flow are stressed. In these boundary conditions, the planner may anticipate network bottlenecks, propose and assess adequate improvements.

Usually, bottlenecks are solved by oversizing and increasing compression power, however this solution is far from offer the optimized solution. In emerging countries, where capital is scarce (or the opportunity cost of the capital is high), it is paramount to evaluate a diversity of alternatives.

Our study has shown that UGS can be a feasible option for solving bottlenecks and should always be considered part of the solution for network idleness (main hypothesis of our study). Its effects in pipeline sizing can be relevant, decreasing required diameters and reducing costs. Further, it inserts in the network a double function point, able to demand when intermittent demand is low, and to deliver when intermittent demand peaks. Actually, despite requiring higher investments than a single pipeline solution, UGS facilities can also benefit from revenues associated with gas trading arbitrages and cost reductions. This positive combination can result in lower gas transmission tariffs, thus fostering natural gas competitiveness to final users.

Integration between natural gas network and power transmission was not assessed in the scope of this work. However, UGS facilities can increase gas supply reliability. Such aspect is relevant for gas delivery contracts that include high penalties for delivery not accomplished. A future analysis should investigate operational savings from this aspect.

Moreover, UGS facilities create trading points in the network, which may even favor gas trading hubs and market regulation. This is a relevant issue to be studied in emerging economies where the trade of gas is used based on long-term contracts between suppliers and consumers indexed to rigid clauses.

UGS geological conditions are a relevant aspect concerning storage fields' development. In our analysis, we freely placed a UGS facility nearby a region. Due to geological conditions, such placement might be less simple. However, in fossil fuels producing regions, depleted fields occur quite often and salt aquifers are also available. A detailed analysis for implanting a UGS facility should put efforts on developing storage fields near to gas networks, thus increasing those facilities benefits.

The present study did not address an increasingly restrictive scenario for greenhouse gases (GHG) emissions as the one preconized by the Paris Agreement. However, planners should bear in mind that this scenario is likely to happen. Therefore, reducing GHG emissions should be one of the main concerns for planners and decision makers [271], also when they evaluate the expansion of the natural gas industry. In this case, a possible option could be converting methane to hydrogen. Therefore, future network development should investigate a possible synergy between natural gas infrastructure and the perspective to produce hydrogen from natural gas to pave the way for cleaner sources. In this case, UGS can be also a game changer, by allowing the storage of natural gas in order to regularize the hydrogen production and insertion in the network, also controlling the quality of the natural gas-hydrogen pooling.

At the end, our results indicate that UGS should be better investigated especially in emerging countries, and this must be done with the support of appropriate methodologies and tools. This can create a virtuous cycle where a better logistic planning reduces gas tariffs and stimulates the demand that justifies the logistic and supply expansion.

4 Blue Sky Mining: strategy for a feasible transition in emerging countries from Natural Gas to Hydrogen

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4.1 Abstract

Natural gas is often considered a transition fuel to a deep decarbonized world. However, for this to happen, new technologies should be fostered, among which a natural gas-based H_2 industry can become a key-option. This study tests the hypothesis that the development of a natural gas-based H_2 industry equipped with CO_2 capture can monetize natural gas remaining resources, mitigate CO_2 emissions and facilitate the transition to the renewable energy-based H_2. To do that, this study evaluates a stepwise strategy for setting up the development of H_2, departing from the idle capacity in the existing natural gas industry, to progressively create a H_2 independent supply. Findings indicated that this strategy can be feasible, according to the case study assessed at relatively moderate crude oil prices. Nevertheless, CO_2 storage can become a constraint to deal with the co-produced CO_2 from the steam methane reforming units. Therefore, it is worth developing storage options.

Keywords: Energy Planning, Hydrogen, Natural Gas Resources, Infrastructure, Hydrogen Energy.

4.2 Introduction

Upon transitioning from the intensive use of fossil fuels to renewable energies and ultimately to renewable hydrogen, the main actions are driven to the development of clean hydrogen production processes at scale, as most of the hydrogen currently produced has fossil origin. An eight-fold increase on the availability of hydrogen would be required up to 2050 [74]. Therefore, a variety of technological options, raw materials, and energy sources for hydrogen production must be made viable, taking into consideration that low environmental impact technologies will be preferred[28].

Dincer and Acar [70] have made a thorough analysis of nineteen hydrogen production methods, which were compared based on energy and exergy efficiencies, production cost, global warming potential, acidification potential, and social cost of carbon[29]. They found that fossil fuel reforming has the highest (83%) energy efficiency and lowest cost, while biomass gasification has the highest (60%) exergy efficiency compared to other selected options. Navas-Anguita et al. [71] approached the specific case of road transportation decarbonization using hydrogen and considered different scenarios for banning the use of hydrogen from fossil-based origin (2030, 2035 and 2040) to conclude that hydrogen production by steam methane reforming with carbon capture and storage would satisfy the demand for road transport in the short-to-medium-term. The real cost-effectiveness use of fuels should consider externalities such as damage to forestry from acid rain, climate change as a result of greenhouse gas emissions, and health impacts from air pollution in cities, none of which are internalized in the form of levies, such as carbon taxes [272]. In this sense, Al-Qahtani et al. [72] presented a comprehensive assessment of the most promising ten hydrogen production technologies considering simultaneously their cost and externalities due to impacts on human health, ecosystem quality and resources depletion, by means of a correlation gathering those variables. The internalized cost of environmental externalities was combined with the levelized cost of hydrogen to generate estimates of the "real" total cost of hydrogen. The authors evaluated

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[28] Presently, 96% of world H_2 comes from fossil fuels [65], being the steam methane reforming (SMR) the source of over 70% of global H2 supply [73].

29 Nazir et al. [76] classified the hydrogen production from fossil fuel methods according to two basic approaches, hydrocarbon reforming and hydrocarbon pyrolysis; while an early work from van der Burgt, Cantle and Boutkan [369] analyzed the synthesis gas via coal gasification, and applied both hydrogen and CO2 for fueling combined cycle power facilities. More recently, Kaplan and Kopacz [33] assessed four variants of coal gasification to hydrogen with CCS in Poland, performing a sensitivity analysis for each case. The authors observed that coal reserves might be unexplored if there is no kind of stimulus to this technology.

the influence of each variable on total cost of hydrogen, which was strongly impacted by the environmental externalities in fossil-based hydrogen, ranging from 57% to 76% in steam methane reform with and without carbon capture and storage, respectively; 62% in methane pyrolysis; 78% and 88% in coal gasification with and without carbon capture and storage, respectively. The steam methane reform with carbon capture and storage presented the lowest unabated total cost of hydrogen, US$4.67/kg$H_2$, and was classified as the most effective hydrogen production route, while the levelized cost of hydrogen production was found to be US$1.88/kg$H_2$ and US$1.26/kg$H_2$ for steam methane reform with and without carbon capture and storage, respectively[30]. The same type of result highlighting the cost advantages of steam methane reform can be found in other studies. For instance, Muritala et al. [75] and Nazir et al [76] [77] [78] compared the main technologies for producing hydrogen from fossil fuels and indicated that steam methane reform is the most mature and used technology worldwide and should maintain its place for producing hydrogen in the future.

Particularly, as for the hydrogen transportation and storage infrastructures, logistics might be one of the challenges for expanding hydrogen market under the energy transition [67]. Therefore, hydrogen deploying strategies often include the use of an existing natural gas infrastructure [67] [81]. Injecting H_2 at low blend volumes (e.g. 15%) in natural gas pipelines is considered an attractive (lower cost) destination for near-term produced hydrogen [69] [82] [73] [273] [274] [275] [276].

Actually, Messaoudani et al. [277] reviewed main issues concerning hydrogen blending in natural gas transmission pipelines and point some key issues for attention concerning the Joule-Thompson effect,

[30] Alternative processes for generating blue hydrogen were also proposed in the scientific literature. For instance, Abbas, DuPont and Mahmud [290] evaluated Hydrogen production from methane decomposition into hydrogen and carbon as a possible fashion to reduce CO_2 emission and showed that thermal decomposition may become competitive to SMR Labanca [330] adopted a plasma pyrolysis process using natural gas as feedstock generating solid carbon black instead of CO_2. This process was proved to be environmentally promising. However, compared to the SMR process, it yields half the amount of conventional SMR and required high amounts of electricity.

minimum ignition temperature and gas flammability. Despite these issues, the authors considered natural gas pipelines can transport hydrogen with minor changes, depending on the blending percentage applied[31].

These findings create the basis to explore how the main and abundant present source of methane, natural gas reserves, and its industrial infrastructure may strategically contribute to the energy transition and to the design of a new hydrogen energy era.

Technically recoverable world natural gas (NG) resources amount 810 trillion cubic meters [87] and proved reserves 198.8 trillion cubic meters [278]. Such vast resources could supply world natural gas demand for the next two centuries [81]. In addition, many emerging countries rely on rich fossil fuels reserves to support development and generate economic growth. Latin America and the Caribbean, for instance, present a steadfast production increase [87], from traditional players like Venezuela, Bolivia, Trinidad & Tobago, Brazil and Argentina [279], to newcomers like Guyana, which is preparing to explore its recently-discovered resources [280].

Natural gas has been often regarded as the transition fuel to a low carbon economy [59] [60] [61] [62] [63]. However, some authors disagree with addressing the transition required by the goals of the Paris Agreement via increasing natural gas direct combustion. As greenhouse gases – GHG – emissions have already reached high levels, some scenarios to comply with the Paris Agreement indicate the urgency to halt the use of fossil fuels [281]. According to [55] [282] estimates, GHG emissions from the combustion of current global fossil fuel recoverable resources would emit around three times the 1,100 Gt of carbon dioxide (CO2) remaining budget (between 2011 and 2100) to keep global warming below 2ºC with a 50 per cent chance. Actually, a rapid fossil fuels phase-out is needed to meet environmental goals and avoid more aggressive climate change effects [52], meaning that natural gas unabated production should be reduced by 57% in 2050 compared to 2020 values. Moreover, a delay in responding to the rapid phase-out of fossil fuels may result in enormous economic losses, mainly in fossil fuels-based economies, and

[31] Blending was also considered for underground facilities. Reitenbach et al [370] assessed the underground storage with blending of hydrogen in the natural gas. Le Duigou et al [371] analyzed underground hydrogen storage (UHS) options in France, performing feasibility analysis for salt caverns and evaluating its applicability for other countries.

some authors consider the transition to a low-carbon economy inevitable [64][32]. Therefore, deploying a strategy to offer feasible alternatives to emerging countries to both explore their fossil resources and cut GHG emissions is important. If the Paris Agreement limits were fully applied, fossil fuel producers would have to curb their production creating a severe reduction in their wealth expectation that might reach US$ 100 trillion [283], mostly due to large volumes of stranded reserves[33], while ambitious technical solutions like Direct Air Capture of CO_2 remain unconsolidated [284].

In sum, to define a strategy to minimize stranded reserves is paramount for fossil-fuel abundant and depending regions [83] [285]. At the same time, hydrogen can become key in deep decarbonization scenarios [65] [66] [67] [68] [69], although its production mostly relies on steam methane reform, as of today. Therefore, the hypothesis of this study is that the blue H_2[34] may be an option to monetize natural gas resources, while bridging towards a low carbon economy [79]. CCS with Steam Methane Reforming (SMR) plants can reduce carbon emissions in up to 90%, if applied to process and energy CO_2 emission streams [80]. Moreover, a proposed hydrogen deploying strategy should include step-by-step the use of the existing natural gas infrastructure [67] [81], both the hydrogen production units and the gas pipelines and storage sites, in order to create a market (the learning-by-doing and using) for the hydrogen.

This is the aim of this study: to propose a step-by-step strategy to foster the production and use of hydrogen, starting from the blue hydrogen. Such strategy departs from the conventional NG industry to progressively create a H_2 mass industry. In other words, benefiting from the idle capacity in existing conventional fossil fuel facilities to stablish and raise an independent H_2 industry.

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[32] The COVID-19 pandemic did not change the urge for a transition to low-carbon economy [86], since CO_2 emissions decrease due to the economic crisis caused by the pandemic should not endure with economic recovery [87]

[33] Stranded assets will no longer be able to provide economic return as planned at some time prior to the end of their economic life due to changes associated with the transition to a low-carbon economy [53]. This unbalance would occur due to disruptive changes that yield lower internal rate of return for fossil fuels production in a lower demand and prices scenario than those conditions anticipated at the investment decision point [348].

[34] In this study, we apply the following definitions [79] [82]: H_2 is classified as Grey, Blue and Green. Grey H_2 is gas produced by thermochemical conversion (such as steam methane reforming) of fossil fuels without carbon capture. Blue H_2 is also produced by thermochemical conversion of fossil fuels but now equipped with CCS. Green H_2 is a renewable gas produced mainly by water electrolysis using renewable electricity sources such as solar PV, wind and others, and also from biomasses.

To the best of our knowledge, no study has up to date delimited this type of stepwise strategy for setting up a blue H_2 development, departing from the idle capacity in the NG industry. A blue hydrogen production strategy remains a challenging universal issue. For instance, in the United States of America, information on national production is not easily gathered. Sun et al. [286] developed a methodology assessing H_2 production in SMR facilities. Furthermore, they estimated emitted CO_2 from those facilities in order to give subsides for future studies. Collodi et al. [287] evaluated the performance and cost of a green field modern SMR plant producing H_2 from natural gas as feedstock/fuel operating in merchant plant mode. The authors mention some projects in the area, including a pilot plant injecting CO_2 from SMR processes for EOR production in the USA, two in construction (Canada and United Emirates) and evaluate better capture techniques. Findings showed overall capture rate from 53 to 90%. Díaz-Herrera et al. [288] evaluated a Blue hydrogen SMR plant in Mexico and Anguita et al [289] assessed SMR in Spain. While the latter identify the barriers for developing projects, the former indicate that SMR should meet the blue hydrogen market needs by 2040. Finally, Abbas et al. [290] developed SMR models for small scale and evaluated CO_2 emissions impact.

This study aims to close this gap by proposing a case study for Brazil, considering its near-future gas production expansion, the already existing H_2 production in the country's oil refineries and the existing NG pipelines. The case study illustrates a strategy and procedures that can be well replicated in other countries/regions where there is an already installed NG industry.

This study firstly describes in **section 4.3** the applied Materials and Methods, starting from its main premises and, then, detailing the proposed strategy and the methodology to assess it. **Section 4.4** shows a case study, **section 4.5** presents and discusses the findings of the study, while **section 4.6** concludes it by raising its main lessons. The Supplementary Material of this paper details the data from the case study and provides additional tables and figures of the results found.

4.3 Materials and Methods

4.3.1 Premises

The Blue H_2 strategy herein proposed intends to comply with a steadfast environmental commitment and offers windows for reaching next maturity levels. The main premises that support this strategy must deal with regulatory and technical assumptions.

4.3.2 Regulatory Aspects

This work considers that countries and regions might possess poorly-developed markets for H_2, but may count on a minimum established infrastructure for natural gas, like pipelines and traditional H_2 production units (HPU) from natural gas. For countries or regions where H_2 regulatory maturity is yet to be established, we propose a minimum of two years lag time prior to defining a regulatory framework.

4.3.3 Natural Gas Infrastructure: Pipelines, Processing and H_2-NG Blending

For the purpose of this study, transport networks include high-pressure pipelines (above 2 MPa) and distribution networks include medium and low-pressure pipelines (0.2 to 2 MPa). Natural Gas goes through processing in Natural Gas Processing Units (NGPU) prior to being transported and distributed to final users. Those units adjust NG composition to its quality regulation (CH_4 % mol > 85) [257], separating methane and ethane from heavier fractions (the so-called C_{2+}). Simulated new NG processing facilities are similar Comperj[35], presenting a capacity of 21 Mm^3/d of raw NG. Gas volumes are expressed in Normal cubic meters.[36]

Blending volumes limits of NG and H_2 in pipelines may vary [273] [291]. However, most authors agree that 15 % v/v is a safe value. This study applies this limit, considering pipelines maximum declared

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[35] Comperj is the most recent facility designed in Brazil, still under construction. It includes SMR and NGPU units.

