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Introduction

Jan Van Impe, Grégoire Léonard, Satyajeet Sheetal Bhonsale, Monika Polanska, and Filip Logist (eds)

The 35th European Symposium on Computer Aided Process Engineering (ESCAPE|35) was held at KU Leuven/Campus Gent, Belgium, July 6–9, 2025. Continuing a tradition that began in 1991 under the auspices of the EFCE Working Party on Computer Aided Process Engineering (CAPE), the ESCAPE series stands as a premier annual event for the global Process Systems Engineering (PSE) community. ESCAPE returned to Belgium for the second time – following the 1998 edition in Bruges – and took place as part of KU Leuven's 600th anniversary celebrations. The 35th edition was organised jointly by KU Leuven/BioTeC+ and University of Liège/PEP.

The 2025 conference embraced the theme "Closing the Loop 2.0", underscoring the evolving role of PSE in enabling a circular economy. The program highlighted both core process engineering disciplines – such as modeling, control, design, and optimization – and cutting-edge approaches involving artificial intelligence, machine learning, and quantum computing, applied across diverse sectors including energy, chemicals, biotechnology, and advanced materials.

ESCAPE|35 received 673 abstract submissions, of which 563 were invited for a 5-to-8-page full paper or a 2-page short paper after a first review round. Upon rigorous re-review of all papers submitted, 423 full paper contributions have been published in full open access (and LAPSE and DOI indexed) by PSE Press as a separate volume of the *Systems & Control Transactions* series. Another 140 contributions have been made available as two pages short papers published by EUROSIS-ETI.

The scientific contributions were organized into thematic sessions, poster presentations, workshops, and demonstrations, within ten thematic tracks:

- T01: Modelling and Simulation
- T02: Sustainable Product Development and Process Design
- T03: Large Scale Design and Planning/Scheduling
- T04: Model-Based Optimisation and Advanced Control
- T05: Concepts, Methods and Tools
- T06: Digitalization and AI
- T07: CAPEing with Societal Challenges (Green Deal, Energy Transition, ...)
- T08: CAPE Education and Knowledge Transfer
- T09: PSE4Food and Biochemical (*new in 2025*)
- T10: PSE4BioMedical and (Bio)Pharma (*new in 2025*)

Tracks T09 and T10 were introduced in this year's edition to broaden the application scope of PSE methods in food, biochemical, (bio)pharma and biomedical systems – fields of increasing relevance to the community.

We extend our sincere thanks to all authors, reviewers, topic coordinators, plenary and keynote speakers, and members of the Scientific and Organizing Committees. We gratefully acknowledge KU Leuven and University of Liège for their support and express our heartfelt appreciation to our numerous sponsors. This edition also marks the inaugural collaboration with PSE Press as the official publisher of the ESCAPE proceedings (full papers volume) – a milestone in promoting high-quality, open access dissemination of PSE research. Many thanks to EUROSIS-ETI as well for publishing the short papers volume, ISBN indexed.

We hope these volumes capture the scientific excellence, collaborative spirit, and forward-looking vision that defined ESCAPE|35 and continue to serve as a valuable reference for researchers and practitioners in the years ahead.

ESCAPE|35 - European Symposium on Computer Aided Process Engineering

Ghent, Belgium. 6-9 July 2025

Peer Review Policy

TERMINOLOGY

- **Conference Paper:** This is a peer-reviewed research paper describing an **original** research contribution and published in the conference proceedings.

APPLICATION

- All conference papers are subject to peer review.

PUBLICATIONS

- All conference papers which have passed peer review and have been accepted by the conference chairs will be published in the conference proceedings.

PEER REVIEW PROCESS

Initial Screening

The conference chairs will screen the initial submissions (one-page abstracts) of contributed papers. At their option, chairs may choose to reject these submissions for any reason, but the primary reasons for rejection at this stage are (a) subject does not match conference themes and topics; (b) in appropriate, unprofessional, unethical, or dishonest material; (c) duplicate submissions; (d) abandoned submissions; (e) multiple submissions from same presenter; (f) obvious poor quality; (g) reasonable suspicion of machine-generated text; (h) need to limit acceptances because of conference space constraints. Chairs may also transfer papers between sessions at this stage.

