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A generic techno-economic optimization methodology for concurrent design and operation of solvent-based PCC processes

Kaveh R. Khalilpour^{1,2*}, Ali Zafaranloo³

¹ School of Information, Systems and Modelling, University of Technology Sydney, Australia

² School of Chemical and Biomolecular Engineering, The University of Sydney, Australia

³ Faculty of Information Technology, Monash University, Australia

*Corresponding author, Emails: kaveh.khalilpour@uts.edu.au

Abstract

A techno-economic equation-based methodology is developed for optimal design and operation of integrated solvent-based post-combustion carbon capture (PCC) processes using a rate-based model for the interaction of gas and liquid. The algorithm considers a wide range of techno-economic design and operation parameters such as number of absorber/desorber columns, height of columns, diameter of columns, operating conditions (P, T) of columns, pressure drop, packing type, percentage of CO₂ mitigated, captured CO₂ purity, amount of solvent regeneration, flooding velocities of columns, and number of compression stages. A case study conducted to showcase two common objective-functions i) minimizing total capital investment, and ii) minimizing levelized capture costs, both for a 300 MW coal-power plant in Australia. The former objective leads to the lowest possible total capital cost of \$312.4M corresponding to levelized carbon capture cost of 58.1 \$/tonne-CO₂. For objective (ii), however, the lowest levelized carbon capture cost is found to be around ten percent lower (52.8 \$/tonne-CO₂), though it leads to a higher total capital cost (\$325.2M). The results indicate that the design and operation variables are markedly interactive, and no unique optimal design exists which can deliver all desired outcomes at once. Therefore, decisions on the selection of right variables become dependent on the decision-makers techno-economic objectives.

Keywords: Climate Change mitigation; post-combustion carbon capture (PCC); process design and economics; process systems engineering; optimization; solvent; MEA.

1 **1. Introduction**

2 The World Energy Investment Outlook by the International Energy Agency (IEA) has highlighted
3 that “carbon capture and storage provides an increasingly important hedge for fossil fuel assets
4 against the possibility of under-utilization or early retirement.” The IEA suggested that by 2050,
5 in order to stabilize global warming, global CO₂ emissions from all fossil fuel energy technologies
6 should be reduced to half of their emissions levels in 2007 (IEA, 2016). Approximately 12% of
7 the targeted reduction in CO₂ emissions could be achieved by applying carbon capture and storage
8 (CCS) technology (IEA, 2016). The UN's Intergovernmental Panel on Climate Change (IPCC) has
9 modelled four pathways on capping global warming at 1.5°C (IPCC, 2018). In most of these
10 pathways, the share of fossil fuel power generation with CCS has increased. This is to expand the
11 share of gas (to ~8%) to the benefit of reducing the use of coal (to ~0%) for global electricity
12 generation in 2050.

13 Amongst the alternatives for carbon capture, solvent-based post-combustion carbon capture (Sol-
14 PCC) technology is known as a feasible option for large-scale CCS projects, since it can be
15 effectively-integrated within fossil fuel-based plants with minimum changes involved, compared
16 with other alternatives (Metz et al., 2005). It is also comparatively reliable due to its several
17 decades of application for enhanced oil recovery (EOR) (Herzog et al., 1997) and currently
18 different other industrial applications such as beverage production (Aaron and Tsouris, 2005;
19 Desideri and Paolucci, 1999). Figure 1 illustrates the schematics of a PCC process. The pre-cooled
20 flue gas passes through the absorber column (packed or tray) where the lean solvent enters from
21 the top of the absorber in a countercurrent course. In the absorber, the solvent removes the CO₂
22 from the flue gas through an exothermic physicochemical interaction; the warmer rich solvent then
23 exits from the bottom of the absorber while the cleaned flue gas leaves the absorber overhead
24 towards the stack. In the desorber column, the rich solvent is stripped of CO₂ by thermal treatment
25 (solvent re-boiling). The lean solvent is recycled to the absorber column while the CO₂ is sent,
26 through the overhead, to the compression unit.