[36] Normal conditions are 20ºC and 101.3 MPa [169]

capacity. Embrittlement is one of the most present concerns in injecting H_2 in NG systems [291], [277] and it could lead to leakage [74] [273] [292]. Therefore, H_2 blending would start in networks disposing of relatively new facilities (built after 2000) [101]. This study considers that investors might replace pipelines after 10 years or built H_2 dedicated networks. Blending might take place in both transport and distribution networks, but in this work, we consider only blending in transport pipelines.

4.3.4 Hydrogen Production and Steam Methane Reforming (SMR)

Being focused on NG conversion, this study does not evaluate alternatives methods for producing H_2 in addition to the conventional SMR, whose feedstock is the processed (dry) Natural Gas. For this facility, this study assumes that by 2025 all authorized units will become operational, hence adding full Grey H_2 capacity for refining use. H_2 facilities planned according to the present strategy will produce according to the Steam Methane Reforming (SMR) process and sized for producing 5.76 MNm^3/d H_2.

4.3.5 Carbon Capture and Storage and Enhanced Oil Recovery

Carbon emissions related to the H_2 production process have to be captured. In this study, enhanced Oil Recovery (EOR) techniques are used to inject CO_2 in oilfields. CO_2-EOR is a proven technology used since mid-1980's in the USA [293] and for more than 20 years in Europe [294]. Several fluids may be used for oil recovery and Mechanical Vapor Recompression (MVR) is a suitable technology to increase recovery outputs [295] [296]. It has been also used to store more than 260 million metric-tons of anthropogenic CO_2, being suitable for producing low-carbon H_2 [297]. EOR technologies meet 50% of the CO_2 storage projects in the world [296].

Planned CO_2 pipelines flowing supercritical fluid, in offshore operation, are 250 km long, with 25 MPa design pressure and built with API65XL type steel. [298] [299] [300]. Revenues from oil production increase with CO_2-EOR provide monetary resources to expand infrastructure.

4.3.6 Basic Strategy

The energy transition strategy from fossil fuels to low carbon economy through H_2 is divided into three steps: Fossil Fuel Domain (short term), Transition (medium term) and Green Energy (long term). Those steps describe a process where fading characteristics of the previous step give place to rising forms of the next. Therefore, blurred areas may appear, mainly in years between steps.

The stepwise strategy developed in this work focuses on the short and medium-term steps (first and second steps), addressing boundary conditions for these two steps rather than detailing the third one. The reason for this is that we consider whether an effective transition is feasible, a H_2 market independent from fossil fuel logistic chain would be reached. In such conditions, Green H_2 would become a natural choice, fostering independent producers to connect to a future and developed H_2 network. Therefore, along this 3-steps strategy, we take advantage of the existing infrastructure to comply with current and future energy demands. In addition, progressive milestones are landed for opening space to reach an independent H_2 market.

4.3.6.1 Short-Term Step – Fossil Domain

This first step benefits from the current H_2 idle production capacity, which also defines network injection points and the start-up time for mixing H_2 into NG networks until a maximum pre-defined blend, according to thermodynamic parameters (Wobbe Index, e.g.) and pipeline specification. Besides, H_2 investments are dependent on decision makers linked to fossil fuels companies. This step is effective as long as idle capacity is available, bearing in mind that new facilities should become available for producing Blue H_2.

Current H_2 production capacity is strongly related to oil refining capacity where Grey H_2 is produced for hydrotreating purposes or chemical use. Production idle capacities provide H_2 volumes that can be made available to be blended into natural gas networks. Since refineries are already connected to NG networks, H_2 would be injected in those city gates (delivery points) with minor engineering changes [273]. In such circumstances, NG traders might profit from carbon credits by selling a mix of NG and H_2 [79] and H_2 gains shares in NG markets. Meanwhile, investor will have time to develop EOR projects, processing, transporting and H_2 producing facilities. **Figure 23** shows how information is collected, addressing H_2 injection in the NG network.

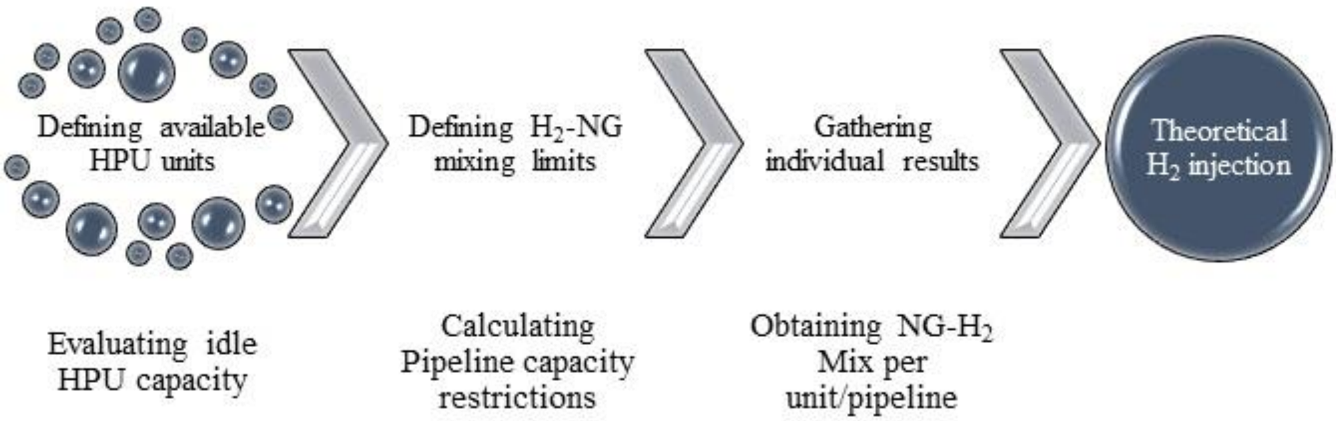

Figure 23: Stepwise method for obtaining reliable H_2 theoretical injection volumes – first step

The theoretical H_2 injection volume blends offers the possibility to evaluate a ramp up for H_2 injection in existing facilities. In Europe, [301] estimates a blend up to 10% in NG networks when preparing exclusive H_2 pipelines by retrofitting existing systems. In the USA, [273] evaluates that within a range between 5 and 15% H_2 v/v no additional risk is added to deliver gas to households and other consumers. Some specialists go further to a blend up to 20%, depending on the local natural gas composition and the pipeline network, recalling that blended H_2 is an old technology, applied since mid-1800 in the USA in a blend varying from 30 to 60%, called “manufactured gas” or “town gas” [74]. According to the same authors, if infrastructure and appliances upgrades are done under control, pure H_2 networks are possible. Main adaptations would require leakage control improvements, retrofitting remaining steel pipelines against H_2 embrittlement or replacing them with noncorrosive and non-permeable materials, such as polyethylene or fiber-reinforced polymers.

To evaluate the energy delivered and estimate maximum H_2 volumetric blends the Wobbe index may be used so as to meet customer energy demands[37]. This index is obtained as follows [276]:

$$W = \frac{H_S}{\sqrt{\frac{\rho g}{\rho a}}} \qquad \textbf{Equation 8}$$

Where:

W = Wobbe index
Hs = High heating value (HVV), J/m^3
$\rho_{g,a}$ = gas/air densities

The Wobbe index is directly proportional to the quantity of combustion energy supplied through a nozzle for a burning process, and it depends on the gas composition [292]. In general, gross calorific values and densities are available in standard conditions. For Wobbe calculation, the standard condition must be the same for air and gas densities, so as for calorific value. In this study, a maximum of 15% v/v blend was applied considering pipelines maximum declared capacity and the Wobbe index was evaluated for a similar range.

Finally, in this first step, existing H_2 production units produce essentially Grey H_2. Blue H_2 starts from compensating emissions from existing H_2 production in Year 5 and not sooner. At least a pipeline or some infrastructure should be built for CO_2 transport to injection field and for CO_2 capture. Estimates indicate that pipeline design and construction time takes no less than 5 years, time that would be needed before starting emissions compensation [302].

4.3.6.2 Medium-Term Step – Transition Period

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[37] This study criteria keep existing consumption devices instead of installing or converting equipment.

The second step aims at developing a Blue H_2 supply to support decision makers to meet decarbonization while monetizing it. It considers NG supply increase and requires both greenfield plants for increasing H_2 production capacity and CCS infrastructure deployment for storing CO_2, since planned facilities for H_2 production must be associated with CO_2 injection field and connected to the CO_2 pipeline. CO_2 from H_2 production increasingly fills export pipeline as oil production from CO_2-EOR increases. Facilities dedicated to H_2 production are built, notwithstanding refinery capacity, preferably next to Natural Gas Processing Units (NGPU). Collected CO_2 in these units are transported to a main pipeline next to the production zone. Market development allows building a relationship client–customer between H_2 producers and fossil fuels producers, increasing the independence of the latter from the former.

After developing a H_2 market for energy use, Grey H_2 decreases. Traditional producers are stimulated to neutralize H_2 emissions and regulation is assumed mature for both H_2 and CO_2 transport modals. Contractors build new pipelines and government launches bids for operators, who sale H_2 transport service for carriers meeting consumers' demand. In the future, Green H_2 producers may also connect to the network, connecting medium- and long-term strategies and completing transition for green energy.

4.3.6.3 Pipeline Sizing and Cost Estimation

Considering the preliminary approach of this study, CO_2 pipeline sizing was performed on a simplified flow for compressible fluids considering Darcy's formula. Churchill's correlation was chosen for calculating friction factor [303]. Complementary data for pipeline sizing like wall thickness were obtained from Brazilian Standard NBR-12712 [304]. Addressing adequate pipe sizing, [246]indicated a practical rule of thumb including pressure losses between 15 and 25 kPa/km. This practical approach was applied in this work. Reference costs for CO_2 pipelines is given by **Equation 9**. In spite of displaying values that might not be updated, [305] brings a practical approach, allowing immediate evaluation of pipeline costs per tCO_2. This correlation was obtained from those values.

$$C = 9.3235M^{-0.596}, R^2 = 0.9993 \qquad \textbf{Equation 9}$$

Where:

C = Cost US$/t$CO_2$/250km)
M = Mass flow rate (MtCO_2/y)

Recent studies have addressed CO_2 pipeline costs. Kjärstad [306] shows that ship transporting is advantageous over pipelines in Nordic countries due to low volumes required.

Equation 10

approaches a correlation obtained from values found for a 730km offshore pipeline in Norway [306].

$$C = 39.9M^{-0.596}, R^2 = 0.9853 \qquad \textbf{Equation 10}$$

Where:

C = Cost (€/tCO_2/250km)
M = Mass flow rate (MtCO_2/y)

According to the authors, for volumes higher than 1.3 MtCO_2, pipelines become a less costly transport solution compared to ships. Knoope [307] found costs for a 300 km pipeline about 0.11-0.64 M€$_{2010}$/km for 0.30 m diameter and 1.5-13 M€$_{2010}$ /km for 1.30 m diameter.

A detailed method for pipeline cost calculation is out of the scope of this work. However, it may be found in [308] and [307]. For some specific aspects, like CO_2 hub formation, Costa et al. [309] designed a model based on a Kernel density estimator for the Iberian Peninsula. Gathering lessons learnt from pipeline construction, [310] summarizes key costs drivers for pipelines in the following items:

• Piping (type and grade of material)

• Equipment (such as compressors, booster stations, valves, crack arrestors, etc.)

• Trenching (i.e., earthworks, excavation, backfilling)

• Distance

• Diameter

• Terrain

• Labor

• Engineering (e.g., design, project management, regulatory/permitting activities)

4.4 Case Study Description

This study simulates the proposed strategy in the Brazilian NG infrastructure. Brazil is a potentially high-producing H_2 country, whose 1P and 3P Natural Gas reserves total 364.6 $x10^9$ m^3 and $550.0x10^9$ m^3, respectively [89], and the NG production is expected to increase up to 253 million m^3/day in 2029 [125] and 501.7 million m^3/day in 2050 [311][38]. These perspectives point towards an infrastructure development, similar to other Latin American and emerging countries with plenty NG remaining resources [278], [87].

4.4.1 Existing Infrastructure Facilities

The Brazilian gas transport (interstate, high pressure) infrastructure has 9,409 km of pipelines from 8 to 38 inches[39] [101] and the maximum operating pressure (MAOP) between 20 and 100 kgf/cm^2 [248].[40]

This network relies on 3 operating and 1 authorized Liquefied NG regasification terminals with total capacity of 62 Mm^3/d [101], 14 Natural Gas Processing Units (NGPU) totaling 107,210 Mm^3/d of nominal capacity [169], 36,290 km of distribution (intrastate, low pressure) pipelines and 4,650 km of production flow pipelines [101].

IEA expects a growth in NG production in Central and South America (CSA) in the period from 2020 and 2040. Brazil does not diverge from this expectation [87]: In the "Stated Policies Scenario", IEA

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[38] From this point on, million m^3/day will be indicated as Mm^3/d and, for year, d will be replaced by "y".

[39] Pipelines are usually traded in diameters named in inches (nominal size). The above values range from 203.2 to 965.2 mm (SI units).

[40] 1961.33 to 9806.65 kPa.

expects a production increase from 174 to 244 billion cubic meters in CSA between 2019 and 2040. In the same period, Brazilian NG production should double, going from 26 to 58 billion m^3. The Brazilian government [311] also forecasted growth scenarios for NG production in the next decades. Those projections indicate that by 2027 NG processing infrastructure might reach its full capacity.

Since H_2 blending should take place in networks possessing relatively new facilities and around 20% of the pipeline network length was built before 2000, it is likely that those pipelines would not be adequate for H_2 blending due to regular use wear. Therefore, initial H_2 production curve is smooth, considering currently grey H_2 production, and might not use all facilities in the beginning years.

4.4.2 CO_2 Storage Potential

Brazil´s CO_2 storage potential is above 100 $GtCO_2$ [312]. Recently, [313] estimated the CO_2 storage potential of 108 Mt of CO_2 in salt caverns built in ultra-deep Brazilian pre-salt layers. Rockett et al. [314] mentioned a total storage capacity of ca 2,000 Gt CO_2 in Brazil, assessing specific storage capacities of 1,800 Gt CO_2 and 167 Mt CO_2 respectively for Campos and Santos basins, while calculated, in a more accurate approach, 950 Mt CO_2 for 17 specific fields in Campos' basin. Likewise, [293] estimated for Campos' basin a 1.1 Gt CO_2 storage potential considering CO_2-EOR techniques.

Nevertheless, conservatively this study departs from forecasted oil production to estimate possible CO_2-EOR in the studied time frame. In Brazil, CO_2-EOR is a currently used technique [315]. Ravagnani [316] evaluates that 2.58 tCO_2 are injected for obtaining $1m^3$ of oil with EOR technique. Similar ratio can be obtained from values described in [317], around 2.45t CO_2/m^3 oil. Alternatively, [293] estimates between 0.26-0.31 t CO_2 per incremental oil barrel produced.

EOR production factor increase depends on several factors, and [317] indicates values ranging between 7 - 23% of total oil in place (OIP), with an average of 13%. Other authors [318] corroborate that range for miscible mixtures between CO_2 and oil in EOR. Concerning Chinese oilfields, Hill [319] estimated 6% to 10% of total oil in place (OIP) production increase. However, the authors highlight that China does not inject supercritical CO_2, which stimulates miscibility and increases productivity. More recent studies reported incremental oil recovery ranging from 6.09 to 22.83% OIP for techniques of CO_2-EOR [320].

Future oil production in Brazil is expected to increase. In fact, daily production should rise by 60% in 2050, compared to 2020. In this study, we consider that part of this growth production might be spurred by CO_2-EOR techniques. In this case study we consider this forecasted oil production for estimate CO_2-EOR storage availability and compare it to CO_2 storage needs from H_2 production. If expected CO_2-EOR storage availability is higher than CO_2 produced in H_2 plants, the maximum H_2 production generation is reached. Otherwise, it sets a curb for H_2 production, assumed to be Blue H_2 in this study. Future oil production in Brazil is expected to increase from 3.24 million bbl/d in 2020 to 5.30 million bbl/d in 2050 [125] [126].