Conference chairs will then invite authors of the one-page abstracts that have passed the initial screening to submit a conference paper for peer review.

Conference Paper Peer Review

Conference chairs act as editors. They will assign peer reviewers to assess the quality of the conference papers and manage the peer review process for each paper. Peer reviewers are generally selected from the International Scientific Committee who are scientists, engineers, or researchers with technical expertise in the conference topic. Peer reviewers must be considered technical experts in their field, hold a PhD, and have published peer reviewed scientific works previously. Each work must be reviewed by a minimum of two peer-reviewers.

A “single-blind” peer review system is used, in which the peer reviewers have access to the identities of the authors, but the authors are never given the identities of the peer reviewers. This is consistent with most journal peer-review procedures in our field.

Peer reviewers will be given a set of quality criteria that may include scientific and technical quality, quality of writing, originality and novelty, appropriateness for the conference topic and theme, interest to the community, and other factors of merit. Peer reviewers are expected to be rigorous and critical in their technical assessments and adhere to the highest standards in the field in order to ensure high quality. Peer reviewers are asked to comment on their assigned conference papers and issue a recommendation to the conference chairs based on this quality criteria. Reviewers may recommend one of the following:

- **Accept Paper.** No technical changes are necessary before publication. Only typographical, spelling, grammar, or other minor changes are necessary which do not require technical review.
- **Accept Paper with Minor Revisions.** Some minor technical issues need to be addressed either through technical changes to the manuscript or through rebuttal to reviewer comments. The reviewer does not believe the issues are significant enough to require additional technical review by the reviewers. The reviewer has provided enough commentary such that the editor can decide if the minor issues have been addressed in a future revision.
- **Revise Paper with Re-Review.** Major technical issues need to be addressed either through technical changes

to the manuscript or through rebuttal to reviewer comments. The reviewer believes the issues are significant enough to require that the revised manuscript receive additional review by the reviewers.

- **Reject Without Reconsideration.** The technical issues are so significant that it is unlikely that an acceptable manuscript could be produced by the deadline; or, the manuscript is out of scope, inappropriate, or computer-generated.

Peer reviewers may be asked to provide numerical scores or rankings, as well as provide written comments intended for the chairs and/or the authors. Peer reviewers are encouraged to provide specific and constructive feedback that will aid the authors in improving the work and provide advice to the chairs.

The conference chairs are responsible for making the final decision on each paper and may require several rounds of author changes if necessary to meet quality standards. Conference chairs are not required to follow the recommendations of the peer reviewers in making these decisions. It is possible that conference chairs will choose to not accept some papers that still pass through rigorous technical peer review, especially when limited by available space or when papers do not sufficiently promote conference objectives. Conference chairs may also transfer papers between sessions as desired.

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To help determine conflicts of interest, and for all other ethical guidelines, we use the Systems and Control Transactions ethical guidelines described at: <https://psecommunity.org/contributor-guidelines>

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Comparative Analysis of Conventional and Novel Low-Temperature and Hybrid Technologies for Carbon Dioxide Removal from Natural Gas

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ABSTRACT

Natural gas production is expected to increase, leading to the exploitation of low-quality reserves that contain high levels of acid gases, such as carbon dioxide. The aim of this work is to compare various innovative and conventional technologies for the removal of CO₂ from natural gas, considered as a binary mixture of methane and carbon dioxide, with CO₂ contents ranging from 10 to 70 mol%. The processes are simulated using Aspen Plus® V9.0 and compared in terms of energy consumption, which is evaluated through the net equivalent methane method. The results show that novel low-temperature and hybrid technologies, which combine distillation and physical absorption, are the most energy-efficient for CO₂ removal from natural gas with high acid gas contents, while conventional physical absorption processes are optimal for natural gas with low to moderate acid gas contents.

Keywords: natural gas, carbon dioxide removal, physical absorption, hybrid technologies, low-temperature distillation.

INTRODUCTION

Global electricity consumption is projected to rise in the coming decades. To meet this growing demand sustainably, renewable energy sources and, among fossil fuels, natural gas are expected to see the most significant growth. As natural gas consumption increases, it will also become necessary to extract it from low-quality reserves, which often contain high levels of acid gases, such as carbon dioxide (CO₂) and hydrogen sulfide [1].