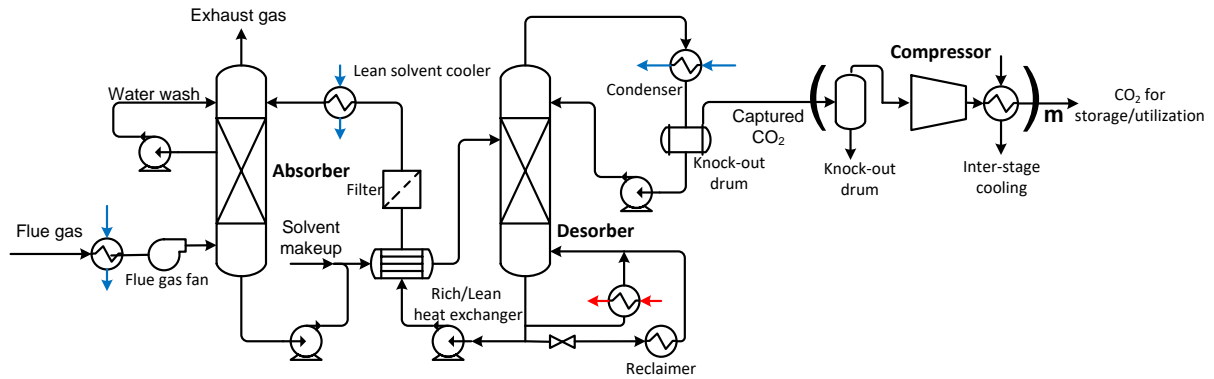


Figure 1: Schematic of the solvent-based PCC process configuration (Wang, 2017).

1
2
3 Despite notable developments in Sol-PCC, the implementation of this technology in power plants
4 still experiences notable barriers due to its high capital and operating costs (Biliyok, 2013; Metz
5 et al., 2005; Rubin, 2007). Previous studies (Abu-Zahra, 2007b; Dave, 2011) have indicated that
6 the operating costs come mainly from the desorber's reboiler though the magnitude varies
7 depending on the type of CO₂-emitting plant, solvent mix, and different design & operation
8 features. This energy requirement leads to a significant reduction in overall plant efficiency
9 (Khalilpour and Abbas, 2011; Rubin, 2013; van der Spek, 2017a). Techno-economic studies have
10 shown significant potentials to integrate and improve the feasibility of Sol-PCC technologies (van
11 der Spek, 2017a, b); however, uncertainty and variability in their results known as a major issue
12 with this analysis. Van der Spek et al. (2017b) recently showed that despite several attempts to
13 harmonize techno-economic estimates, the capital cost evaluation for the same PCC process could
14 vary by a large margin of 65%, due to inherent uncertainties in early stages of costing studies.
15 They speculated that these variabilities of capital costs originated from the differences in
16 equipment sizing methods and predictions for equipment costs, which later could be propagated
17 into the levelized cost of electricity and operating costs. Hence, rigorous techno-economic analyses
18 for integration of Sol-PCC processes with CO₂-emitting plants seem essential to achieve optimum
19 design and operation conditions. The critical parameters influencing the efficiency of Sol-PCC
20 processes are solvent type, solvent concentration, configuration of absorption and stripping
21 columns, operating conditions of absorption/desorption columns, the percentage of CO₂ avoided,
22 captured CO₂ purity, and amount of regeneration. Abu-Zahra et al. (2007a) investigated the impact
23 of several parameters using Aspen Plus simulation environment and highlighted the importance of
24 rigorous design optimization for cost reduction of Sol-PCC. Khalilpour and Abbas (2011) provided

1 a concise summary of various pathways for performance improvement and discussed the great
2 potential of process optimization for improving the overall efficiency of the Sol-PCC process
3 integrated with power plants.