As premise, only part of this production growth will be based on CO_2-EOR. Based on previous studies [320], we considered technical learning would allow gains in EOR starting from 7% up to 23 % daily production, in analogy to the above references.

A CO_2 pipeline is sized considering supercritical flow to convey captured gas to injection facilities. Such case is relevant when both H_2 and oil production sites lie close to each other. In Brazil, it occurs quite often, since production frontiers are offshore and several HPU facilities are installed close to the shore. Natural Gas Processing Unities (NGPU) are even closer to the shore, which means that those facilities may be feasible locations for future H_2 producers in an independent market.

4.4.3 Pipeline costs

For countries where CO_2 supercritical pipeline costs are not available, the analogy with natural gas pipelines is a usual approach, as proposed in [307], where the author highlights that the traditional costs were based on superseded costs from North American natural gas pipelines, and further proposed a change in those models by an updated model. Since in Brazil most resources are deployed offshore, recently-built and projected production flow pipelines that connect offshore fields and processing units onshore might be a good approach for cost evaluation.

Values sources vary from 2012 to 2019 and were equaled in the same base date according to [321] and [322] for exchange rates and base date prices. These values were compared to those indicated in specific costs for CO_2 pipelines previously cited [305] [306] and updated to base year 2019 according to [175].

4.4.4 H_2 Production Potential

As mentioned before, H_2 production requires mainly dry NG, free from heavier fractions and composed by lighter fractions, such as methane and a low portion of ethane [323]. Therefore, not all raw NG volumes are available for producing H_2. Processing factor in Brazilian NGPU may be obtained from historical data [169]. In 2019, 22,930 Mm^3 NG were processed in Brazil, generating 20,970 Mm^3 dry NG. This leads to a processing factor of 0.91, or 91 % of the produced NG reaches the required qualification to produce H_2. Heavier fractions (rich gas) are sold as ethane, LGP (propane, butane) and naphtha (C_{5+}). For the purposes of this study, we apply this processing factor in all raw NG streams.

Not before 2 years blending actions in the NG networks should start, since in Brazil, as in other emerging countries, H_2 blending is not yet regulated. Currently valid regulation for NG does not mention H_2 in transport pipelines [257].

Authorized refinery capacity totals 2,411 million barrels/day of processed oil in 19 facilities. Nonetheless, H_2 generation capacity (HPU) is restricted to 11 refineries, all of them connected to NG network, totaling 25,838.44 kNm^3/d or 31,598.44 kNm^3/d. Average capacity use is 74.4%, and idle capacity is 25.6% [324] [102] [325].

Recently, the Brazilian government published forecasts revealing a vast production potential for natural gas [311] [125] [126]. Such optimistic forecast for natural gas production compares a business-as-usual production scenario to a "new gas market" scenario, featuring a surplus between those two scenarios departing from 53 Mm^3/d in 2020, reaching 245 Mm^3/d.

Under a conservative perspective that considers that the NG supply of the business-as-usual scenario would have a guaranteed market, this study expects that the Blue H_2 might spur the "New Gas

Market", offering a low carbon option for monetizing these resources thus decreasing CO_2 emissions. Therefore, we suppose that the NG forecast in the reference scenario would be used in conventional application. However, NG surplus provided in the New Gas Market possibility could be employed in Blue H_2 generation, including new facilities and required infrastructure.

Likewise, in the current strategy we anticipate processing extra capacity from year 6 onwards. Therefore, Blue H_2 production will come from greenfield projects, increasing current H_2 production.

Therefore, the H_2 potential production related to this NG supply expansion, via SMR based Brazilian existing HPU, is obtained from [323] and corresponds to a weight ratio of 0.4208 kg H_2/kg NG. Potential H_2 may be found in **Table 22**.

Table 22: Potential H_2 (elaborated from [311] [125]**)**

	NATURAL GAS PRODUCTION, MNm³/d			**HYDROGEN PRODUCTION, MNm³/d**	
	A	**B**	**C**	**D**	**E**
YEAR	**Conventional use (Business as usual)**	**NG Surplus (available for new uses)**	**Maximum forecasted production (A+B),**	**Potential from NG surplus (B)**	**Max Potential H_2 (from A+B)**
0	77.7	53.6	131.3	**1,124.9**	**2,755.8**
1	73.4	52.7	126.1	**1,105.3**	**2,645.6**
2	71.1	43.5	114.6	**912.8**	**2,404.6**
3	70.0	44.1	114.1	**925.8**	**2,395.2**
4	66.6	49.5	116.2	**1,039.8**	**2,438.1**
5	68.6	53.4	122.0	**1,119.9**	**2,559.3**
6	81.5	55.8	137	**1,171.9**	**2,883.0**
7	98.0	57.9	155.9	**1,214.5**	**3,270.8**
8	115.3	53.0	168.3	**1,111.7**	**3,530.8**
9	136.8	43.7	180.5	**917.1**	**3,787.0**
10	136.8	43.7	180.5	**917.1**	**3,787.0**
20	156.8	150.2	307.0	**3,151.0**	**6,441.5**
30	256.3	245.4	501.7	**5,150.6**	**10,529.1**

4.4.5 HPU and NGPU Capacity Expansion

Processing unit costs were obtained from [326]. This cost was updated to the base date[41] and converted to US$, obtaining a current value of US $395.58 million. For the H_2 production, Yan et al [327], addressed Blue H_2 production obtaining capital costs ranging from £188.7 to 293.0 (US$ 232.42 to US$ 360.89) million and operational costs from £237.5 to 329.8 (US$ 292.53 to US$ 406.21) million, while Yan et al. [328] analyzed H_2 purification in Pressure Swing Adsorption (PSA) processes. Other studies, like [329] obtained operational cost for H_2 production for conventional SMR 0.130 €/Nm^3 (0.1444 US$/Nm^3). Considering Brazilian facilities, Labanca [330] evaluated costs ranging from 2080.0 to 2655.4 US$/t H_2. In the present study, we have adopted the following values to estimate production costs and required investments for evaluating Blue H_2: applied unitary costs were 2655.4 US$/t H_2 for SMR [330] and US $25.90 million/ m^{3}d NG [326].

4.5 Results and Discussion

According to the strategy proposed by this study, the short and medium-term steps (first and second steps) were essential for developing a H_2 market. This section will present global results for H_2 production and CO_2 emissions discussing each step, as previously expressed. The strategy refers to the proposed steps, rather to the time span between them. For instance, if regulatory framework is ready in a country or region, this lag time could be leaped, and all strategy anticipated.

4.5.1 Short-Term Step – Fossil Domain

Currently, the installed capacity for producing H_2 is 25.8 MNm^3 H_2/d (0.112 EJ/y)[42]. If authorized SMR facility starts up, it might reach 31.6 MNm^3 H_2/d (0.137 EJ/y). This first step benefits from the

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[41] Base year in 2019, and obtained rates are available in [321].
[42] Considering reference H_2 density value 0.0838kg/m^3 @ 20ºC, 1 atm and High Heating Value 11.915 MJ/m^3

current H_2 idle production capacity, which also defines network injection points and the start-up time for mixing H_2 in NG networks until a maximum pre-defined blend, according to thermodynamic parameters (Wobbe Index, e.g.).

H_2 blending becomes possible from year 2 onwards and full installed capacity 25.8 MNm^3 H_2/d might be reached if main H_2 producers increase operation for injecting in the network. It is possible to see blending volumes in the left axis (**Figure 24**a), increasing up to 5.4 MNm^3 H_2/d in Y10.

Grey and Blue H_2 forecasts may be observed in (**Figure 24**b). Total H_2 production might reach 0.40 EJ in 2030 (Y10). Grey H_2 would depart from the current production of 0.087 EJ and would peak (0.137 EJ) by year 7, after capacity increase. Therefore, within this step, Blue H_2 should depend on new SMR facilities. As a CO_2 pipeline should operate from year 5 onwards, Blue H_2 production will receive a strong push forward, flowing CO_2 captured from new SMR facilities.

Equation 11

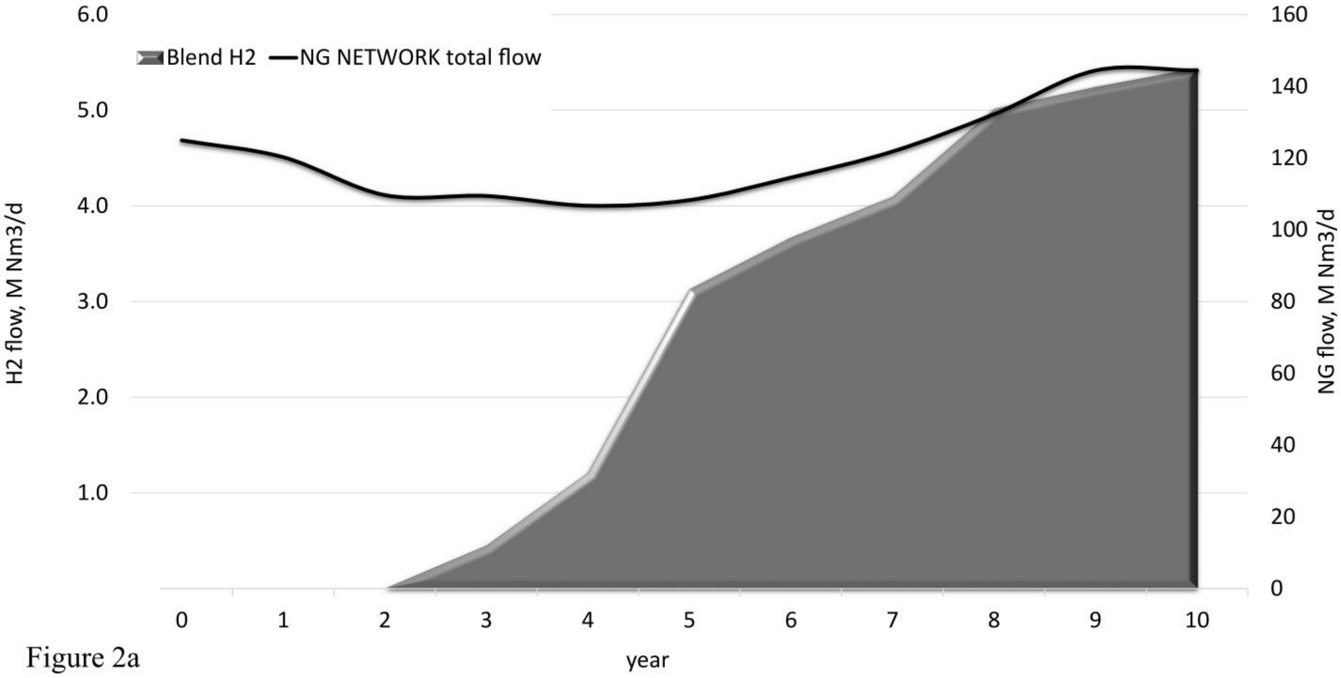

Figure 2a

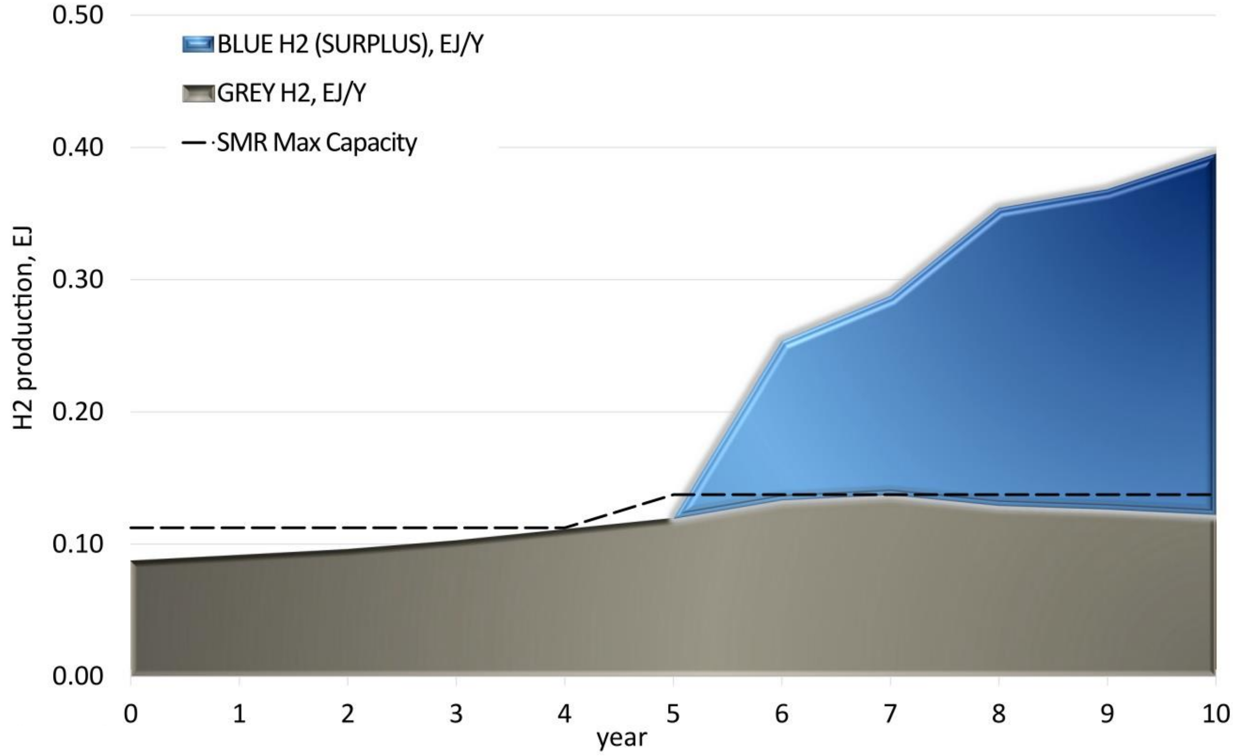

Figure 24: H_2 results during the Fossil Domain: (a) H_2 blending volumes in the network; (b) H_2 production.

Extra H_2 capacity production for Blue H_2 would be required from year 6 onwards. Two extra SMR units producing 5.76 MNm^3H_2/d[43] would be required to meet NG estimated production. Likewise, considering that existing NG processing facilities might be equally busy, then two dedicated processing units of 21 MNm^3 H_2/d would be required for treating forecasted NG production up to Y10.

This first transition is not a rigid landmark, but it would occur when new H_2 production facilities become available. This strategy extends from year 6 to year 10, period in which Blue H_2 slowly displaces Grey H_2 and further increases.

This slow transition from installed Grey H_2 capacity to Blue H_2 should be explained. Firstly, it occurs slowly due to Grey H_2 facilities residual development. Secondly, it is likely that facilities designed for producing Grey H_2 take some time to compensate their emissions postponing their conversion prior to becoming Blue H_2 producers, since CO_2 capture and transport facilities are not originally in the scope of those facilities. At last, some of them may not be installed close enough to the CO_2 transport network. Figure 24b displays this initial transition from Grey to Blue H_2. However, some compensation may be possible. Therefore, installed Grey H_2 loses some fraction, mostly linked to blended gas.

During the Fossil Domain, H_2 investments are totally dependent on decision makers linked to fossil fuels companies. Capacity use departs from average 74.4% in Y0. Most of the H_2 production capacity (0.11 EJ/y) is strongly related to oil refining capacity and mostly Grey H_2 is produced for refining purposes or chemical use. This step would take as long as new facilities become available for producing and trading H_2. However, during this period H_2 trading may find a constraint, which is the maximum installed capacity of H_2 conversion in Brazil in year 0. H_2 blending in the network for commissioning purposes starts in Y3 (grey H_2) in selected spots in the network, overall percentage of 0.41% in Y3, increasing up to close to global 15% in Y7. Yet, it is relevant to evaluate local blending should not

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[43] It is worth to notice that this pace of deployment of new facilities is a challenge from the technological and commercial point of view. Historical data shows that building those facilities face several restrictions and in a practical approach it may not occur. In addition, it is relevant observe that such scale for one single unit is higher than the larger unit operating in Brazil (see section 7.3 supplementary material).

overcome blending limits. Between Y5-10, it is possible to foresee at least one 100%-H_2 pipeline ramp up, which would influence overall H_2 use.