The aim of this work is to compare various innovative and conventional technologies for the removal of carbon dioxide from natural gas, considered as a binary mixture of methane and carbon dioxide. It first examines the performance of the physical absorption process using propylene carbonate (PC) as a solvent, along with a hybrid process in which it is applied downstream of low-temperature distillation. These results are, then, compared with previously studied technologies, including physical absorption with dimethyl ethers of polyethylene glycol (DEPG), low-temperature distillation, and hybrid processes that combine distillation and absorption [2].

The low-temperature distillation process considered here is the one described by Langé et al. [1]. It consists of two distillation columns operating at different pressures: the bulk CO₂ removal is performed in a high-pressure distillation column, typically operated at 50 bar such that CO₂ freeze-out is avoided, and the natural gas production at commercial grade is performed in a low-pressure column, typically operated at 40 bar (anyway lower than the critical pressure of methane).

The Fluor Solvent™ process, which uses PC as the solvent, was commercialized by Fluor in the early 1960s. Propylene carbonate is particularly advantageous, as noted by Bucklin and Schendel [3], when hydrogen sulfide is not present in raw natural gas. The bulk distillation + physical absorption finishing with PC is a new process that has been proposed for the first time in a patent by Xu [4]: no other references are in fact present in the literature about combined purification technologies for the natural gas purification in which propylene carbonate is involved.

The PC absorption process and the bulk low-temperature distillation + PC absorption process are

simulated using Aspen Plus® V9.0 [5]. The energy analysis is conducted using the net equivalent methane method. The processes are compared in terms of methane equivalent consumption, methane losses, and net produced purified methane, offering guidance on the optimal process based on the composition of the raw natural gas.

METHODS

Inlet and outlet stream conditions

The feed gas conditions are assigned in terms of temperature (35 °C), pressure (50 bar) and total flowrate (5,000 kmol/h). The raw natural gas is assumed to be a binary mixture of methane and carbon dioxide, having a CO₂ content ranging from 10 mol% to 70 mol%. When the CO₂ molar fraction is below 10 %, amine absorption is known to be a proven and cost-effective technology [1]. A CO₂ molar content of 70 % represents a sort of upper limit, indicating a reserve with an extremely low methane content [6].

The conditions for the purified gas are selected based on the requirements for pipeline network application. Therefore, the limit on the CO₂ content is set equal to 2 mol% [7]. The temperature of the purified natural gas is set to 25 °C, and the pressure is set to 50 bar, matching the operating pressure of the purification unit in the analyzed processes.

The CO₂ product stream is assumed to be injected underground for Enhanced Oil/Gas Recovery or sequestration and the specifications are assigned in terms of temperature (14.06 °C), pressure (50 bar) and maximum limit on hydrocarbons content of 2 mol%.

Net Equivalent Methane method

The energy analysis is based on the “net equivalent methane” (NEM) method [8], which consists in the evaluation of the equivalent quantity of methane that must be burned to power a specific equipment piece. By using the same basis for the various types of energy, the NEM method allows a fair comparison between different processes. The energy requirements considered include: supplying electric power, heating above ambient temperature, and cooling below ambient temperature. Heating below ambient temperature and cooling above ambient temperature do not consume methane, as service water can be used to provide or remove heat, respectively.

Supplying electric power

The gas compression and liquid pumping need electric power to be supplied. This electric power is assumed to be obtained by means of a methane-fired combined-cycle power plant. The amount of methane equivalent can be determined according to Eq. (1):

$$NEM = \frac{W}{\eta_{cc} \cdot LHV_{CH_4}} \quad (1)$$

where W indicates the mechanical power, η_{cc} is the combined-cycle efficiency, assumed equal to 0.55, and LHV_{CH_4} is the lower heating value of methane, which is 50 MJ/kg.