4 It is a legitimate question concerning the lack of rigorous design methodologies for Sol-PCC, given
5 the high industrial demand. The answer is rooted in the absorber and desorber columns' reactive
6 separation. The modeling and design of gas-liquid interaction systems
7 (absorption/desorption/distillation) is a conventional chemical engineering problem. The literature
8 is relatively rich with modeling/design methodologies for absorption/desorption columns with
9 non-reactive interaction (both rate-based and equilibrium). However, when chemical reactions
10 accompany these processes, the so-called reactive absorption/desorption systems become
11 significantly complex (Astarita, 1967, 1983; Danckwerts, 1970). This is due to the high interaction
12 of process thermodynamics, the existence of multiple reactants (some in the ionic state), and
13 mass/heat transfer within the system. For this reason, reactive absorption/desorption systems are
14 not yet fully understood (Kenig and Górak, 2005). The initial interest in reactive separation was
15 derived mainly from the need for natural gas sweetening, e.g., (Danckwerts and Sharma, 1966;
16 Pandya, 1983; Sanyal et al., 1988). In recent decades, however, the number of publications in this
17 field has notably increased with the attention to capturing CO₂ from flue gas (Freguia and Rochelle,
18 2003; Mores et al., 2011). Studies in this regard often have been modelled the system with
19 simulators, while others with equation-based models. Nevertheless, there are discrepancies across
20 the simulation software packages. For instance, Luo et al. (2009) compared the results of four
21 different pilot plants with six simulators (Aspen RadFrac/RateSep, Promax, CHEMASIM,
22 Protreat, and CO2SIM) and found that the employed simulators were not capable of predicting
23 consistent results for critical parameters like reboiler duty, concentration and temperature profiles.
24 This deficiency even applies to well-known solvents such as MEA.

25 Furthermore, in recent years there has been a growing trend of rigorous methodologies for the
26 integration of Sol-CCS processes with dynamic electricity market, e.g. (Khalilpour, 2014; Mac
27 Dowell and Shah, 2015). Despite this, very few studies have integrated “operation” models with
28 “design,” e.g., (Damartzis et al., 2016; Khalilpour and Abbas, 2014a; Lawal, 2012). In the
29 mainstream literature, modeling tasks are carried out based on an existing pilot plant to find the
30 optimal operating conditions. However, a correct and optimal design task for a new (PCC) plant
31 requires parallel modeling of both process design (heights, diameters, and so forth) and operating

1 conditions (pressures, temperatures, flow rates, and so forth). This critical approach has received
2 very little attention in the literature concerning PCC (Damartzis et al., 2014), and hence its
3 importance is evident from the high capital expenditure (CAPEX) of a PCC process being close to
4 that of a power plant. Khalilpour and Abbas (2014a) developed an equation-based methodology
5 for optimal synthesis and design of absorption and desorption columns considering the rate-based
6 interaction of the gas and liquid. The design methodology deliberates the influential techno-
7 economic parameters such as a number of absorber/desorber columns, height, and diameter of
8 columns, operating conditions (P, T) of columns, pressure drop, packing type, the percentage of
9 CO₂ avoided, captured CO₂ purity, amount of regeneration, and flooding velocities of columns.
10 The authors reported that the design and operation parameters are so markedly interactive that
11 decisions as to the selection of the right values for the variables require techno-economic study
12 and the setting of a unique objective such as NPV (net present value). Then the optimal operation
13 and design parameters could be found under the umbrella of the economic objective function. The
14 users could give the objective function based on their specific goal which might be more towards
15 minimization of capital costs or operational costs. Such goals may vary based on different
16 locations. For instance, CSIRO's study suggests that while the main barrier to the implementation
17 of CCS technologies for energy-importing countries (e.g., China) is to improve the energy
18 efficiency of PCC process, the challenge for developed countries such as Australia is the reduction
19 of process capital expenditures through an optimal process design (Dave, 2011). According to this
20 study, capital costs account for 73% of the costs of electricity generation with carbon capture in
21 Australia (and similarly developed countries), whereas it is only 33% for China. It is evident from
22 this example that the design objective for these two design scenarios would be different and thus,
23 the development of an economic model combined with technical variables could assist companies
24 in easier decision-making.