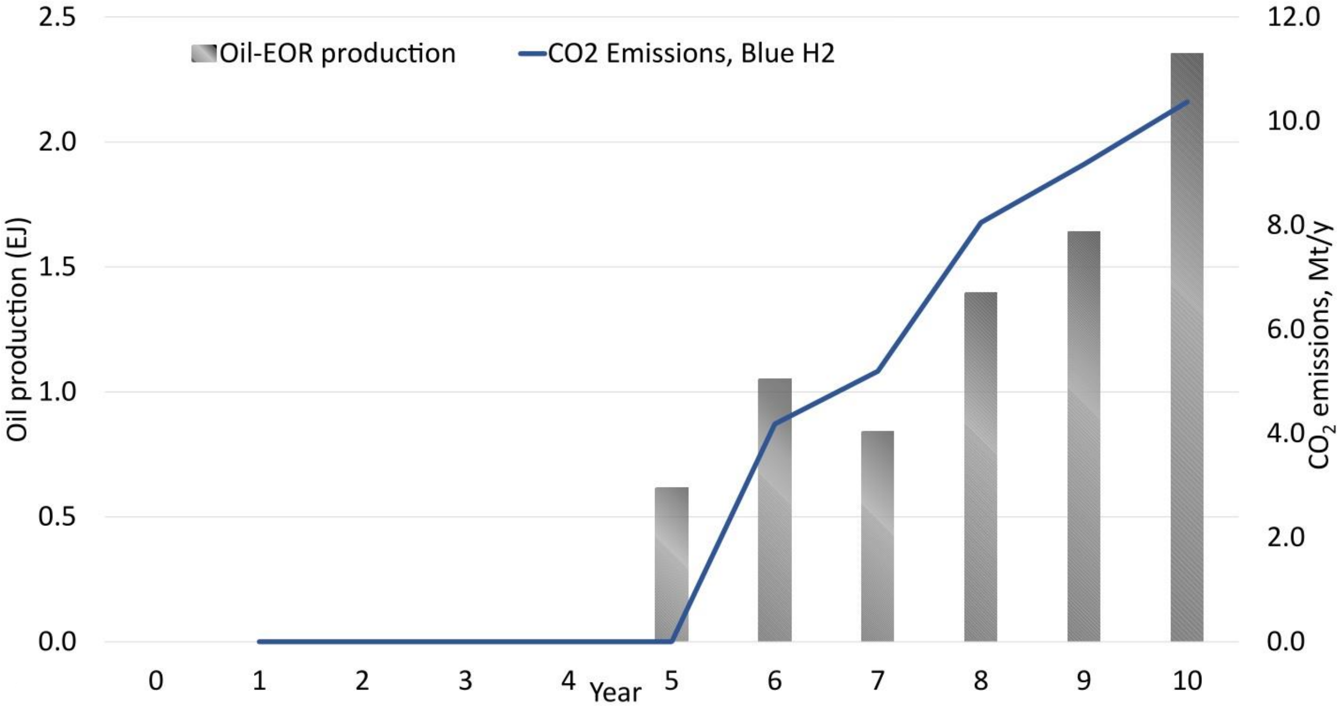
H_2 production reaches full capacity in year 6 when the authorized Comperj SMR facility starts operation. This new facility does not meaningfully change installed capacity use because its capacity is mostly committed to refining process. Surely, it implies that planners should prepare and design new SMR facilities previously. Simultaneously, Blue H_2 production begins in Y5, reaching 0.4 EJ in Y10. In the present strategy, two new SMR facilities would be required in year 6. Those units would meet H_2 generation requirements up to year 11.

H_2 production increases more than fourfold in the first ten years, 75% of this being Blue H_2, prior to develop internal market according to the current strategy. In Y10, Blue H_2 is 0.3 EJ, while Grey H2 reaches 0.1 EJ.

In order to avoid a constraint after Y5 due to a lack of CO_2 for EOR, the proposed strategy considers a CO_2 pipeline for making the production of Blue H_2 possible. **Figure 25**a shows CO_2 emissions and oil production using the CO_2-EOR technique.

CO_2 emissions from the indicated SMR facilities would start at 3.0 Mt CO_2 in year 5, reaching 11.0 Mt CO_2 in year 10. In principle, these volumes are independent from CO_2 storage capacity for EOR production, since they are based on NG availability. But, if oil production requires less CO_2 than SMR supplies, Blue H_2 is curbed. For new facilities, only Blue H_2 is allowed in this strategy.

EOR presented an increasing pace, according to oil production. During this period, CO_2 use in EOR techniques is more than enough for the forecasted oil production, and EOR stands for 15% of overall oil production (**Figure 25**b).



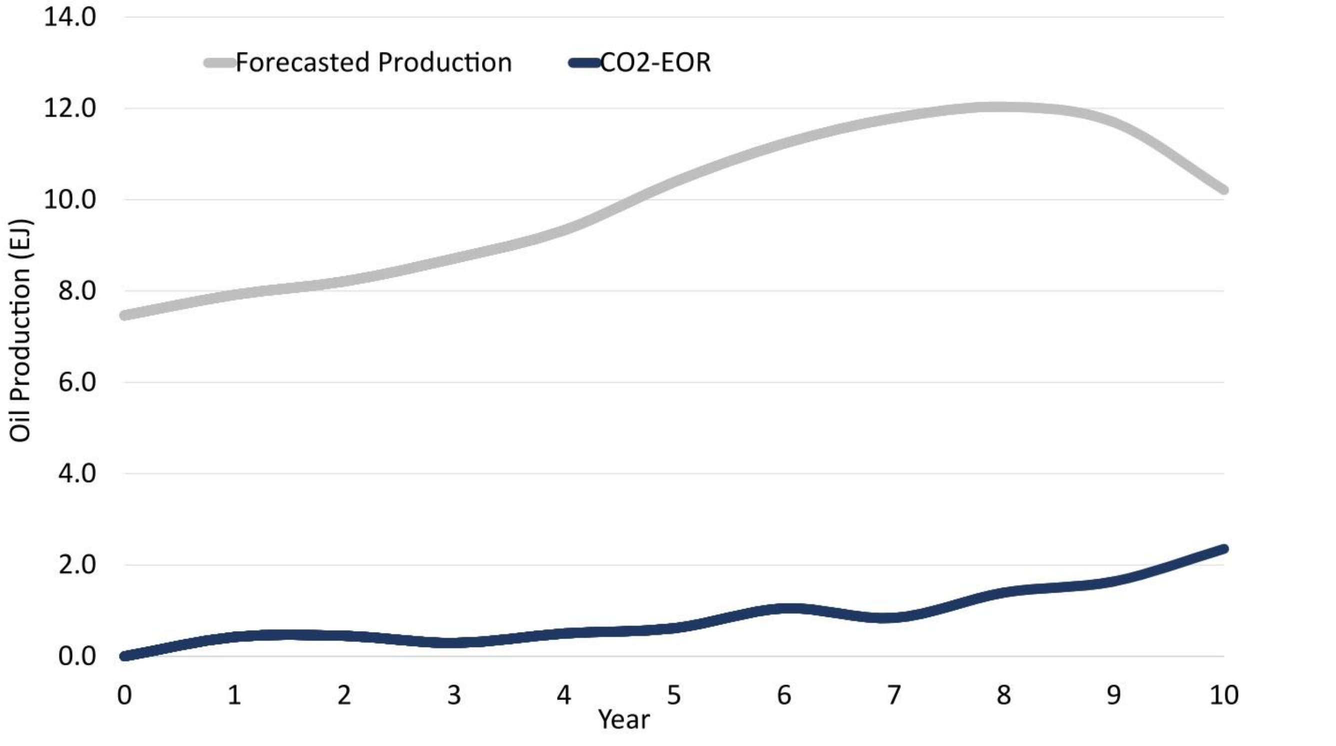


Figure 25: EOR Results in the first ten-year period: (a) additional oil production and injected CO_2; (b) total oil production (Y1-Y10), with EOR derived production highlighted in blue

Blended Natural gas delivery depends on transport pipelines and requires specific analysis, since capacity sizing would involve locational aspects in order to investigate eventual bottlenecks in the network [302]. However, in this work some considerations are entailed related to energy delivery through blending.

In Brazil, Wobbe index ranges from 46.5 to 53.5 MJ/m^3 in transport networks [257]. Calculated H_2 Wobbe index is 46.5 MJ/m^3 [331]. Although maximum allowed blend in this work is 15% v/v, we simulated energy losses per volume up to 21.2% v/v H_2/NG blending. Energy losses due to blending may be seen in **Figure 26**.

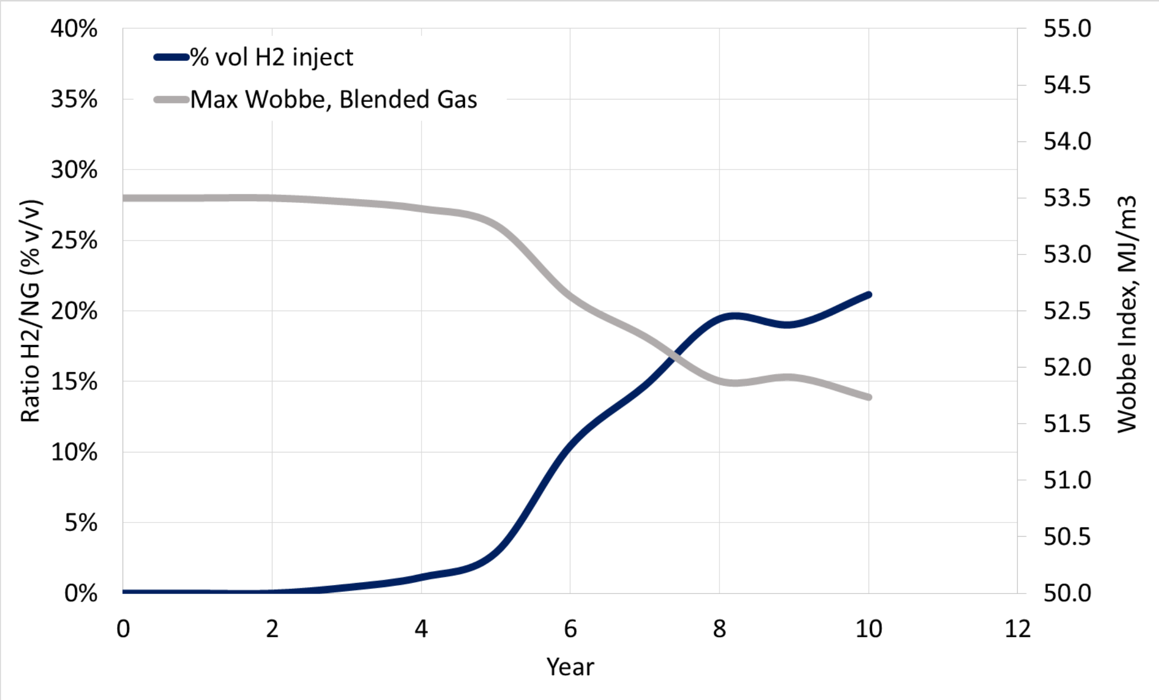


Figure 26: Wobbe index of different H_2/NG blends

Blending causes losses of 3.3 % on delivered energy for 21% H_2 in blending, which means that if NG might be supplied in the maximum allowed Wobbe number, 53.5 MJ/m^3, blending H_2 to NG would supply energy equivalent to 51.0 MJ/m^3. For 15% blending it would represent less than 3%. Regulatory tolerance of 13.1% is much higher than variation caused by H_2 blending, indicating that H_2 blending would likely be absorbed by NG clients.

4.5.2 Medium-Term Step –Transition Period and Forward

This second step happens after both greenfield plants for producing H_2 and CCS infrastructure operate reliably. Since market development allows building a relationship client–customer between H_2 producers and fossil fuels producers, NG pipelines may be replaced by H_2 pipelines, and full-H_2 networks become available. Households and industry adapt their equipment, turning them able to use H_2. After blended H_2 was spread, safety tests should guarantee those applications. New facilities for H_2 production are designed in association with CO_2 storage fields and turned available by connection through a structuring pipeline. Captured CO_2 from H_2 production increasingly fills export pipeline as oil production from CO_2-EOR increases. **Figure 27** shows obtained results.

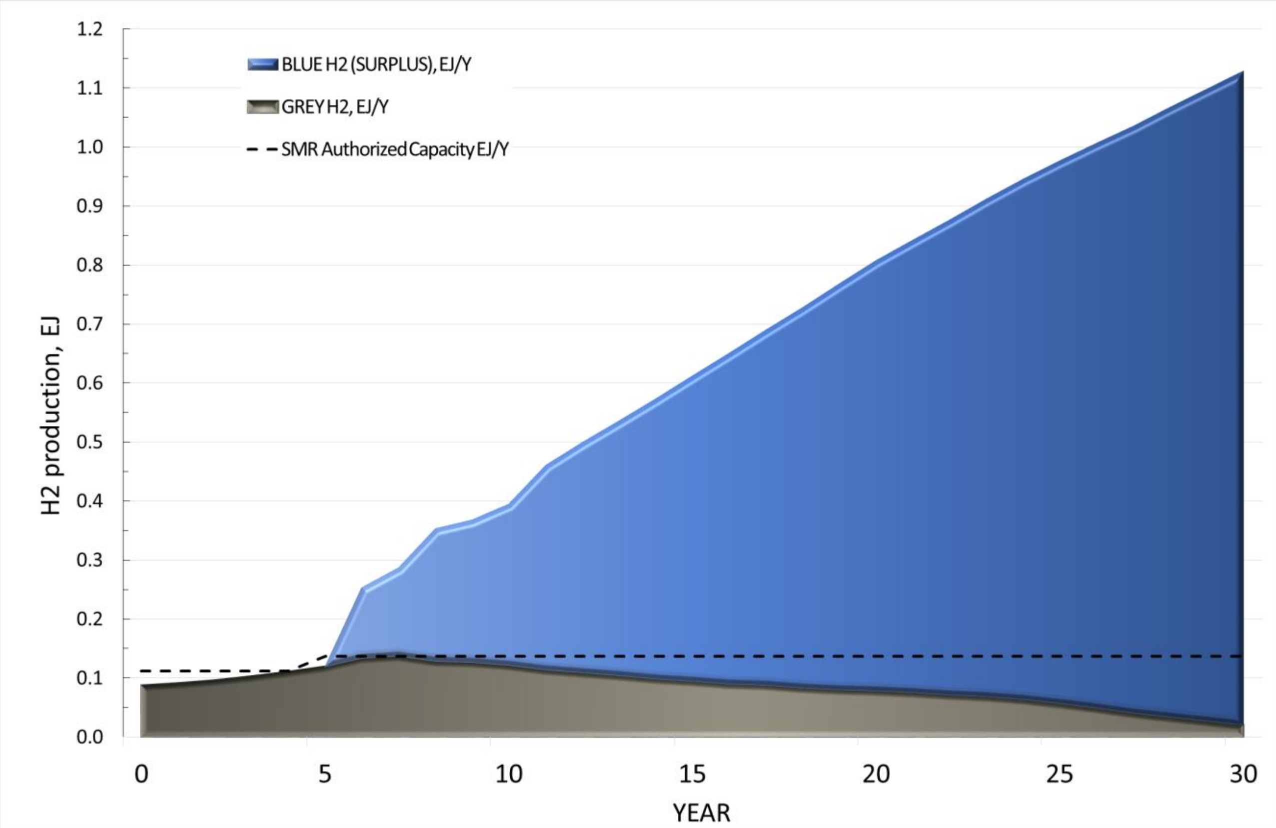


Figure 27: Blue and Grey H2 production in the first ten-year period

During the transition domain, H_2 investments gain relative independence from decision makers linked to fossil fuels companies. Although it departs from a condition in which most of H_2 production capacity is still related to oil refining, Blue H_2 gains pace, attracting investors. SMR units' locations displace from refineries and may be installed close to NGPUs, thus injecting blended H_2 in the NG network or connecting to exclusive H_2 pipelines.

