DIMETHYL ETHER FROM SYNGAS DERIVED FROM VINASSE: ECONOMIC AND ENVIRONMENTAL BENEFITS OF PROCESS ENERGY INTEGRATION

Gabriela de França Lopes[1]*, Caroline Teixeira Rodrigues[1], Gabrielly Mylena Benedetti Tonial[1], Luiz Mario de Matos Jorge[1], Paulo Roberto Paraíso[1]
[1]Department of Chemical Engineering, State University of Maringa, Colombo Avenue 5790, 87020-900, Maringa, Brazil.
*gabidflopes@gmail.com, caroline.rodrigues.eq@gmail.com, gabriellybtonial@gmail.com, lmmjorge@uem.br, prparaiso@uem.br

ABSTRACT

Dimethyl ether (DME) stands out as a clean fuel for various applications, especially as a substitute for diesel and LPG. The feasibility of its production has been investigated, with process integration potentially contributing new dimensions of sustainability to the process, both environmentally and economically. In the context of the need to seek alternatives that are advantageous in technical, economic, and environmental aspects, energy integration plays an important role. This study aims to achieve energy integration in the direct synthesis process of dimethyl ether from syngas derived from vinasse, assessing the benefits for the process with the network of heat exchangers generated. Integration calculations were performed using Aspen HYSYS® software with its Aspen Energy Analyzer tool, and cost evaluations of the integrated process were carried out with the Aspen Process Economic Analyzer tool. With energy integration, costs for hot utility are eliminated by 100% and cold utility by 13.6%. This resulted in a reduction of carbon equivalent emissions by approximately 9,850 tons per year and a reduction in the cost of the simulated DME stage by about 4.8 per ton, leading to a final unit cost of $248.12/t considering all production stages. Thus, this study contributes to advancing the feasibility of producing this important biofuel, providing significant economic and environmental benefits.

KEYWORDS: *Biofuel, Simulation, Cost, Pinch Analysis,* CO_2

I. INTRODUCTION

Among the great diversity of chemical processes that currently exist, those that can contribute to sustainable development are increasingly being sought. In the context of the need to seek alternatives that are advantageous in technical, economic, and environmental aspects, energy integration plays an important role. It involves relating hot streams that need to be cooled and cold streams that need to be heated to exchange energy between them, helping to achieve their goals with the lowest cost and efficient energy use [1,2]. Pinch Analysis is a structured approach designed to enhance energy efficiency in industrial processes. It involves a series of techniques for evaluating heat transfers, establishing energy goals, pinpointing inefficiencies, and proposing process enhancements by discovering potential opportunities for resource recovery. [3].

The term "Pinch" defines the thermodynamic boundary for the maximum possible heat recovery from a process, with the composite curve—illustrating temperature versus enthalpy—serving as the essential tool for this analysis, providing a visual depiction of overall heat availability, requirements, and the achievable heat recovery. [4]. Composite curves are constructed by combining hot and cold streams of a process to produce the hot composite curve (a single hot composite stream representing the general heat source of the process) and the cold composite curve (a single cold composite stream representing the general heat demand of the process). The intersection at the minimum temperature difference indicates the target for the maximum achievable heat recovery (MER) within the process. [4].

Process integration has been developed beyond the approach of heat and energy integration, within the new dimensions of sustainability in industry, such as cleaner use of fossil fuels, waste management, and emission reduction [5,4]. In the context of biofuels, dimethyl ether (DME) is being promoted as a clean fuel for various applications, especially as a substitute for diesel and LPG [6]. It is produced from syngas, a mixture of hydrogen, carbon monoxide, and smaller compounds [7], being CO_2 hydrogenation, CO hydrogenation, water-gas shift, and methanol dehydration, the main reactions involved in DME direct synthesis [8].

Lopes [9] performed a rigorous modeling and simulation of the direct synthesis of dimethyl ether from syngas derived from vinasse from a sugar-alcohol industry, evaluating this production both technically and economically. The process, illustrated in Figure 1, consists basically of stages of compression, a reactor, an absorption column, a flash-tank, and distillation columns to recover the solvent and purify the DME.