25 In this paper, we aim to provide a generic methodology for supporting techno-economic decision
26 making for optimal synthesis, design, and operation of Sol-PCC systems. The approach developed
27 here concurrently optimizes the critical design and operation variables for achieving the best
28 decision over the lifespan of a plant.

1 **2. Problem statement**

2 Consider a CO₂-emitting process (e.g., power plant, a steel company, and cement industry) with a
3 baseline flue gas flow rate of F_b^{FG} . The flue gas composition is known. The given planning horizon
4 is Y years ($y: 1, 2, \dots, Y$), each year with TPY total periods of a given fixed length Δt (min, hr, day,
5 week, etc.). The current optimization study is occurring in the base year ($y = 0$).

6 The government has introduced its emission reduction regulations in the form of carbon taxes over
7 a given timeframe, and thus the plant must comply with the new policies. The company has
8 selected Sol-PCC process as its strategic emission reduction approach and is assessing to build a
9 Sol-PCC plant with baseline design capacities of DC tonnes of CO₂ capture per period of Δt , and
10 an annual capacity factor of CF . With the addition of a Sol-PCC plant, the company will need
11 extra energy for running the pumps, compressors, and reboilers. If the company is an electricity
12 generator, this excess in-house demand will evidently imply a reduced electricity export. For a
13 power-consuming plant (cement, steelmaking, etc.), this will mean additional power procurement.
14 In a liberalized market, the price of electricity is variable and defined by market dynamics
15 (Khalilpour, 2014). Herein, we assume that the company, with access to historical periodical data,
16 has projected the average pool price of electricity, EEP_y , at year y . The prices of heating energy
17 (for reboiler) and cooling energy are HEP_y and CEP_y , respectively.

18 Our decision-making optimization algorithm is illustrated in Figure 2. Any optimization process
19 consists of a few key components, including assumptions, input parameters, variables, constraints
20 and an objective function.

21 **Inputs:** Table 1 shows a list of inputs. First, the decision-maker (power plant, steelmaking
22 company, cement industry, etc.) defines the desired decision parameters which are “inputs” to the
23 program (A in Figure 2) including flue gas composition, desired carbon capture rate, preferred list
24 of solvents, column packings, equipment specifications as well as costs.

25 **Variables:** Table 1 also shows a list of variables. These variables are of two types. Some are
26 directly linked with economic objective function (No 1-9 in Table 1, also presented as a section B
27 in Figure 2). There are however some other variables which are determined in the synthesis/design
28 stage (No 10-33 in Table 1) and are indirectly linked to the objective function. Once the decision-
29 maker supplied the input parameters, the optimization initiates to find the best combinations of all
30 these variables to achieve the optimal goal.

1 **Table 1:** List of input parameters and unknowns (variables) for the Sol-PCC process system synthesis and design

Inputs	Variables	
<ul style="list-style-type: none"> • Desired rate of CO₂ capture (weight per time) • Available flue gas flow rate and its detailed composition (CO₂, H₂O, N₂, etc.) • Solvent types, composition, and operating (T, P) range • List of candidate packings and their properties • List of equipment suppliers and types (pumps, compressors, heat exchanger, drums, etc.) 	<ol style="list-style-type: none"> 1) CO₂ capture efficiency (%) of the PCC plant 2) Temperature of the inlet flue gas to absorber 3) Temperature of the inlet gas to desorber 4) Temperature of the inlet solvent to absorber 5) Lean loadings 6) Rich loadings 7) Packing type and size 8) Pressures of absorber columns 9) Pressures desorber columns 10) Number of absorber columns 11) Column diameter of absorber column 12) Packing height of absorber column 13) Size of absorber demister 14) Solvent flow rate of absorber 15) Pressure drop of absorber column 16) Number of desorber columns 	<ol style="list-style-type: none"> 17) Column diameter of desorber column 18) Packing height of desorber column 19) Size (area) of desorber demister 20) Gas flow rate of desorber 21) Pressure drop of desorber 22) Reboiler temperature 23) Condenser size 24) Reflux drum size 25) Reboiler size 26) Lean/rich Heat-exchanger size 27) Recycled solvent cooler size 28) Blower size 29) Pump size 30) Number of compressors 31) Sizes of compressors 32) Sizes of inter-stage cooling heat exchangers of compressors 33) Sizes of pre-compressor knock-out drums