Heating above ambient temperature (> 25 °C)

The supply of heat to the process at temperatures higher than the ambient one is achieved through the use of low-pressure steam. The necessary amount of steam is provided by a boiler fed with methane: the equivalent methane flowrate consumed can be computed according to Eq. (2):

$$NEM = \frac{Q_{hot}}{\eta_b \cdot LHV_{CH_4}} \quad (2)$$

where Q_{hot} is the required thermal power, and η_b is the boiler efficiency, assumed equal to 0.80.

Cooling below ambient temperature (< 25 °C)

The removal of heat from the process at temperatures lower than the ambient one requires the use of a proper refrigeration cycle. This refrigeration cycle requires mechanical work to be operated, which is considered to be provided by a combined-cycle plant powered by methane. To calculate the amount of methane equivalent to the required mechanical duty, first it is necessary to compute the coefficient of performance (COP) of the refrigeration cycle from Eq. (3):

$$COP = \left(\frac{T_o}{T_f} - 1 \right)^{-1} \cdot \eta_{II} \quad (3)$$

In Eq. (3), the term in brackets is the coefficient of performance of an ideal Carnot cycle, that is calculated knowing the temperature of the hot reservoir (the ambient temperature $T_o = 25$ °C) and that of the cold reservoir (the final temperature reached at the outlet of the cooler, T_f). η_{II} is the second law efficiency, which is defined as the ratio between the efficiency of the system and the theoretical maximum possible one. η_{II} is assumed equal to 0.60.

By definition of the COP, the mechanical duty W can be computed given the cooling duty, denoted as Q_{cold} , to be removed from the system (Eq. (4)).

$$W = \frac{Q_{cold}}{COP} \quad (4)$$

Therefore, the amount of equivalent methane can be determined according to Eq. (5):

$$NEM = \frac{Q_{cold}}{\eta_{cc} \cdot COP \cdot LHV_{CH_4}} \quad (5)$$

PROCESS SIMULATION

The processes are simulated using Aspen Plus® V9.0 [5]. Physical absorption is modelled with the “Acid gas:

After simulating the base configuration of the processes, energy-saving schemes, incorporating heat integration based on pinch analysis, are considered for each process.

The feed gas (FEED) is mixed with recycle streams

Regeneration occurs through a series of three flashes at progressively decreasing pressures, with the first two being adiabatic. The pressure levels are chosen based on an example of a real plant reported by Mokhtab et al. [7]. Specifically, the pressure of the first flash is kept equal to 31.7 bar, and the pressure of the second flash is initially set to 13.1 bar, as in the reference example. However, the intermediate flash pressure may need some adjustments to meet the CO₂-stream purity requirements for reinjection. Results indicate that this adjustment is necessary when the feed molar CO₂ content is below 20 %. Above this threshold, the CH₄ molar fraction in the CO₂-OUT stream naturally becomes very low due to the reduced amount of methane processed. The last flash operates at atmospheric pressure. After conducting a sensitivity analysis, a pressure of 18 bar, as used by De Guido et al. [2] for absorption with DEPG

Figure 1. PFD of the propylene carbonate absorption process.

The vapor stream from the last flash can be used for reinjection purposes. Atmospheric flash vapors are recompressed to 50 bar in COMPR-3 and, then, cooled down to the bubble point temperature in a battery of two heat exchangers: COOLER-3 and COOLER-4. In the former, the CO₂ stream is cooled to ambient temperature (25 °C) using service water, while in the latter the final required temperature of 14.06 °C is reached employing a refrigeration cycle: decoupling these contributions is important, as only the duty related to the last cooler is considered in the energy consumption calculation.

Since the maximum allowed residual CO₂ molar content in the purified gas is 2%, the regenerated solvent purity must be at least 98% to provide the necessary driving force for absorption. To ensure an adequate margin, the lean solvent molar purity is set at 98.5%. Solvent purity can be controlled by modifying the FLASH-LP duty.

absorber.

The PFD of the bulk low-temperature distillation combined with the PC absorption process is illustrated in Figure 2. The distillation unit treats the raw gas to reduce the CO₂ content to 20 mol%. The final gas purity is, then, achieved through PC absorption. This process is only simulated for CO₂ molar contents greater than 20 % since below this threshold, the process becomes a simple PC absorption operation, eliminating the need for hybrid technology.