As a comparative standard, this study refers to the Europe Decarbonization pathway [79]. In this reference, two main scenarios are described, starting from a current H_2 demand of 329 TWh (1.2 EJ). The European "current policy scenario" previewed to reach 0.5 EJ in 2040 and 0.54 EJ in 2050. As for the “accelerated decarbonization pathway”, 2270 TWh in 2050 (8.17 EJ) H_2 demand, 1600 TWh (5.76 EJ) of which green H_2. Blue H_2 would stand for 600 TWh (2.16 EJ) in 2050 in Europe. Thus, non-green H_2 use would reach 670 TWh (2.4 EJ) in 2050. Compared to this reference, Figure 10 shows that total H_2 production might reach 0.8 EJ, in (Y20) and 1.13 EJ in (Y30), respectively 0.7 and 1.11 EJ corresponding to Blue H_2. Grey H_2 would go from the current production of 0.08 EJ to reach 0.02 EJ, about 25% from this value in 2050. Comparatively, those values are lower than the expected values in the “accelerated decarbonization pathway” [79], which plans to demand 2.16 EJ blue H_2 in 2050 in Europe. According to this strategy, Blue H_2 production reaches in 2050 tenfold of the current total H_2 production capacity in Brazil. This is a meaningful change in the country´s natural gas market.

After year 11, Blue H_2 associated emission rate decreases. It happens because in the initial years there is a need for a leap in Blue H_2 production. A single facility, such as a CO_2 pipeline meaningfully changes H_2 production profile, introducing Blue H_2. EOR demands for CO_2 storage are lower than the CO_2 produced according to the H_2 potential, thus curbing its growth. Considering CO_2 storage capacity from EOR production and emissions reduction, the current strategy reaches, 21.1 Mt CO_2 in (Y20) and 28.8 Mt CO_2 in (Y30), as may be observed in **Figure 28**a.

EOR Oil production presents a steady growth from the beginning of the second decade on. This occurred due to the assumed premise regarding EOR that established values between 7 to 23% from production should come from EOR due to increasing technology learning favoring EOR participation in total oil production. However, it meets part from total forecasted oil production in Brazil [311] [125] [126], reaching 22% total production (**Figure 28b**).

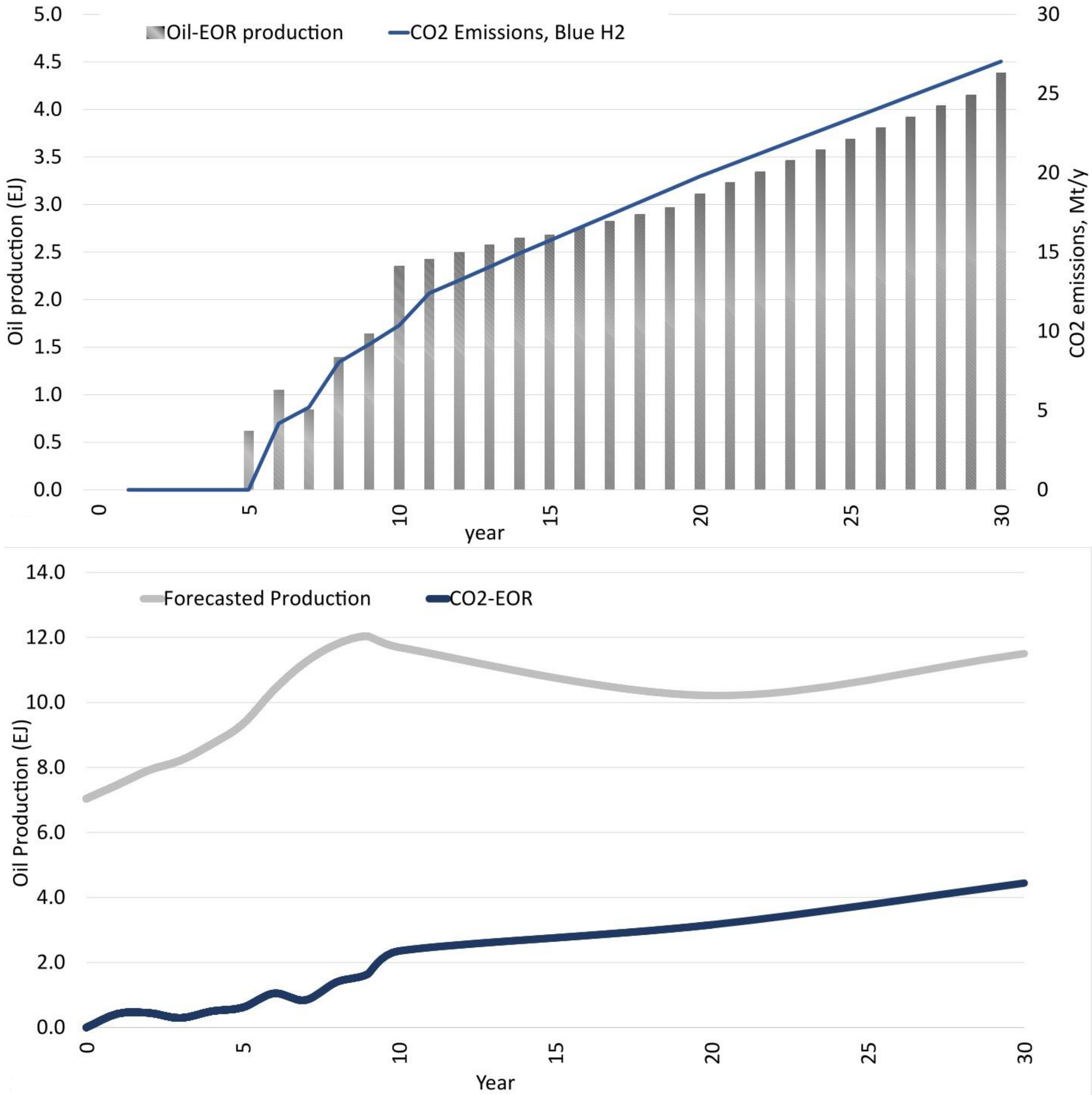


Figure 28: EOR Results in the long-term: (a) additional oil production and injected CO_2; (b) total oil production (Y1-Y10), with EOR derived production highlighted in blue

EOR availability imposes restrictions to Blue H_2 production. However, if those restrictions are relaxed by considering new storage modes, potential H_2 production reaches 1.12 EJ in 2050. **Figure 29** shows H_2 production behavior in this situation. Developing other storage options than EOR might be also a potential option, as mentioned before Costa *et al* [313] evaluated a meaningful storage potential in salt caverns offshore in Brazil and such an option should also be considered.

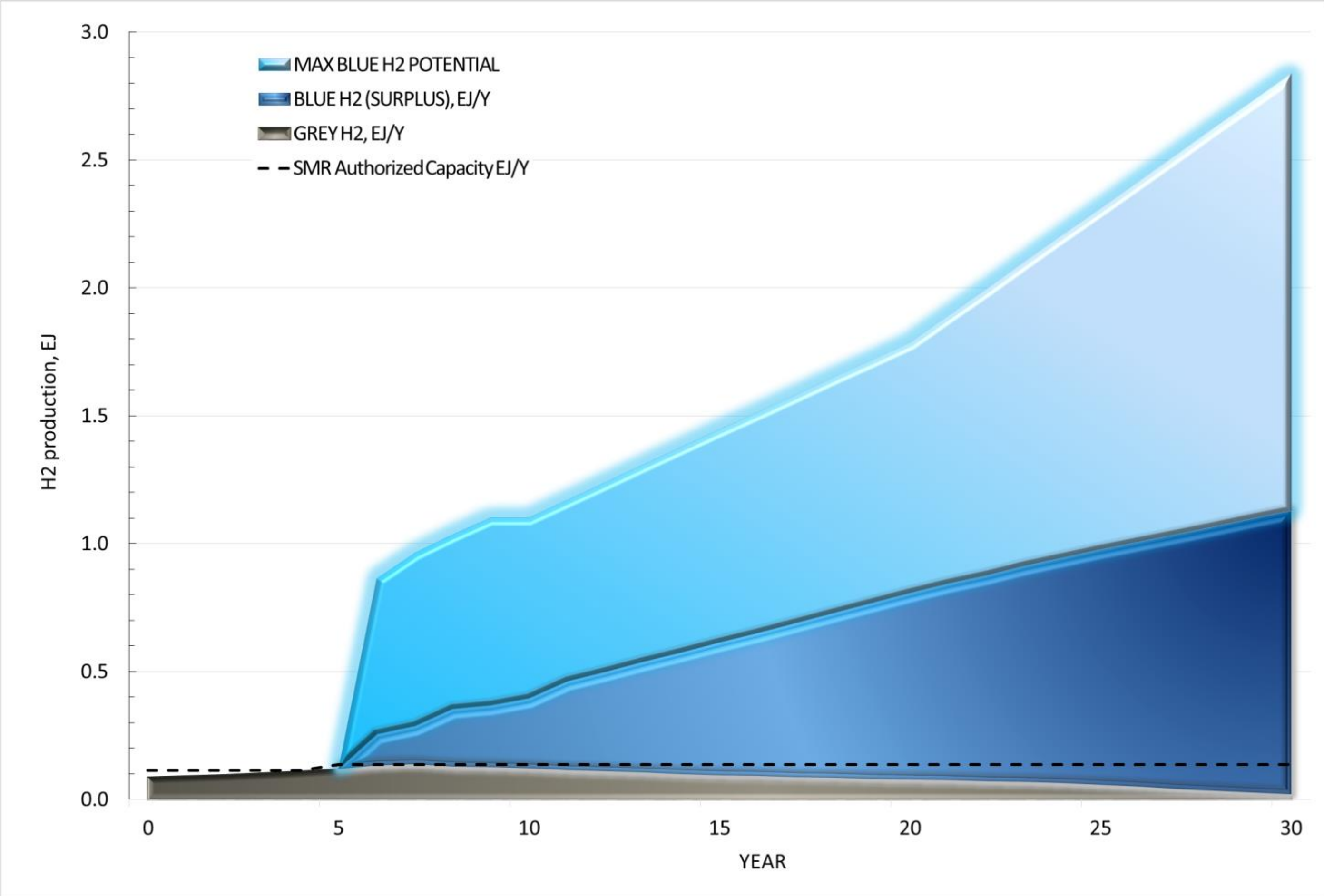


Figure 29: Blue and Grey H_2 production in the first long-term

From **Figure 29** it may be concluded that storage capacity may curb Blue H_2 production. Therefore, it is relevant to develop alternative storage options other than EOR. Such a strategy is relevant not only to increase storage capacity but also to foster Blue H_2 independence from Oil industry. In this case, investors should strongly consider NGPU and SMR capacity increase. Even in a modest growth scenario, business as usual, this simulation indicates 1 NGPU in the first decade, 1 more in year 20 and 4 more until Y30. Considering this strategy and the New Gas Market, 2 NGPU would be required in year 6, 1 more in year 7 and 2 more until year 15. In year 30 such an increase in gas production would total 11 NGPU. From year 10 onwards these new facilities installed for monetizing NG resources increase, not necessarily linked to refining needs. However, since H_2 networks replace NG networks, eventual new refineries could benefit from this infrastructure. Once H_2 becomes an independent business, new refineries could dismiss such facilities, becoming just a H_2 buyer. From year 12 to year 30 at least one SMR unit would be required each two years to comply with H_2 projected production. Only in year 22 no new SMR would be required. Global SMR unit requirements are 11 through 30 years.

Regarding the oil production compared to CO_2-EOR it seems that the estimated values may be reachable, thus making it possible to store CO_2 generated from H_2 production. In fact, for this level of EOR production, CO_2 produced in both in new and existing SMR units may be stored. On the one hand, such condition indicated that Blue H_2 production would be limited in this study only by NG availability and SMR facilities. On the other hand, a decrease in EOR production might also curb Blue H_2 production.

4.5.3 Pipeline Sizing and Cost Evaluation

As depicted in **Table 23**, CO_2 captured from SMR facilities reached 27.0 Mt in year 30. Then, two options were addressed. In the first, a single 44 inches pipeline was designed with a head loss of 20.1 kPa/km (a 42 pipeline was not selected due to pressure loss found 25.3 kPa/km). In the second option, a 36 inches pipeline was required to comply with full load of 15.7 Mt CO_2 in year 15 and a 32 inches pipeline to an additional load of 11.3 Mt CO_2 in year 30. The head losses found were, respectively, 18.8 and 17.8 kPa/km.

Table 23: Pipeline sizing

CO2 flow, Mt/y	Nom Diam., in	Length km	Pres. Loss, KPa/km
27.0	44	250	20.1
27.0	42	250	25.3
15.7	36	250	18.8
11.3	32	250	17.8

Average cost from offshore pipelines built in Brazil in the last decade was US$ 211.62/m.in (US$ per meter and per inch nominal diameter). On the Other hand, IPCC [305] offered a curve that indicated ratios US$/t$CO_2$ (for a 250 km pipeline). More recently, Kjastard et al. [306] indicated similar ratio unitary value in €/tCO_2, for pipelines analyzed in Norway. Those values may vary according to CO_2 volumes and were updated to 2019 (Y-1). Results may be compared global in **Table 24:**

Table 24: Pipeline costs

Nominal Diameter, in	Unitary Cost, 2019	Estimated Cost, MUS$ 2019	Cost Source
44	2.23 US$/t$CO_2$	1,803.72	IPCC [305]
42	2.43 US$/t$CO_2$	1,702.47	
36	3.08 US$/t$CO_2$	1,449.14	
32	3.74 US$/t$CO_2$	1,268.98	
44	6.26 US$/t$CO_2$	5,071.68	[306]
42	6.82 US$/t$CO_2$	4,786.79	
36	8.65 US$/t$CO_2$	4,074.03	
32	10.52 US$/t$CO_2$	3,567.18	
44	211.62 US$/m.in	3,066.30	Historic data
42		2,926.92	
36		2,508.79	
32		2,230.03	

Despite a large variation obtained from those sources, sizing reveals gains of scale. CO_2 flows around 15.7 Mt CO_2 were observed in year 15 of this simulation, while in year 30 total value of 27.0 MtCO_2 is reached. Comparison of global costs indicates that a larger pipeline would require less investments than two pipelines to convey the same quantity. However, a detailed feasibility study should be elaborated.

According to Kayfeci et al. [332] and Penner [333] apud Labanca [330], unitary costs for SMR unities should be between US$ 2080 to US$ 2655. Based on these data, costs for SMR units in the first 10 years would be between US$ 3,369.60 and US$ 4,301.10 million. In all other years of the analysis, CO_2 requirements for EOR would be higher than CO_2 generated within the H_2 production, which means that Blue H_2 production would not be capped by oil production.

In this preliminary approach, investment capital costs for producing Blue H_2 in the first decade would involve the facilities and costs presented in **Table 25**.

Table 25: Calculated investment for Blue H_2 in the short term (Y1 to Y9)

	Gas Flow	Units	Investment, M US$
NGPU	79.74 M m^3/d	3	1,631.82
SMR	14.59 M m^3/d	3	5,096.87
CO2 Pipeline	27 Mt/Y	1	3,066.30
Total Investment			**9,794.99**

Incomes are based on a value of US$ 40/bbl, starting from year 5, when first CO_2-EOR facility produces. Findings show that by year 10 (9,581.49 MUS$) -11 (14,256.19 MUS$) investments would equal oil revenues from additional production due to EOR. This result does not consider earnings from H_2 or NG sales.