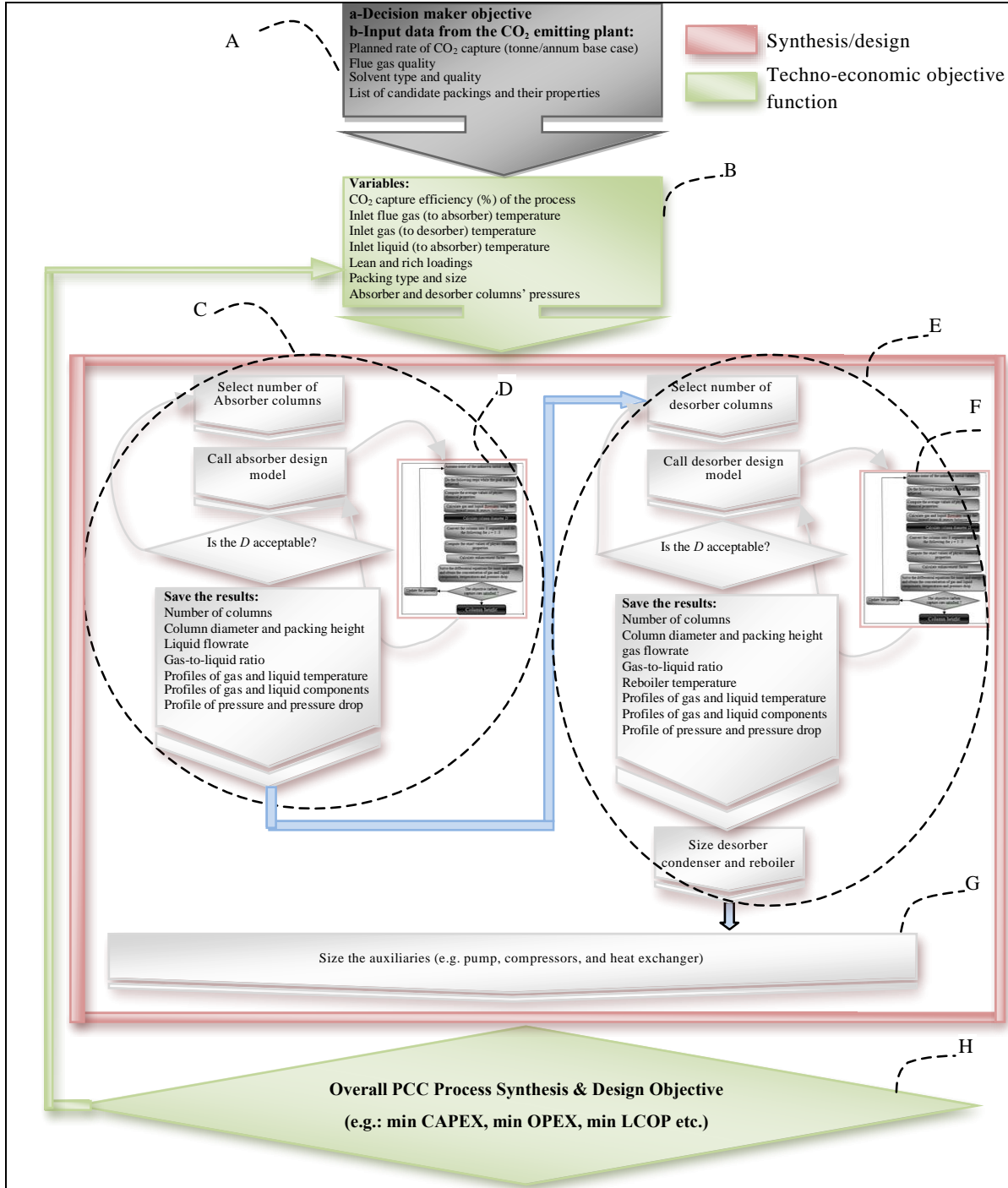
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3 **Constraints:** In any techno-economic assessment, there are several constraints involved. These
 4 could be high-level economic constraints, such as the maximum available investment budget, or
 5 could be technical limitations enforced by the physics or chemistry of the system. For instance,
 6 equipment size could theoretically have any value, but manufacturers might supply equipment in
 7 certain sizes. Absorber/desorber columns height can take any theoretic magnitude while within a
 8 practical perspective, manufacturers often enforce a maximum allowable diameter and height.