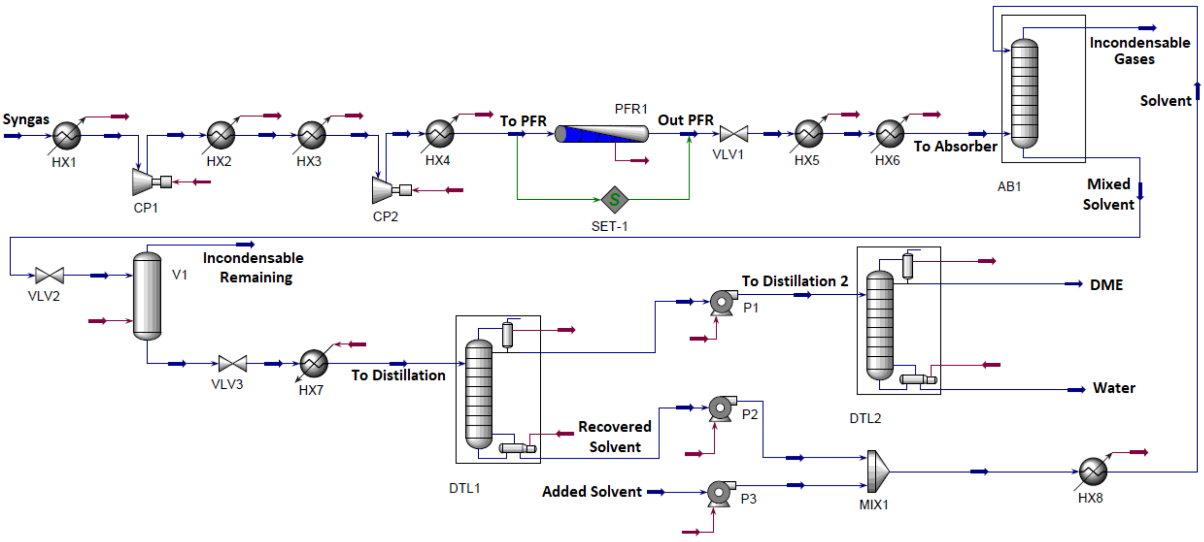


Figure 1. DME production model from synthesis gas designed on the Aspen Hysys® by De França Lopes et al. [10]

In the process, besides the reactor and columns, there are heat exchangers with no energy integration. The cost analysis of the Lopes [9] system reveals that the capital expenditure totals $47,062,900, with an annual operating cost of $14,075,000 and utility costs amount to $11,214,900 per year. Additionally, the system results in carbon emissions of 197,208,000 kg per year [9]. Therefore, the objective of this work is to perform energy integration in this process and assess the benefits obtained for the process from both economic and environmental perspectives.

The paper is organized into several sections. Section II provides a detailed description of the research methodology, including both energy integration and process cost calculations. Section III presents the results and their discussion, covering the selected heat exchanger network and comparing the costs and carbon emissions of DME production before and after integration. Finally, Section IV summarizes the main conclusions of the study.

II. METHODOLOGY

The energy analysis was performed using Aspen HYSYS® software through its Aspen Energy Analyzer (AEA) tool. Table 1 presents the data of the process streams, and the heat exchange required between them.

Table 1. Process stream data considered in the integration.

Stream	Division	Inlet T (°C)	Outlet T (°C)	Enthalpy (kJ/h)	HTC (kJ/h.m².°C)	Cp (kJ/kg.°C)
1	1.1	236.33	161.90	2.14E+07	9146.49	3.59
	1.2	161.90	98.39	1.60E+07	7054.66	3.15
	1.3	98.39	0.00	2.19E+07	4242.15	2.78
2	-	0.01	50.00	2.04E+07	4201.23	2.82
3	3.1	269.81	231.66	5.73E+06	554.21	2.27
	3.2	231.66	184.64	6.87E+06	555.73	2.21
	3.3	184.64	177.80	1.69E+07	4901.11	37.38
4	-	318.28	275.00	8.21E+06	867.41	2.86
5	-	302.16	90.00	3.95E+07	433.23	2.81
6	-	136.85	80.00	1.04E+07	206.69	2.77

The design of original process includes ten heat exchanger units, requiring 147,000,000 kJ/h of cold utility and 20,400,000 kJ/h of hot utility. Thus, the heaters and coolers have an investment cost of US$540,000 and an operational cost of US$108.28 per hour, requiring a total cost of US$118.20 per hour.