The present strategy does not evaluate the detailed feasibility of each facility. Instead, it assesses monetizing NG resources in order to avoid stranded reserves, thus paving the way for a just energy transition, avoiding job losses and economic setbacks. Hence, the present strategy showed that it seems possible monetizing NG resources trough Blue H_2 strategy. Such a strategy involves simple calculation but executes a stepwise method to address monetizing fossil fuels in an increasingly curbing environmental framework. Providing low carbon methods are essential not only in the present but also in the future, when restriction to carbon emissions should become stronger.

4.6 Conclusion

This study modeled a strategy to monetize NG resources by means of increasing oil production by EOR technology. This strategy consisted in assessing NG production data and calculating H_2 production potential from NG. Brazil would reach a H_2 production of 1.12 EJ in 2050, relying only on endogenous natural resources. Comparatively to Europe business as usual scenario (0.54 EJ), it is a bold increase, standing for a tenfold rise compared to current H_2 production for Brazil. Compared to Europe, Brazil would reach about half of the projected Blue H_2 demand 2.16 EJ in the accelerated decarbonization pathway.

Furthermore, total H_2 production potential would reach 0.7 EJ in 2050, considering fossil resources. Monetizing such reserves seem to be feasible, once relatively low oil prices (US$ 40/bbl) would quickly pay investments done (9 years).

Storage capacity may curb Blue H_2 production, therefore, it is relevant to develop alternative storage techniques other than EOR. Such a strategy is relevant not only to increase storage capacity but also to foster Blue H_2 independence from oil industry.

The present strategy showed that it is possible to monetize NG resources trough Blue H_2 strategy. Monetizing Natural Gas resources may be a tricky business in a near future, regarding environmental restrictions. The current study offers an original strategy for fossil fuel producers to monetize those resources in such a restraining scenario.

However, a future detailed study should be developed, including an economic feasibility analysis. In addition, earnings from NG sales and regulatory issues should be further discussed, so as to account for local taxes and subsidies. Finally, a detailed study to assess and properly size the transportation network, including aspects such as fluid dynamics and network constraints is also an important future development. Those issues that were not addressed current study are relevant suggestions for future work

.

5 *Conclusion and Future Studies*

The present work had the global objective of evaluating strategies to monetize natural gas resources under infrastructure constrains. This main objective of this thesis was divided into three major research questions that led to the preparation of three scientific papers focused on natural gas liquids, transport and storage infrastructure and blue hydrogen production. Brazil was used as a country case study in all three papers, because it has meaningful conventional and unconventional reserves, which require feasible options for monetization.

All technical solutions of the presented strategies are technologies in advanced development or already proved, and evaluating them under the perspective to avoiding stranded reserves is unusual. This thesis tried to fill this gap. Actually, this work evaluated how natural gas technologies can impact the energy planning in a systemic way, mainly regarding rich natural gas resources and avoiding stranded reserves.

The evaluated strategies have in common the idea that industrial facilities can bring wealth by creating jobs, generating income and producing goods with downward linkages to different industrial sectors. However, in the last decades Brazil is passing through a process of deindustrialization. For instance, the two methanol producers in Brazil closed in the last 5 years, chlorine and soda facilities stalled and the monopsonist for petrochemicals prefer importing from its newly-built ethene factory in Mexico rather than producing in Brazil. Actually, importing finished industrial goods has become a common strategy in Brazil and this might undermine some of the evaluated strategies in this thesis

Nevertheless, the strategies assessed by this thesis converge in a strong requirement for engineers and technicians to develop and carry on those projects. Oil and gas production need high- skilled human capital. A petroleum producer country, such as Brazil, can transition from the oil & gas sector to other options, including H_2 as an energy carrier, by benefiting from the skilled labor already in place.

Natural Gas Liquids (NGL)

The first analysis carried out in this study compared two strategies to monetize NGL fractions: petrochemical feedstocks and energy use. Both processing strategies presents positive NPV values for all simulations. Then, processing natural gas should be an attractive business in either strategy. Petrochemicals offer a higher but riskier NPV, which might suffer high influence on the gas composition.

The Fuel strategy presents advantages of being a well-stablished and oligopolistic market in Brazil, which is able to flow production by a capillary wholesale structure. But average NPV values are lower than in the petrochemical strategy. Costs are lower for the Fuel strategy, which reinforces that option that seems to involve lower risks. The Petrochemical strategy presents higher NPV values, but with a larger standard deviation. Market risks for Petrochemical strategy also involve a diversity of factors, which investors should be acquainted with.

It could be expected that leaner compositions would not yield enough volumes for meeting the minimum required scale to feed a steam cracker. However, the ethane steam cracker scale is not the limiting factor for this route even under leaner compositions

The Petrochemical strategy has outdone the Fuel strategy for moderate and rich gas compositions (> 7% C2 and/or >3% C3+) considering transport specifications. Those moderate and rich compositions challenge the limiting values of ethane in transport pipelines established in Brazilian regulation, by delivering lean gas compositions close to the limiting values or even going beyond them. In a scenario when these rich compositions profiles prevail, processing units may be overloaded by ethane streams and the petrochemical strategy deals with that by creating a value chain for ethane.

Discount rates were estimated according to the Brazilian figures at different time frames. However, since it is a rather fluctuating value in emerging countries, such as Brazil, it becomes a risky component of the assessments made. The stochastic assessment of the NPV that was undertook in this study helps to deal with the uncertainty, but does not solve this this risk. Further studies should deepen the impact of the opportunity cost of capital into the strategies assessed in this work.

Underground gas storage (UGS)

The second assessment made in this study propose and apply a method for evaluating bottlenecks in existing networks and optimizing seasonal and variable gas demand by offering regular supply using UGS. Results indicated that pipelines should be designed integrated to the existing network where they are inserted. Simulation runs allowed the comparison between single and integrated solutions, offering options for investigating supply and demand variations. In these boundary conditions, the planner may anticipate network bottlenecks, assess and propose adequate improvements. Often bottlenecks may be solved by oversizing or increasing compression power, although this is far from offering the best solution.

The analysis provide evidence that UGS is a feasible option for both solving bottlenecks and reducing network idleness. It reduces diameters in pipeline sizing and benefits from revenues associated with gas trading arbitrages. UGS acts as a swing point, demanding gas to compensate low demands from intermittent customers, and delivering it when the network is challenged by peaks. This lowers the gas transmission tariffs.

Although the study did not evaluate the type of UGS to be applied nor assessed the existence of geological sites in the region, it is worth noting that the chosen region is home of the largest aquifers in South America (Guarani), thus at least two possible geological formations may favor the project: depleted field and saline aquifers. The best option should be studied in future analyses.

Natural gas to hydrogen conversion (with associated carbon capture)

Not seldom industrial facilities keep idle capacity when market demands vary. Currently, steam methane reformers are the most applied technology for hydrogen production. Therefore, taking advantage from those facilities' idle capacity can pave the way for transitioning from grey to green hydrogen through blue hydrogen. Moreover, natural gas (NG) conversion to hydrogen equipped with carbon capture facilities can be monetized when CO_2 from hydrogen production is used in increasing oil production by EOR technology. This strategy consisted in assessing NG production data and calculating H_2 production potential from NG in Brazil.

Results showed potential capacity for H_2 production in Brazil of 1.1 EJ in 2050.[44] In addition, average idle hydrogen production capacity would yield an amount of H_2 that is technically allowed to blend with natural gas in most of the existing transport pipelines. Finally, potential oil production increase by introducing EOR would pay for investments for installing CO_2 offshore pipeline.

Final Remarks

Natural gas is a highly cost-intensive industry that presents high and irreversible fixed costs. In addition, long-term contracts require meeting demands for a variable market. Delivery prices often are high, preventing investments as long as oil prices are used as reference for trading contracts. In addition, natural gas is a fossil fuel, and replacing coal might not be a strategy effective enough to abate greenhouse gas emissions, which places the need to carry the energy transition process to a low carbon uses of natural gas that go beyond coal replacement.

All in all, planners should care about three factors: avoiding stranded reserves; monetizing natural gas resources; storing and delivering NG products. Infrastructure is on the hinge of all these factors. Natural gas needs to be processed, conveyed, stored and sold in a chain that should add value and bring both social and environmental benefits for the society.

This study did not deepen the analysis on natural gas price formation, for instance evaluating supply contracts and delivery modes (pipelines, LNG, etc.). Nonetheless, these aspects can be relevant for reaching a feasible strategy.

A synergy between those strategies could be found when evaluating the possibility of a natural gas hub formation in Brazil, or even a gas-petrochemical hub, similar to Mont Belvieu, in USA. Installing a UGS facility may spearhead a hub formation, if some relevant aspects of infrastructure concerning gas processing, SMR plants and steam crackers are observed.

Synergies can be found on locational definitions, mainly if UGS are installed in depleted fields. Therefore, UGS site location is a crucial definition, and usually precedes other decisions, since it depends

[44] As comparison, this could be extrapolated for Latin America, that could potentially reach 3.3 EJ in 2050 relying only on endogenous natural resources

on geological conditions. Suitable places for developing UGS sites should in principle include regions where depleted hydrocarbon fields exist. Surely saline formations, aquifers or abandoned mines can be investigated, but it is likely that those options would depart from less geological knowledge than depleted field, and they would be likely more expensive projects due to this aspect.

UGS placement may profit from two extra regional pre-conditions: existing natural gas infrastructure as pipelines and/or processing units, and future perspective of producing natural gas. These preconditions may not only abruptly reduce costs but also favor reaching customers. It may help when exploring frontiers are found close to mature fields as some the pre-salt fields in Brazil.

Another possible positive synergic aspect to be found in a location previously selected for those above-mentioned technologies is the existence of multimodal infrastructure. Regions of mature oil and gas exploration usually present a reasonable multimodal infrastructure, like airports, railways, roads and ports is advantageous for flowing feedstocks and products. In this regards, proximity of consumer center may be also advantageous for start.

Additionally, only for the Petrochemical strategy, regional proximity of existing steam cracker units connected by pipelines may offer a synergic aspect, since ethane transportation is a barrier to develop petrochemicals. In fact, all these above-mentioned aspects as synergic may become infrastructure barriers if they do not occur. Therefore, decision makers should be careful when defining to deploy this integration strategy. In Brazil, regions like the Recôncavo basin, in Bahia, and the Campos basin, in Rio de Janeiro fills most of those infrastructure aspects.

In a transition scenario, lean natural gas streams, mostly methane, can be used for Hydrogen production, given the idle SMR capacity in Brazil. The produced hydrogen can be blended into transport networks up to 15% v/v and the captured CO_2 emissions from this process can be used to enhance oil production offshore. In the Campos Basin, for instance, there are meaningful offshore reserves in pre-salt area that can be enhanced this way and mature fields that require advanced recovery technologies. In addition, the region that has the largest processing capacity in the country is connected by transport pipelines to the refinery REDUC, in the metropolitan area of Rio de Janeiro. This refinery is placed close to an ethane steam cracking facility.

These locational aspects allow a synergic effect between the hydrogen and the petrochemical strategies, on the one side. On the other side, underground storage sites can be placed in mature or depleted fields close to oil exploitation frontiers, like pre-salt, where EOR techniques can be applied, thus integrating all three strategies. Finally, since petrochemicals may fix carbon in long-term strategies, it is more desirable under decarbonization scenarios when compared to producing fuels, contributing to meet the Paris Agreement goals.

Nonetheless, the market structure is a relevant barrier common to the three strategies. In markets like Brazil, where natural gas and derivates supply chain is highly concentrated by some actors, and competition rarely occurs, the challenge is to find strategies that facilitate the entrance of new investors.

Regulatory framework should play an essential role under these. Actors that have full or mandatory market enforcement are not willing to share it. In Brazil, recent changes in the main law regulating natural gas sector, and consequently in the regulatory framework, seem to indicate a trend to a competitive market. Nevertheless, those changes are yet to be proved feasible and steady. In the case of the Petrochemical industry, the Brazilian market structure points to high entry and exit barriers, due to a monopsonist and monopolistic structure. Investing in NG infrastructure is a capital-intensive business, often relying on middle and long-term feasibility.

Each analyzed strategy was developed considering different time frames and locations. The results showed that the strategies are not qualitatively exclusive, since a decision maker can choose to process raw natural gas, use part of the dry NG for producing blue hydrogen, and apply NGL for both fuel and petrochemical strategies. This can be done based on a hub created around a UGS facility connected to pipelines. Yet, the policy of investing on blue hydrogen can be in some level conflicting to the idea of increasing oil production. In addition, to invest in UGS facilities may require trading natural gas only as a fuel rather than as a petrochemical feedstock.

In brief, the main lessons from this thesis can be highlighted as following:

- NGL can be an important driver to monetize gas resources and have higher expected return as chemical feedstock than when used as fuels.
- High pressure gas pipelines are the most cost-effective transport mode to convey large amounts of natural gas, and underground storage in geologic structures is a feasible way to store it and regulate supply and demand.
- Underground gas storage can optimize gas pipelines networks and help to deal with seasonal markets. In addition, UGS may underpin a value chain for gas-based industries.
- Transporting and storing NG are relevant services that offer opportunity for investors. Moreover, UGS may attract demand unfolding a value chain for gas-based industries.
- Producing hydrogen from natural gas can bridge fossil fuels industry to low carbon when equipped with CO_2 capture and storage. In fact, in a contemporary analysis, IEA [35], developed a similar rationale as the presented strategy highlighting the role of blue hydrogen for energy transition. According to IEA, 50% of the natural gas use would be directed to hydrogen production worldwide, resulting in global 925 billion cubic meters of natural gas and 1.8 Gt CO2 being captured by 2050.
- Natural gas processing by outputting valuable liquids can be a supportive option for reducing the break-even price of the gaseous fractions of the raw gas, and establish diversified markets (including petrochemicals).
- Finally, converting natural gas into hydrogen from idle capacity in existing facilities is relevant to deal with energy transition towards decarbonization in addition to valuing fossil fuel resources.

<u>Future developments</u>

This thesis evaluated strategies for different gas fields and scales. Further studies are needed, however, to both complement the evaluations made and expand them to other scopes.

1 – Develop a case based on an existing depleted field in a mature petroleum production area.

A future study could evaluate a hub formation, departing from a UGS facilities in depleted fields, connected to processing units, steam crackers and steam methane reforming units. For this purpose, this thesis indicates a brown field analysis, taking advantage from as much as existing facilities as possible. The following additional factors should be regarded: geological pre-conditions; idle capacity; transport pipelines; EOR and EGR potentials; limiting distance between facilities; proximity to customer market; complementary innovative technologies. In Brazil, few regions meet the above conditions. This study indicates Campos and Recôncavo Basins should be the most suitable regions for this analysis.

2 - Geological analysis

Geological analyses are expensive. Yet, the definition of the UGS site location is crucial. Depleted fields usually are the best starting point, since they have information from historical use. Actually, some stages of geological assessment for depleted fields can be dismissed due to historical familiarity about the former oil production site. Nevertheless, geological knowledge in a given place may excel in other specific formations like aquifers, saline formations or abandoned mines, depending on the local conditions.

3 – Developing better integration between electricity generation planning and natural gas infrastructure.

Power generation is a major natural gas consumer in Brazil. However, the integrated planning of electricity supply and natural gas network expansion was not made by this study. In the Brazilian electric power system, natural gas fueled plants have a relevant role providing flexibility to cope with fluctuations of hydropower generation, which could even become more variable with climate changes. Therefore, granting flexible and reliable natural gas supply increases energy security. Additionally, as UGS increases reliability, its benefits to the electric power system should be studied and valued.

4 – Studying natural gas regulatory framework in the light of the recent changes

Recently, a new Gas Law was passed in Brazil, ruling changes for infrastructure access, facilities sharing and authorization rules. In principle, it intends to facilitate the construction of UGS facilities and pipelines. The present study did not dig deep into the regulatory framework, but this is surely relevant for informing investment decisions. A comparative analysis of the Brazilian framework with the international success cases could bring relevant lessons to decision makers.