9 **Objective:** Selection of the objective function is the most critical step in any techno-economic
 10 assessment and is entirely related to a company's policies and future planning. A correct objective
 11 function can guarantee a sustainable solution. An objective function might be merely minimization
 12 of total capital investment (C_{TCI}), simply CAPEX, or operating expenditure (OPEX). It could also
 13 be the minimization of levelized cost of the product (LCOP), maximization of internal rate of
 14 return (IRR), maximization of net present value (NPV) of cash flow, and so forth. The formulation
 15 presented in this work is generic, and it offers flexibility for future users to employ the objective
 16 function of interest. It is noteworthy that the current appropriate objective functions are the
 17 minimization of OPEX, NPV of costs, and levelized costs. This is mostly due to the fact that the
 18 carbon capture process is not considered as a lucrative practice as the product of the process (CO₂)
 19 doesn't have positive economic value. As such, attentions are mainly toward minimization of

1 capture costs rather than maximization of profit. Steps in a typical techno-economic process shown
 2 in Figure 2.

3



4

5

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Figure 2: Overall PCC process synthesis and design methodology

3. Problem formulation

3.1. Objective function formulation

Here, we present a techno-economic optimisation algorithm for Sol-PCC process system synthesis, design and operation. The manufacturer supplies equipment cost as a function of size, operating conditions, and material quality. There are several cost models specific for any equipment. There are also some generic cost formulations which could be found in process design handbooks and textbooks. Here we use one of the most popular cost functions introduced by Turton et al. (2008) and provided in CAPCOST software package.

The purchased cost of equipment at manufacturer's site, including free-on-board (FOB) costs, as given by,

$$C_p = C_p^0 F_P F_M \quad (1)$$

where, C_p^0 is a base equipment cost, F_P is cost factor for pressure and F_M is cost factor for material. The base equipment cost, C_p^0 is given by,

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10} X + K_3 [\log_{10} X]^2 \quad X^{min} \leq X \leq X^{max} \quad (2)$$

where X is area or volume of the equipment and $K_1 - K_3$ are constants specific for given equipment. A similar correlation is given for the pressure factor, F_P and expressed as,

$$\log_{10} F_P = C_1 + C_2 \log_{10} P + C_3 [\log_{10} P]^2 \quad P^{min} \leq P \leq P^{max} \quad (3)$$

where P is the design pressure and $C_1 - C_3$ are constants specific for given equipment. Similarly, several direct and indirect costs are involved in the installation of purchased equipment. The summation of all costs makes the bare module cost (C_{BM}). The direct costs are a) purchased cost of equipment at manufacturer's site, b) cost of materials for installation (piping, insulation and fireproofing, foundations and structural supports, instrumentation and electrical, and painting associated with the equipment), and c) labor costs. The indirect costs include a) freight, insurance, and taxes, b) construction overhead, and c) contractor engineering expenses. For any piece of equipment, the C_{BM} is given by,

$$C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P) \quad (4)$$

where B_1 and B_2 are constants. Thus, the base bare module cost can be calculated using,