Energy integration was analyzed considering three different utilities according to the software information: cooling water and refrigerant 1 as cold utilities, and low-pressure steam as a hot utility. Cooling water has an inlet temperature of 20°C and an outlet temperature of 25°C, with a cost of 2.12×10^{-7} US$/kJ, a heat transfer coefficient (HTC) of 13,500 kJ/h.m².°C, and a specific heat capacity (Cp) of 4.18 kJ/kg.°C. Refrigerant 1 has an inlet temperature of -25°C and an outlet temperature of -24°C, with a cost of 2.74×10^{-6} US$/kJ, an HTC of 4,680 kJ/h.m².°C, and a Cp of 4.00 kJ/kg.°C. Lastly, low-pressure steam has an inlet temperature of 125°C and an outlet temperature of 124°C, with a cost of 1.90×10^{-6} US$/kJ, an HTC of 21,600 kJ/h.m².°C, and a Cp of 2,196.40 kJ/kg.°C.

A minimum temperature difference of 3°C was established for the heat exchangers in the integration process, as this value yields the lowest total cost based on the software analysis. In total, 45 heat exchanger network configurations were simulated, examining cases with no stream splits, two splits, and three splits for energy integration. For cost analysis, the equation 1 was used, from Aspen Energy Analyzer:

$$Cost = a \times variable^2 + b \times variable + c \qquad \text{Equation (1)}$$

where
a = 10000;
b = 800;
and c = 0.8.
For the cost analysis, ten years was considered as the plant lifespan and 4320 operating hours per year, with a return rate of 9.7%, according to De França Lopes et al. [10]

The utilities and ideal heat exchanger networks for the process were evaluated from economic and environmental perspectives. For cost evaluations of each process—fixed investment, operating costs, utilities—the APEA (Aspen Process Economic Analyzer) add-on for HYSYS® was used, while the AEA add-on was used for CO_2 emission assessment.

To assess the cost of the process after energy integration, the methodology based on Turton et al. [11] was used. The capital cost (C_R) of the equipment was amortized over the operational life to establish an annual cost, considering interest rates and the plant's useful life according to Lopes [9]. The annualized capital cost (CF) was calculated according to Equations (2) and (3).

$$crf = \frac{i\,(1+i)^t}{(1+i)^t - 1} \qquad \text{Equation (2)}$$

$$CF = C_R . crf$$ Equation (3)

Adding the annualized capital cost to the operational cost of the process provided a total annualized cost (TAC), according to Equation (4). Dividing this by the annual production amount yielded a unit production cost (CPU), through Equation (5).

$$TAC = CF + OC$$ Equation (4)

$$CPU = \frac{TAC}{Q}$$ Equation (5)

Finally, the costs of the initial process stages used by Lopes [9] and the benefits of cogeneration from bagasse were considered to obtain results for the complete production cost of dimethyl ether from vinasse for comparison.

III. RESULTS AND DISCUSSION

The total costs of the evaluated heat exchanger networks were determined, with the most costly network having a total cost of $97.32 per hour, which reduces the cost by 17.7% compared to the network without integration ($118.20 per hour).

The least costly network had a total cost of $27.77 per hour, reducing the cost by 76.5%, and was therefore selected for integration. It has 7 heat exchangers, requires 127,000,000 kJ/h of cold utility, and does not need hot utility or stream splits. It considers only two heat exchangers exchanging energy between streams (HX3 and HX6). The first (HX3) facilitates heat exchange (8,210,000 kJ/h) between streams 1 and 2. The second (HX6) facilitates heat exchange (12,200,000 kJ/h) between streams 5 and 2.

Compared to the network without integration, it is possible to reduce the number of heat exchangers by 3, the demand for cold utility by 13.6%, and the hot utility by 100%. Thus, it is observed that the few integrations between streams were sufficient to eliminate the need for hot utilities. Table 2 presents a comparison between the financial parameters and carbon emissions of the original process and the adapted process with energy **integration.**

Table 2. Utilities considered in the integration.

Parameters	Original Process [9]	After Energy Integration	Variation
Capital Cost (US$)	47,062,900	44,563,800	2,499,100
Operating Cost (US$/year)	14,075,000	13,670,600	404,400
Utility Cost (US$/year)	11,214,900	10,849,400	365,500
Equipment Cost (US$)	26,271,900	25,208,500	1,063,400
Installed Cost (US$)	30,495,400	28,815,800	1,679,600
Utilities (MJ/year)	3,528,576,000	3,352,320,000	176,256,000
Carbon Emissions (kg/year)	197,208,000	187,358,400	9,849,600

It is observed in the table that all process costs have been reduced, with notable decreases of nearly $2.5 million in investment and over $400,000 annually in operating costs, primarily due to the reduction in utilities in the process. Additionally, there is also a reduction in carbon emissions calculated by the AEA tool of nearly 10 million kg per year, mainly due to the utility exchanges performed during energy integration. Table 3 presents a comparison between the original process and the modified process with energy integration concerning the costs per ton of DME for the simulated stage (Synthesis Gas – DME) and for the total of all stages to produce it from vinasse (Vinasse to Biogas, Biogas to Synthesis Gas, and Synthesis Gas to DME).