In addition, after few years being regarded as an economic asset that might thrive, unconventional gas reserves projects reached a stalemate in Brazil. Understanding the limitations for this industry is also a relevant technical and regulatory question, since potential reserves are meaningful and, in this case, the risks for stranded reserves is higher than for associated offshore gas.

Regulatory uncertainties are another relevant issue for the capital-intensive strategies assessed in the present analysis. Therefore, future studies should better represent the institutional challenges.

5 –Wider analyses on CO2 capture and storage

CCS techniques are relevant when regarded as a complementary technique for producing blue hydrogen. In the current strategy, global investment values were used. Thus, regulatory aspects and public policies were not assessed. Further developing these subjects is worthwhile. In addition, chemical ways to fix carbon may be associated to the physical storage of CO_2. For instance, the use of microalgae to fix CO_2 can be a relevant to increase CO_2 pipeline feasibility by building delivery points along the pipe way. In addition, biogas dry reform projects can play similar role, since Brazil is a significant biogas producer.

6 –Developing a feasibility study for the proposed strategy for hydrogen transition

Finally, the monetization of NG resources by means of the Blue H_2 strategy has indicative positive results. Regulatory aspects for injecting hydrogen in natural gas network have not been addressed in Brazil, but regulation does not forbid it, which may be seen as an advantage.

Preliminary results indicated positive revenues for EOR production for monetizing the blue hydrogen industry. However, regulatory framework, taxes and detailed costs were not deeply assessed in this thesis.

In addition, transitioning policies from blue to green hydrogen were not addressed. Another study should identify mechanisms to make progressively attractive to leave fossil sources and adopting clean sources in long-term policies.

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7 *Supplementary Material*

7.1 Strategies for monetizing natural gas liquids from processing plants

Simulation codes and data may be found on https://github.com/matheuspoggio/Natural-Gas-Processing-Plans-NPV-Analysis

7.2 Planning natural gas networks and storage in emerging countries

Pipelines' main characteristics, such as nominal diameter, length, and localization are listed in **Table S-26**

Table S-26: Natural gas transmission Pipelines in Brazil. Based on [334]**.**

Name	Origin*	Destiny	Operation Year	Nominal Diameter (in)	Length, km
Atalaia-Santiago-Catu	Atalaia (SE)	Catu (BA)	1974	14	230.0
Santiago/Catu-Camaçari I	Santiago (BA)	Camaçari (BA)	1975	14	32.0
Atalaia-FAFEN	Atalaia (SE)	Laranjeiras (SE)	1980	14	29.0
Candeias-Camaçari	S. Francisco do Conde (BA)	Camaçari (BA)	1981	12	37.0
Ramal Campos Elíseos II - Ramal de 16"	Duque de Caxias (RJ)	Duque de Caxias (RJ)	1982	16	2.7
Lagoa Parda-Aracruz	Linhares (ES)	Aracruz (ES)	1983	8	38.0
Aracruz-Serra	Aracruz (ES)	Serra (ES)	1984	8	41.0
Reduc-Esvol	Duque de Caxias (RJ)	Volta Redonda (RJ)	1986	18	95.2
Guamaré-Cabo	Guamaré (RN)	Cabo (PE)	1986; 2010	12	455.8
Esvol-Tevol	Volta Redonda (RJ)	Volta Redonda (RJ)	1986	14	5.5
Esvol-São Paulo (Gaspal I)	Piraí (RJ)	Mauá (SP)	1988	22	325.7
Santiago/Catu-Camaçari II	Santiago (BA)	Camaçari (BA)	1992	18	32.0
RBPC-Capuava (GASAN I)	Cubatão (SP)	São Bernardo do Campo (SP)	1993	12	37.0
RBPC-Comgás	Cubatão (SP)	Cubatão (SP)	1993	12	1.5
Reduc-Regap	Duque de Caxias (RJ)	Betim (MG)	1996	16	357.0
Guamaré-Pecém	Guamaré (RN)	Pecém (CE)	1998	10 to 12	382.0
Bolívia-Brasil (Gasbol), Brazilian part	Bolivian Border	Brasil	1999-2000	16 to 32	2593.0
Uruguaiana-Porto Alegre	Uruguaiana (RS)	Uruguaiana (RS)	2000	24	25.0
Uruguaiana-Porto Alegre	Canoas (RS)	Triunfo (RS)	2000	24	25.0

Pilar-Cabo	Pilar (AL)	Cabo (BA)	2001	12	203.6
Lateral Cuiabá	Cáceres (MT)	Cuiabá (MT)	2001	18	267.0
Candeias-Aratu	São Francisco do Conde (BA)	Aratu (BA)	2003	14	15.4
Santa Rita-São Miguel de Taipu	Santa Rita (PB)	São Miguel (PB)	2005	8	25.0
Dow-Aratu-Camaçari	Aratu (BA)	Camaçari (BA)	2006	14	27.0
Atalaia-Itaporanga	Atalaia (SE)	Itaporanga D'Ajuda (SE)	2007	14	29.0
Cacimbas-Vitória	Linhares (ES)	Vitória (ES)	2007	26 to 26	129.4
Carmópolis-Pilar	Carmópolis (SE)	Pilar (AL)	2007	16	176.7
Catu-Carópolis	Itaporanga D'Ajuda (SE)	Carmópolis (SE)	2007	26	67.8
Catu-Carópolis	Catu (BA)	Itaporanga D'Ajuda (SE)	2008	26	197.2
Açu-Serra do Mel	Serra do mel (RN)	Alto do Rodrigues (RN)	2008	14	31.4
Cabiúnas-Vitória (Gascav)	Macaé (RJ)	Serra (ES)	2008	28	300.0
Campinas-Rio (Gascar)	Paulínia (SP)	Japeri (RJ)	2008	28	450.0
Fafen-Sergás	Divina Pastora (SE)	Laranjeiras (SE)	2009	8	22.7
Cabiúnas-Reduc III (Gasduc III)	Macaé (RJ)	Duque de Caxias (RJ)	2009	38	180.0
Japerí-Reduc (Gasjap)	Japeri (RJ)	Duque de Caxias (RJ)	2009	28	45.3
Campos Elíseos-Gas Ring	Duque de Caxias (RJ)	Duque de Caxias (RJ)	2009	20	2.3
Urucu-Coari (Garsol)	Urucu (AM)	Coari (AM)	2009	18	279.0
Coari-Manaus	Coari (AM)	Manaus (AM)	2009	20	383.0
Coari-Manaus (Branches)	Coari (AM)	Manaus (AM)	2009	3 to 14	140.1
Cacimbas-Catu	Linhares (ES)	Pojuca (BA)	2010	28	946.0
Paulínia-Jacutinga	Paulínia (SP)	Jacutinga (SP)	2010	14	93.0
Gascav Connection	Anchieta (ES)	Anchieta (ES)	2010	10	9.7
Rio de Janeiro-Belo Horizonte (Gasbel II)	Volta Redonda (RJ)	Queluzito (MG)	2010	18	267.0
Pilar-Ipojuca	Pilar (AL)	Ipojuca (PE)	2010	24	187.0
Caraguatatuba-Taubaté	Caraguatatuba (SP)	Taubaté (SP)	2011	28	98.0
Guararema-São Paulo	Guararema (SP)	São Paulo (SP)	2011	22	54.0
São Paulo -São Bernardo do Campo (Gasan II)	São Paulo (SP)	São Bernardo do Campo (SP)	2011	22	38.0
Total					**9409.0**

* Symbols in brackets refer to the following Brazilian States: AL – Alagoas; AM – Amazonas; BA – Bahia; CE – Ceará; ES - Espírito Santo; MG - Minas Gerais; MS - Mato Grosso do Sul; MT - Mato Grosso; PB – Paraíba; PE – Pernambuco; RJ - Rio de Janeiro; RN - Rio Grande do Norte; RS - Rio Grande do Sul; SE – Sergipe; SP - São Paulo.

Transport pipeline network growth evolution profile can be observed in **Figure S-30**

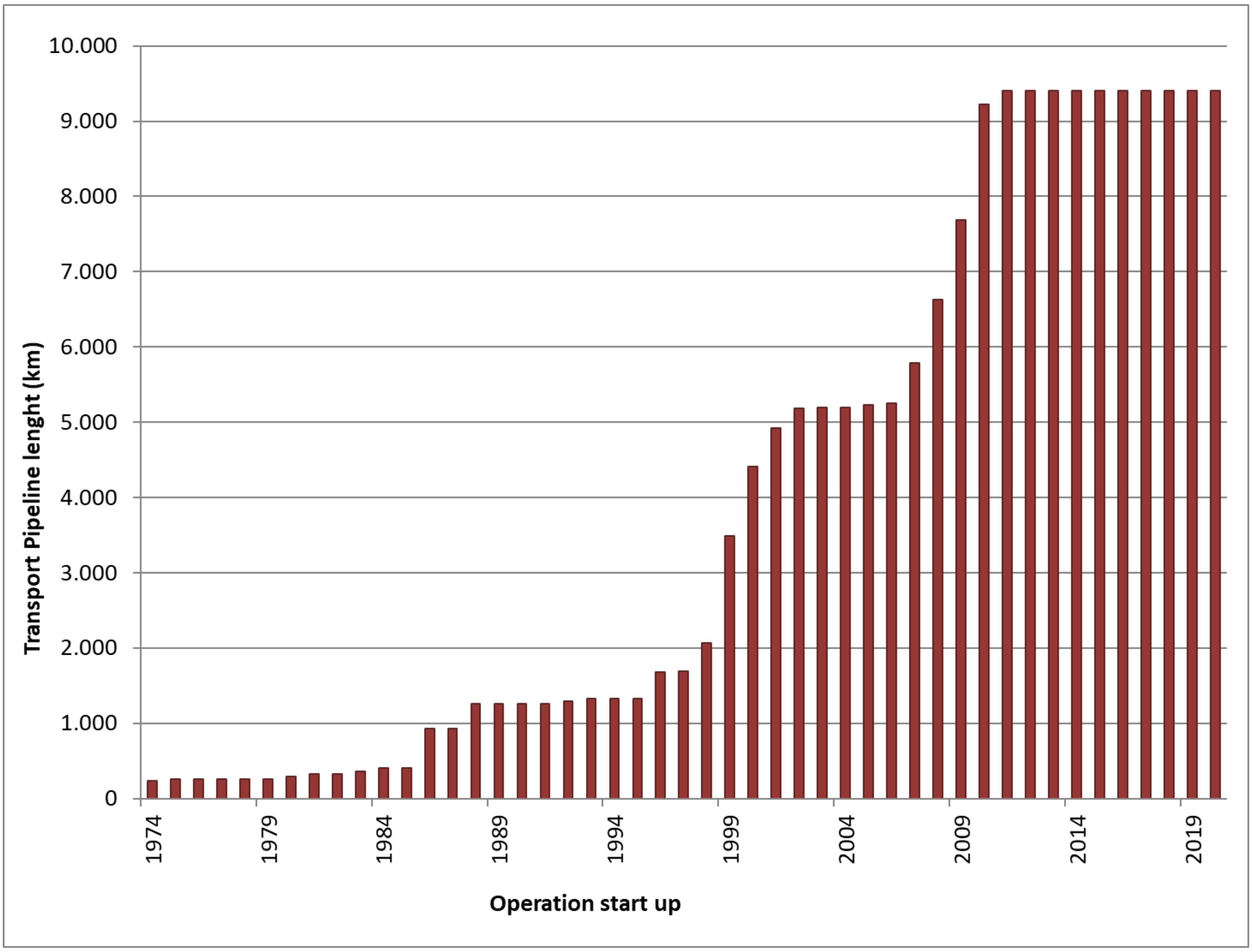

Figure S-30: Transport network historic increase. Based on [334]

7.3 Blue Sky Mining

This supplementary material presents a brief description of the step-by-step procedure developed and applied to assess the strategy of monetization for blue hydrogen.

It begins with a brief but broad approach of the hydrogen production methods and concentrates on the focus of the article, which is the steam methane reforming (SMR). The strategy is then unveiled by a stepwise and concise description of the idle hydrogen production capacity, which addresses the following aspects:

- Evaluating the logistic options for hydrogen and natural gas blending and establishing rules for hydrogen-natural gas blending in gas pipelines;
- Establishing new natural gas pipelines facilities expansion to cope with the increase on hydrogen production volumes;
- Estimating the future natural gas resources availability and prioritizing hydrogen production instead of accumulating stranded reserves;
- Designing the approach to be undertaken for carbon capture storage and utilization, prioritizing the use of CO_2 from blue hydrogen production on enhanced oil recovery in the short term; establishing metrics for enhanced oil recovery (EOR) and forecasting the amounts of oil production from enhanced oil recovery;
- Calculating the required volume of CO_2 potentially sequestered and sizing the correspondent CO_2 pipeline needs.

There is a diversity of technologies for hydrogen production, which is thoroughly treated in the literature. Figure S-31, adapted from Nazir et al. [335], presents an overview of the methods to produce hydrogen from fossil fuels and from renewables.

Concerning the hydrogen production from fossil fuels, which is the motivation of the present study, it has been analyzed under a monetization perspective of taking into account the externalities associated with the "real" cost of hydrogen production [70] [71]. These studies were convergent with others [335] [75] to conclude that the SMR is the most mature technology used worldwide for hydrogen production, that it should maintain that position for the near future, and that it presents the lowest unabated total cost of hydrogen when it is equipped with carbon capture and storage, as of today. These findings create the basis to explore how the main and abundant current sources of methane, natural gas reserves, and the associated industrial infrastructure may strategically contribute to the energy transition and to a new hydrogen energy era.

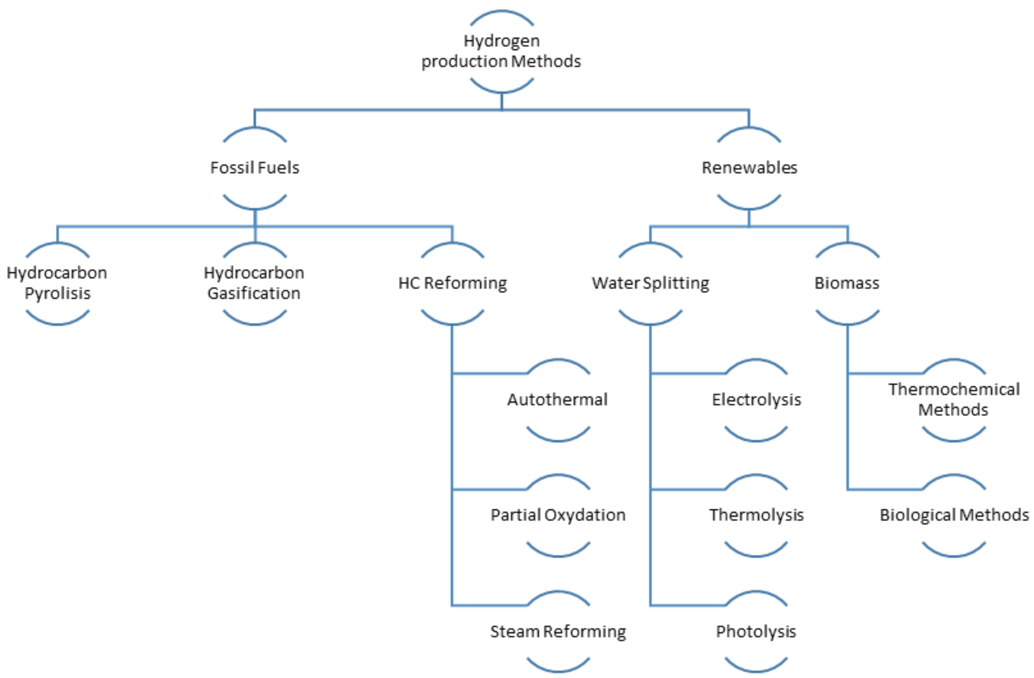

Figure S-31: Hydrogen production methods. Adapted from [335]**.**

The strategy proposed in this paper relies on the use of the SMR idle capacity in hydrogen-producing facilities and consists, essentially, of the following steps:

1) Estimating resources: In a country with prospective reserves, natural gas may be used for producing hydrogen. It was assumed that agents would prefer to produce hydrogen than accumulate stranded reserves. Hence, all extra natural gas production would be used for hydrogen production

2) Assessing the idle hydrogen production capacity: for the case study of this paper, refining capacity and utilization factors are provided by Brazilian official data sources. However, the production capacity can be assessed from other sources, such as Sun et al [286]. In this paper, the following data was obtained [6] - see **Table S-27**:

Table S-27: Hydrogen production capacity in Brazilian Petroleum Refineries

			Yearly Utilization Factor, %				
REFINERY*	**Full capacity, $Nm^3/d \times 10^3$**	**Authorization**	**2018**	**2019**	**2020**	**Avg Idle Capacity, %**	**Available H_2 $Nm^3/d \times 10^3$**
RNEST	3,000.00	575/2017	64.0%	97.2%	102.0%	12.3%	368.00
RNEST (2025)**	6,200.00	565/2011	64.0%	97.2%	102.0%	12.3%	760.53
REPLAN SP	4,070.44	669/2016	48.3%	84.6%	52.4%	38.2%	1,556.26
RPBC	2,870.00	813/2019	93.6%	83.3%	82.8%	13.4%	385.54
REGAP/ REGAP II	2,120.00	156/2014	86.8%	71.4%	53.7%	29.4%	622.57
REPAR	1,870.00	554/2020	74.2%	66.3%	82.7%	25.6%	478.72
REFAP	1,800.00	80/2015	68.1%	61.0%	69.1%	33.9%	610.80
REVAP	1,630.00	521/2020	90.6%	52.5%	87.3%	23.2%	378.16
RLAM	3,985.30	811/2013	55.8%	66.9%	68.3%	36.3%	1,447.99
REDUC	822.83	322/2016	83.2%	88.0%	77.6%	17.1%	140.43
RECAP	550.00	976/2015	75.7%	79.8%	64.9%	26.5%	145.93
LUBNOR	35.00	401/2016	70.4%	78.5%	68.2%	27.6%	9.67
Average			**72.9%**	**77.2%**	**75.9%**	24,7 %	
Total - 2020	**22,753.56**						3946.92
Total - 2025	**34,713.56**						

*** Acronyms used to name refineries in Brazil:** RNEST - Refinaria do Nordeste; REPLAN - Refinaria de Paulínia; RPBC - Refinaria Presidente Bernardes de Cubatão; REGAP - Refinaria Gabriel Passos; REPAR - Refinaria do Paraná; REFAP - Refinaria Alberto Pasqualini; REVAP - Refinaria do Vale do Paraíba Henrique Lage; RLAM - Refinaria Landulpho Alves; REDUC - Refinaria de Duque de Caxias; RECAP - Refinaria de Capuava; LUBNOR – LUBNOR.
**** Estimate**

3) Evaluating logistic options for Hydrogen and Natural Gas blending: as SMR facilities require natural gas supply, natural gas pipelines are already connected upstream to those facilities. Thus, connecting hydrogen facilities upstream to the natural gas infrastructure for blending should require small adaptations in the refinery area.

For the case study of this paper, in Brazil, all refineries are connected to the natural gas network and a list of all pipelines diameters and capacities is available [169] [101]. **Figure S-32** illustrates the Brazilian refineries connected to the network of natural gas pipelines.

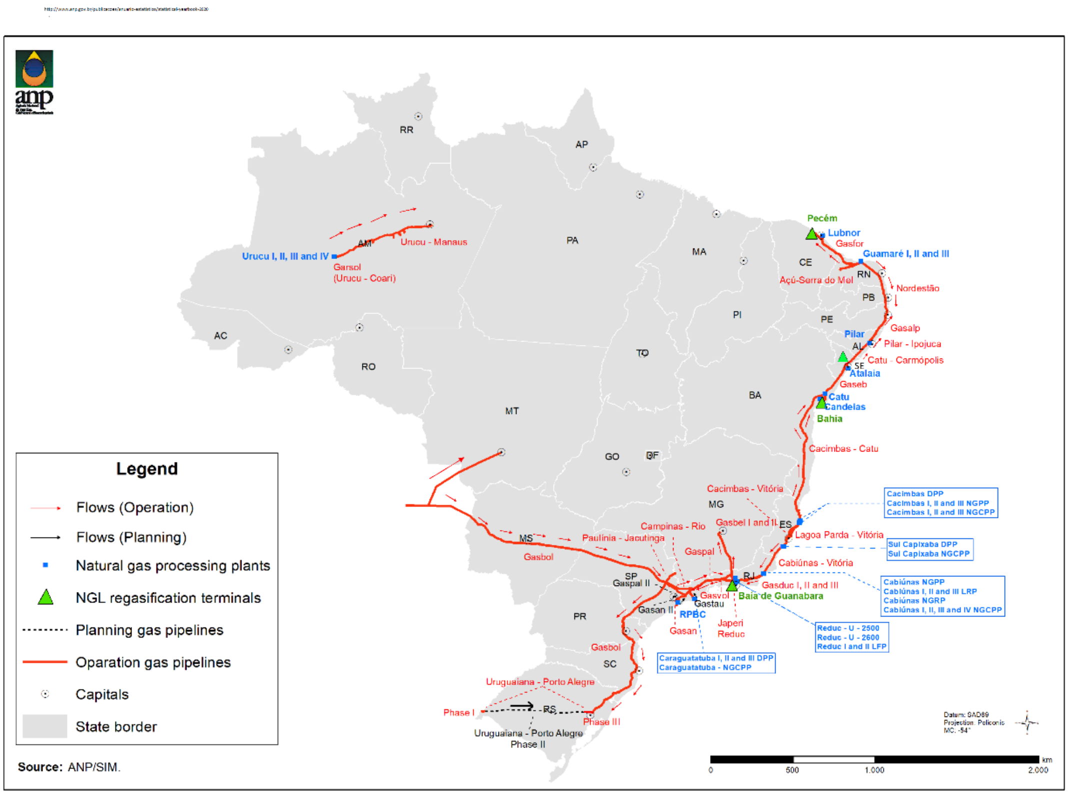

Figure S-32: Brazilian Natural gas Infrastructure [169]

The blending strategy in the work included each refinery and pipelines able to convey hydrogen. In the strategy, the pipeline's natural gas transport capacity was calculated based on the available data. Refineries with available capacity were assessed compared to pipelines full capacity. Based on these capacities, newer pipeline systems were prioritized over the older in order to avoid problems like embrittlement. Ramp up were scattered up to 5 years for each pipeline. **Figure S-33** displays the refineries' contributions ramp up according to the pipeline systems connected to them.

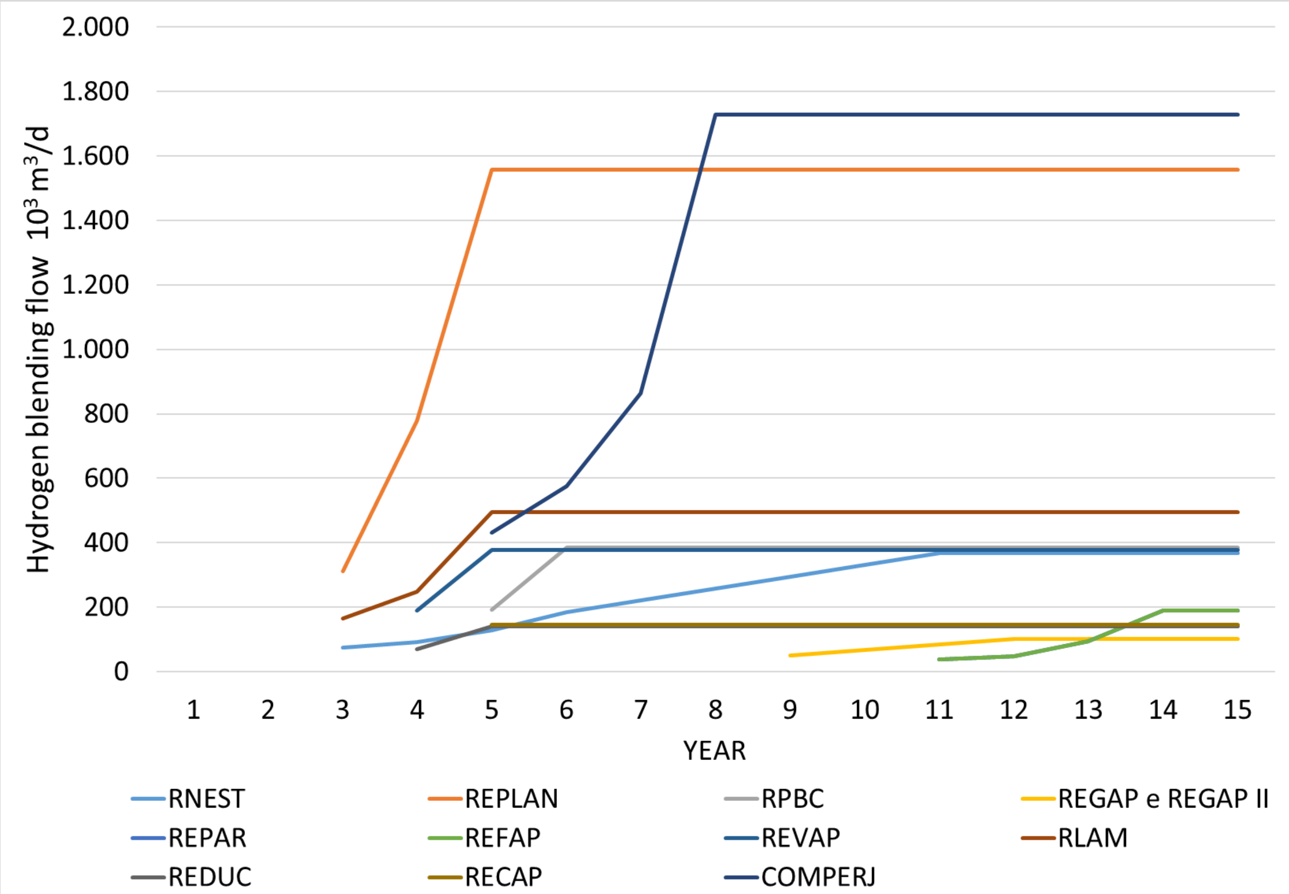

Figure S-33: Blending strategy according to each refinery and pipeline system

4) Establishing in the year 3-5 a stepwise H_2 injection increase based on: (a) hydrogen availability due to idle capacity in SMR facilities; (b) the average Wobbe index in the pipeline that sets an initial maximum blending value.

5) Building CO_2 pipelines: after 5 years, CO_2 pipelines can be built to start compensating GHG emissions from SMR facilities. In the particular case of Brazil, these pipelines should ramp up in 5 five years [336].

6) Estimating oil recovery factors: studies show that EOR techniques might increase hydrocarbons exploitation by 7 to 23% (with an average of 13%) of total oil in place (OIP) [317]. Other authors [318] corroborate that range for miscible mixtures between CO_2 and oil in EOR. Hill [319] estimated an increase of 6% to 10% of total oil in place (OIP) production, although they highlighted that this result is not based on supercritical CO_2 injection, which stimulates miscibility

and increases productivity. More recent studies reported incremental oil recovery ranging from 6.09 to 22.83% of OIP for techniques of CO_2-EOR [320].

7) Projecting oil production from EOR: In Brazil, the forecasts for crude oil production from the Ministry of Mines and Energy [337] [338] were used, see **Table S-28**.

Table S-28: **Oil production forecasts in Brazil. Based on** [337] [338]

Year	Forecasted Production (Millions of Barrels)
2020	3.24
2021	3.44
2022	3.65
2023	3.78
2024	4.01
2025	4.30
2026	4.78
2027	5.17
2028	5.43
2029	5.54
2030	5.39
2040	4.70
2050	5.30

8) Calculating CO_2 volume flow: the required CO_2 flows to be injected in the oil reservoir were estimated from the oil production forecasts. If the required volume for EOR is higher than the CO_2 produced in SMR facilities, than blue H2 production is limited by SMR production. If the opposite happens, then blue Hydrogen production is limited by EOR production.

9) Sizing CO_2 pipelines: the diameters of pipelines are calculated according to the maximum CO_2 yearly flows obtained in the previous step. This estimate keeps the CO_2 flow in the pipelines as a supercritical fluid (above 31.1 ºC and 7.5 MPa). Above such conditions, CO_2 flow is in dense phase and presents minimum pressure losses [307]. Design temperature ranges from 10 to 35ºC. In this study, the design pressure was set at 25.00 MPa [298] [339] and the maximum pressure loss was established as 25kPa/km. The minimum operating pressure of 18.75 MPa is well-above

supercritical conditions. The Darcy's equation was applied, considering the Churchill correlation for friction factor – see equations S-1 to S-5.

$$\Delta P = \frac{\left(kgf/cm^2\right)}{100m} = \frac{\upsilon^2 \times \rho \times f}{2 \times d}$$

Equation S-1

$$f = 8 \times \left[\left(\frac{8}{\text{Re}}\right)^{12} + \frac{1}{(A+B)^{1,5}}\right]^{\left(\frac{1}{12}\right)}$$

Equation S-2

$$A = \left\{2,457 \times \ln\left[\frac{1}{\left(\left(\frac{7}{\text{Re}}\right)^{0,9} + 0,27\frac{\varepsilon}{D}\right)}\right]\right\}^{16}$$

Equation S-3

$$\text{Re} = 998{,}5 \times \frac{d \times \upsilon \times \rho}{\mu}$$

Equation S-4

$$B = \left(\frac{37530}{\text{Re}}\right)^{16}$$

Equation S-5

Where:

ΔP = pressure loss

ν = velocity

ρ = Density

f = friction factor

d/D = pipe diameter

Re = Reynolds number

μ = viscosity

ε = roughness

This is a practical approach, which can be found in both industry manuals (e.g. [303]) and scientific papers [340] [341]. Pipeline wall thicknesses were obtained according to API 5L X65 pipelines apud Silva Telles [299] and Brazilian standard NBR 12712 [342],, as shown in **Table S-29** and **Equation S-6**.

Table S-29: External Diameters and calculated wall thicknesses for API 5L X65 pipelines.

Nominal Diameter, in	External Diameter, mm	Wall Thickness, mm
10	273.1	23.8
12	323.9	28.2
14	355.6	31.0
16	406.4	35.4
18	457.0	39.8
20	508.0	44.3
22	559.0	48.7
24	610.0	53.2
26	680.0	59.3
28	711.0	62.0
32	813.0	70.9
36	914.0	79.7
38	965.0	84.1
40	1016.0	88.6
42	1067.0	93.0
44	1118.0	97.5
48	1219.0	106.3
52	1321.0	115.2

$$e = \frac{P.D}{2.F.E.T.S_y}$$ **Equation S-6**

Where:

e = wall thickness;
P = design pressure (Kpa)
D = external diameter
S_y = minimum flow stress to the material according to NBR 12712
F = design factor according to locational placement
E = joint design factor
T = design temperature

The definition of the pipeline material also set the roughness applied in the previous equations. Density was defined according to Crane [303], while for viscosity, the Sutherland's correlation was used – see equations S-7 and S-8.

$\rho = (349p'.Sg)/T,$ **Equation S-7**

where $p' = 1.013 + p$
$T = 273.15 + t$,
Sg – specific gravity
T = temperature, Kelvin,
t = temperature ºC,
p' = absolute pressure,
p = gauge pressure,
R= Universal gas constant
ρ = density, kg/m^3

$$\mu = \mu_0 \left(\frac{T_0 + C}{T + C}\right)\left(\frac{T}{T_0}\right)^{\frac{3}{2}}$$ **Equation S-8**

Where:

μ = viscosity at temperature T;
μ_0 = viscosity at temperature T_0;
T = Absolute temperature for calculated viscosity
T_0 = Absolute temperature for known viscosity
C = Sutherland's Constant
For most gases, viscosity variation with pressure is small [303]