$$C_{BM}^0 = C_p^0 F_{BM}^0 = C_p^0 (B_1 + B_2) \quad (5)$$

There is also a third category of costs in the development of a plant which include contingency ($C_{Con} = \alpha_1 \sum C_{BM}$) and contractor fees ($C_{CF} = \alpha_2 \sum C_{BM}$). These costs are calculated as fraction of total bare module costs with constants α_1 and α_2 . The total module cost (C_{TM}) is given by,

$$C_{TM} = (1 + \alpha_1 + \alpha_2) \sum C_{BM} \quad (6)$$

When a new plant is being planned, there will be a fourth category of costs including site development, auxiliary buildings, off-sites, and utilities. These costs are calculated as a fraction of base bare module cost ($C_{Aux} = \alpha_3 \sum C_{BM}^0$). Hence, the fixed capital investment (FCI) costs are given by,

$$C_{FCI} = C_{TM} + \alpha_3 \sum C_{BM}^0 \quad (7)$$

Any new plant also needs a working capital (C_{wc}) which is a fraction (α_4) of total module costs. Equation (8) concludes the total capital costs, TCI, or CAPEX formulation,

$$C_{TCI} = C_{FCI} + C_{wc} = (1 + \alpha_1 + \alpha_2 + \alpha_4) \sum C_{BM} + \alpha_3 \sum C_{BM}^0 \quad (8)$$

Table 2 shows a summary of the total capital expenditure functions.

The operating expenditures (OPEX) consist of two segments including manufacturing costs and general expenses. Manufacturing costs include variable costs (all utilities, maintenance, and repairs, operating labor, operating supplies, supervision, laboratory charges, etc.) and fixed costs (depreciation, property taxes, insurances, and rent). The general expenses include administrative expenses, and distribution and marketing costs (when relevant). A detailed OPEX framework is given elsewhere (Abu-Zahra et al., 2007; Peters et al., 2003). OPEX can also be represented by two components, which are fixed and variable operation and maintenance costs (FOM and VOM). The FOM costs comprise of constant elements such as property insurance, maintenance, repairs, operating labor, supervision, administrative, and R&D. The annual FOM is usually presented as a fraction of fixed capital investment ($FOM_y = \beta \times C_{FCI}$). The VOM includes all variable costs such as heating and cooling duties, solvent make-up, as well as the electricity for pumps and compressors. In essence, the annual OPEX could be rearranged and shown by correlation (9) as a summation of FOM and all variable costs,

$$OX_y = FOM_y + VOM_y = \beta \times C_{FCI} + \sum VOM \quad (9)$$

1

Table 2: The total capital expenditure formulation (Turton et al., 2008)