The separated liquid CO₂, with a purity of 99.99 mol%, is pumped to 50 bar and slightly heated to 14.06 °C in HEATER-7 using service water.

The partially purified natural gas is, then, compressed from 40 bar to 50 bar in COMPR-4 before



entering the absorption section. Absorption is carried out at 50 bar, with a PC feed temperature of -15°C , consistent with the simple PC absorption process previously discussed. The compressed gas, containing 20 mol% residual CO_2 , is mixed with vapor recycle streams from the first two flashes in the solvent regeneration section. The resulting stream is heated in HEATER-1 to reach the same temperature, as in the simple PC absorption process. In the absorber, the CO_2 content is reduced to 2 mol%.

The CO_2 -rich solvent exiting the bottom of the absorber is sent to the regeneration section, which operates under identical conditions to those used for the simple PC absorption process when handling a feed stream with 20 mol% initial CO_2 content. Vapors from the last flash are recovered for reinjection purposes.

The regenerated lean solvent, with a molar purity of 98.5 %, is pumped back to 50 bar and cooled to -15°C , preparing it for reuse in the absorption unit.

RESULTS AND DISCUSSION

The results reported in the following are obtained by applying the NEM method to convert the energy consumptions, retrieved from process simulations, into methane consumptions. To enable a meaningful comparison among the investigated processes, optimized process schemes, incorporating heat integration based on pinch analysis, are considered.

The results in terms of NEM consumption and methane losses in the CO_2 -rich streams obtained for the PC absorption process and its corresponding hybrid version, together with the technologies studied by De Guido et al. [2], are reported in Figure 3 and Figure 4, respectively. The methane losses in the CO_2 -rich streams are expressed as a percentage of the methane fed.

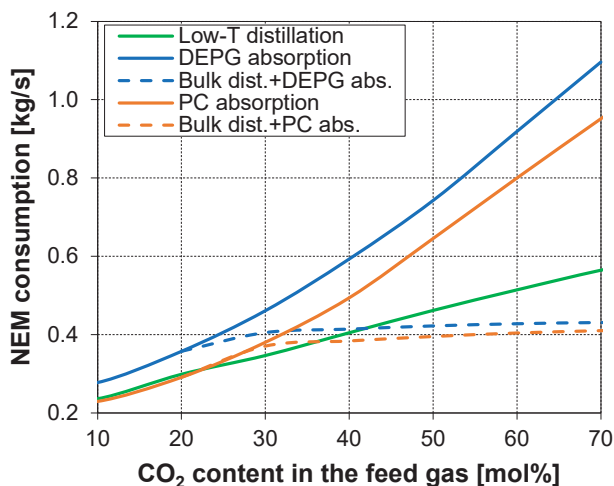


Figure 3. Comparison between CO_2 removal technologies in terms of NEM consumption.

Looking at Figure 3, it can be observed that physical absorption with PC solvent consumes less energy than with DEPG solvent across the entire range of CO_2 contents studied. It also performs slightly better than low-temperature distillation for CO_2 concentrations between 10 and 25 mol%. For CO_2 contents in the feed gas between 25 and 35 mol%, the process with the lowest energy requirements results to be the one based on low-temperature distillation. Above 35 mol% CO_2 in the feed gas, the hybrid process, where the finishing step is carried out using PC physical absorption, becomes more efficient.

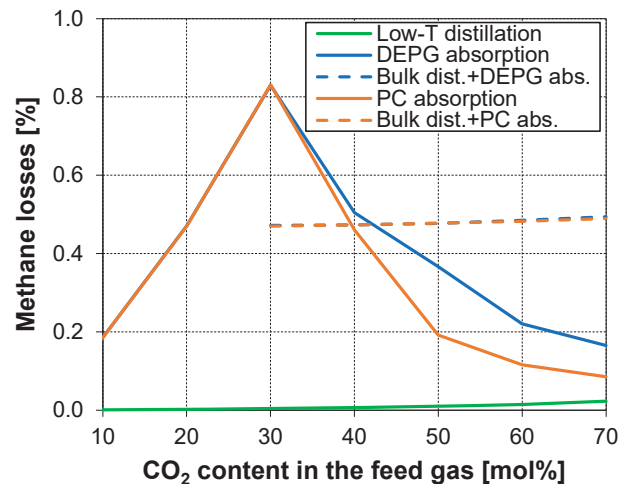


Figure 4. Comparison between CO_2 removal technologies in terms of methane losses.