Table 3. Comparison of DME costs before and after integration.

Costs	Original Process [9]	After Energy Integration
Capital Cost	$47,062,900	$44,563,800
Capital Cost (Cogeneration)	$28,521,248	$28,521,248
Interest Rate (i)	0.0974	0.0974
Capital Recovery Factor (crf)	0.160932	0.160932
Annualized Capital Cost (CF)	$12,163,914/year	$11,761,728/year
Operating Cost	$14,075,000/year	$13,670,600/year
Operating Cost (Cogeneration)	$1,711,274/year	$1,711,274/year
Savings from Cogeneration	$6,795,216/year	$6,795,216/year
Total Operating Cost (OC)	$8,991,058/year	$8,586,658/year
TAC for Synthesis Gas – DME Stage	$21,154,972/year	$20,348,387/year
DME Produced	180,065 t DME/year	180,065 t DME/year
Unit cost of Synthesis Gas – DME Stage	$117.49/t DME	$113.01/t DME
TAC for Vinasse – Biogas Stage	$4,984,891/year	$4,984,891/year
TAC for Biogas – Synthesis Gas Stage	$19,343,750/year	$19,343,750/year
TAC for Synthesis Gas – DME Stage	$21,154,972/year	$20,348,387/year
TAC Vinasse – DME	$45,483,613/year	$44,677,028/year
DME Produced	180,065 t/year	180,065 t/year
Unit Cost of DME (Complete Process)	$252.60/t DME	$248.12/t DME

It is observed in the table that the unit cost of DME for the simulated stage decreased from $117.49 to $113.01 per ton with energy integration, representing a reduction of $4.48 per ton due to the few changes introduced by the integration. For the total of all DME production stages—namely, summing the costs provided in the literature for the stages of producing biogas from vinasse and producing synthesis gas from biogas—the total annualized cost was reduced from $45,483,613 per year to $44,677,028 per year. Thus, a reduction of more than $800,000 per year was achieved. Analyzing the final unit cost of dimethyl ether, the cost was reduced from $252.60 per ton of DME to $248.12 per ton of DME.

IV. CONCLUSIONS

The energy integration in the DME production process from synthesis gas resulted in more efficient utilization of process stream energy, leading to a reduction in DME cost by approximately $4.50 per ton, achieving a final unit cost of $248.12 per ton. This improvement was facilitated by the implementation of a heat exchanger network, which led to a 13.6% reduction in cold utility requirements and a 100% reduction in hot utility needs.

Overall process costs were reduced, with significant decreases of nearly $2.5 million in investment costs and over $400,000 annually in operating costs, primarily due to lower utility consumption. Furthermore, energy integration contributed to a reduction in carbon emissions of about 9,850 tons per year.

Therefore, by implementing energy integration in the process, this study contributes to advancing the feasibility of producing this important biofuel, providing significant economic and environmental benefits, and consequently paving the way for sustainable development. Future work will include integrated modeling and simulation of all stages of dimethyl ether production from vinasse, evaluating different methods of synthesis gas production from biogas, and ultimately achieving a more comprehensive energy integration with even greater potential benefits.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the financial support from Coordination of Higher Education Personnel Improvement - Brasil (CAPES) - Finance Code 001.

REFERENCES

[1]. Relvas, S., Fernandes, M. C., Matos, H. A., & Nunes, C. P., 2000. "Integração de Processos: Uma metodologia de optimização energética e ambiental". Polarpress, Lda., 1st ed., 129 p., Setúbal.

[2]. Beninca, M., 2008. "Integração energética de uma planta de eteno com aspectos de flexibilidade: aplicação da análise pinch em conjunto com a otimização matemática". Dissertação de Mestrado em Engenharia Química, Universidade Federal do Rio Grande do Sul, Porto Alegre, 113 p.

[3]. Hall, S., 2012. "Energy Conservation". In: Branan's Rules of Thumb for Chemical Engineers (5th ed.), Butterworth-Heinemann, pp. 375-385.

[4]. Manan, Z. A., Nawi, W. N. R. M., Alwi, S. R. W., & Klemeš, J. J., 2017. "Advances in Process Integration research for CO2 emission reduction: A review". Journal of Cleaner Production, Vol. 167, pp. 1-13.