From Figure 4 it is possible to notice that up to 30 mol% CO_2 content, the methane losses for the two physical absorption technologies considered are the same, due to the imposed specification of 2 mol% methane content in the CO_2 product stream. Above a CO_2 content in the feed gas of 30 mol%, the percentage of methane lost in this stream falls below the limit of 2 mol % and losses are related to the solubility of methane in physical solvents at atmospheric pressure, which is the pressure set in the last regeneration flash, and at the temperature reached in this non adiabatic flash, which is about 11°C when PC is used as solvent, and 61°C when DEPG is used. The propylene carbonate absorption process shows the lowest methane losses because methane's relative solubility in PC is less than in DEPG (0.038 vs 0.066 at 25°C [9]) and due to the lower operating temperature of the FLASH-LP. It is also worth noting that, in the low-temperature distillation process, methane losses are essentially negligible due to the imposed specification on CO_2 product purity. For hybrid technologies, methane losses show a flat trend. The lost methane is almost independent of the CO_2 content in the feed gas, as the bulk separation is performed in the distillation

section, where a high-purity CO₂ stream is removed. Methane losses are similar for both PC and DEPG hybrid technologies.

Net purified methane is defined as the percentage of methane in the raw gas that exits the process in the sales gas, minus the amount of methane burned to operate the process. This parameter takes into account both the equivalent methane consumption, which is a measure of energy requirements, and methane losses, which depend on the nature of the separation process (distillation and/or absorption). Referring to the graph in Figure 5, the best process selection is indicatively:

- PC absorption or low-temperature distillation in the range 10 - 15 mol% CO₂;
- low-temperature distillation in the range 15 - 50 mol% CO₂;
- hybrid processes, with a slight preference for bulk low-temperature distillation + PC absorption, above 50 mol% CO₂.

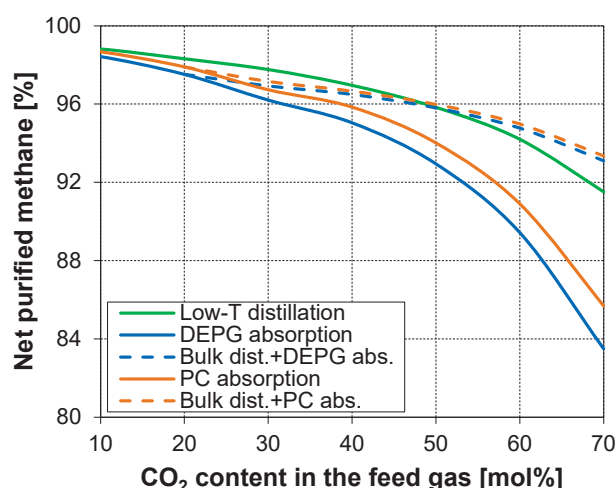


Figure 5. Comparison between CO₂ removal technologies in terms of net purified methane.

CONCLUSIONS

The analysis carried out in this work is relevant to the upgrading of low-quality natural gas through CO₂ removal and underground storage, offering a climate change mitigation solution by utilizing methane, the cleanest fossil fuel, and securely storing CO₂. The focus is on identifying the most energy-efficient CO₂ separation technology for natural gas, which mainly contains methane and carbon dioxide, depending on the CO₂ content.

For moderate CO₂ contents, below 15 mol%, both physical absorption with propylene carbonate and low-temperature distillation are good options, with propylene carbonate outperforming other physical solvents (e.g., DEPG) due to lower CH₄ losses with the solvent. For

higher CO₂ contents, from 15 to 50 mol%, low-temperature distillation is the most convenient process, in fact, by avoiding the use of a solvent, the energy requirements of the plant are less sensitive to the CO₂ content in the feed. For very high CO₂ concentrations (> 50 mol%), hybrid technologies are optimal, with the propylene carbonate-based process being the most efficient one.

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