[5]. Varbanov, P. S., & Seferlis, P., 2014. "Process innovation through Integration approaches at multiple scales: a perspective". Clean Technologies and Environmental Policy, Vol. 16, pp. 1229-1234.

[6]. Azizi, Z., Rezaeimaneshi, M., Tohidian, T., & Rahimpour, M. R., 2014. "Dimethyl ether: A review of technologies and production challenges". Chemical Engineering & Processing: Process Intensification, Vol. 82, pp. 150–172.

[7]. Delparish, A., & Avci, A. K., 2016. "Intensified catalytic reactors for Fischer-Tropsch synthesis and for reforming of renewable fuels to hydrogen and syngas". Fuel Processing Technology, Vol. 151, pp. 72–100.

[8]. Falco, M., Capocelli, M., & Centi, G., 2016. "Dimethyl ether production from CO2 rich feedstocks in a one-step process: thermodynamic evaluation and reactor simulation". Chemical Engineering Journal, Vol. 294, pp. 400–409. https://doi.org/10.1016/j.cej.2016.03.009

[9]. Lopes, G. F., 2019. "Simulação da Produção de dimetil éter a partir de gás de síntese para uma indústria sucroalcooleira". Dissertação de Mestrado em Engenharia Química, Universidade Estadual de Maringá, Maringá, 96 p.

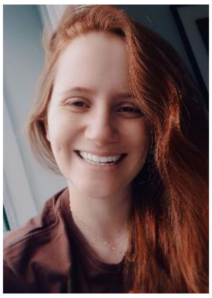
[10]. De França Lopes, G. F., Bonfim-Rocha, L., Jorge, L. M., & Paraiso, P. R., 2020. "Dimethyl Ether Production from Sugarcane Vinasse: Modeling and Simulation for a Techno-economic Assessment". Bioenergy Research. https://doi.org/10.1007/s12155-020-10089-9.

[11]. Turton, R., et al., 2012. "Analysis, Synthesis, and Design of Chemical Processes". 4th ed., Upper Saddle River, NJ: Prentice Hall.

Gabriela de França Lopes

Holds a bachelor's degree in chemical engineering from the State University of Maringá (2014), with a master's (2019) and Ph.D. (2022) from the Graduate Program in Chemical Engineering at the same university. Served as a postdoctoral researcher at the State University of Londrina in partnership with Geo Bio gascarbon (2024). Also holds a degree in Production Engineering from Unicesumar (2023). Specializes in Process Modeling and Simulation, focusing on technical and economic analyses of energy production from sugarcane industry residues.

Caroline Teixeira Rodrigues , Holds a bachelor's degree (2013) and a master's degree (2019) in Chemical Engineering from the Federal University of Goiás and a Ph.D. (2022) from the Graduate Program in Chemical Engineering at the State University of Maringá.



Gabrielly Mylena Benedetti Tonial , Holds a bachelor's degree in chemical engineering (2018) from the Federal University of Technology - Paraná, Francisco Beltrão Campus, and a master's degree in chemical engineering (2021) from the State University of Maringá. Currently, she is a CAPES-funded doctoral fellow in the Graduate Program in Chemical Engineering at the State University of Maringá. Her work focuses on process modeling and simulation, as well as optimization, with an emphasis on heat integration analysis using Pinch methodology.

Luiz Mario de Matos Jorge, Graduated in Chemical Engineering from the State University of Maringá (1990). Holds a master's degree in chemical engineering from the University of São Paulo (1992) and a Ph.D. in Chemical Engineering from the University of São Paulo (1998). Has expertise in Chemical Engineering, with research focused on catalysis, kinetics, chemical reactors, and process modeling and simulation. Investigates fundamental aspects of both non-reactive systems, such as grain drying and hydration, and reactive systems, including steam reforming of methane, biogas, methanol, ethanol, glycerol, hydroprocessing of vegetable oils, and Fischer-Tropsch synthesis.

Paulo Roberto Paraíso, Holds a bachelor's degree in chemical engineering from the Federal University of Minas Gerais (1980), a master's degree in production engineering from the Federal University of Santa Catarina (1986), and a Ph.D. in Chemical Engineering from the State University of Campinas (2001). Currently, serves as an Associate Professor at the State University of Maringá. Has experience in Chemical Engineering, with a focus on Separation and Mixing Operations, primarily working on the following topics: drying, soybean meal, fluidized bed, and energy.