		Factor associated with the installation of equipment	Symbol	Comments	Formula	
(1) Direct project expenses						
Total Capital Investment (C_{TCI}) or CAPEX		Total Module Cost (C_{TM}) [expansion to existing plant]	Bare Module Cost (C_{BM})	(a) Equipment FOB cost	C_P Purchased cost of equipment at manufacturer's site $\log_{10} C_p^0 = K_1 + K_2 \log_{10} A + K_3 [\log_{10} A]^2$ $C_p = C_p^0 F_P F_M$ Where: $\log_{10} F_P = C_1 + C_2 \log_{10} P + C_3 [\log_{10} P]^2$	
				(b) Materials required for installation	C_M Includes all piping, insulation and fireproofing, foundations and structural supports, instrumentation and electrical, and painting associated with the equipment	
				(c) Labor to install equipment and material	C_L Includes all labor associated with installing the equipment and mentioned in (a) and (b)	
(2) Indirect project expenses						
		Total Module Cost (C_{TM}) [expansion to existing plant]	Bare Module Cost (C_{BM})	(a) Freight, insurance, and taxes	C_{FIT} Includes all transportation costs for shipping equipment and materials to the plant site, all insurance on the items shipped, and any purchase taxes that may be applicable	
				(b) Construction overhead	C_O Includes all fringe benefits such as vacation, sick leave retirement benefits, etc.; labor burden, social security and unemployment insurance, etc.; and salaries and overhead for supervisory personnel	
				(c) Contractor engineering expenses	C_E Includes salaries and overhead the engineering; drafting, and project management personnel on the project	
$C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P)$ $C_{BM}^0 = C_p^0 F_{BM}^0 = C_p^0 (B_1 + B_2)$						
(3) Contingency and fee						
		Total Module Cost (C_{TM}) [expansion to existing plant]	Bare Module Cost (C_{BM})	(a) Contingency	C_{Cont} A factor to cover unforeseen circumstances. These may include loss of time due to storms and strikes, small changes in design, and unpredicted price increases.	$\alpha_1 \sum C_{BM}$
				(b) Contractor fee	C_{Fee} This fee varies depending on the type of plant and a variety of other factors.	$\alpha_2 \sum C_{BM}$
$C_{TM} = \sum C_{BM} + (\alpha_1 + \alpha_2) \sum C_{BM} = (1 + \alpha_1 + \alpha_2) \sum C_{BM}$						
		Total Module Cost (C_{TM}) [expansion to existing plant]	Bare Module Cost (C_{BM})	(4) Auxiliary facilities	C_A	$C_A = \alpha_3 \sum C_{BM}^0$
				(a) Site development	C_{Site} Includes the purchase of land; grading and excavation of the site; installation and hook-up of electrical, water, and sewer systems; and construction of all internal roads, walkways, and parking lots	
				(b) Auxiliary buildings	C_{Aux} Includes administration offices, maintenance shop and control rooms, warehouses, and service buildings (e.g., cafeteria, dressing rooms, and medical facility)	
				(c) Off-sites and utilities	C_{Off} Includes raw material and final product storage; raw material and final product loading and unloading facilities; all equipment necessary to supply required process utilities (e.g., cooling water, steam generation, fuel distribution systems, etc.); central environmental control facilities (e.g., wastewater treatment, incinerators, flares, etc.); and fire protection systems	
$C_{FCI} = C_{TM} + \alpha_3 \sum C_{BM}^0$						
				(5) Working Capital	C_{WC}	$C_{WC} = \alpha_4 C_{TM}$
$C_{TCI} = C_{FCI} + \alpha_4 C_{TM} = (1 + \alpha_4) C_{TM} + \alpha_3 \sum C_{BM}^0$						

2

3

4

1 As CAPEX and OPEX are the main components of the most techno-economic analysis, we are
 2 now able to formulate most types of objective functions. The net present value (NPV) of costs over
 3 the planning horizon, as given by,

$$4 \quad NPV = C_{TCI} + \sum_{y=1}^Y \frac{OX_y}{(1+r)^y} \quad (10)$$

5 in which OX_y is the OPEX of the PCC plant during year y and r is a discount rate. LCOP as a
 6 levelized cost of energy, as given by,

$$7 \quad LCOP = \frac{FCF \times C_{TCX} + OX_1}{DC \times TPY \times CF} \quad (11)$$

8 where DC is the design capacity of the PCC process in terms of unit weight of CO_2 captured per
 9 time interval Δt , TPY is the number of Δt within a year, and CF is the annual capacity factor of
 10 the plant. FCF is the fixed charge factor for levelization of total CAPEX and given by,

$$11 \quad FCF = \frac{r(1+r)^Y}{(1+r)^Y - 1} \quad (12)$$

12 Therefore, the user can select various objective functions including the ones introduced here, i.e.,
 13 CAPEX (C_{TCI}), OPEX (OX_y), NPV, and LCOP.

14

15 **3.2. Equipment sizing**

16 **3.2.1. Auxiliary equipment**

17 This stage includes finding the number of units and their corresponding sizes for the absorber,
 18 desorber, and all other unit operations. While the generic Sol-PCC process has a schematic similar
 19 to Figure 1, the process synthesis and design are a much more complex task as the number of units
 20 and their specific sizes are not known. The Sol-PCC process includes the following units:

- 21 • Flue gas blower
- 22 • Absorber (might require more than one), with packing and demister
- 23 • Desorber (might require more than one), with packing and demister, condenser, and drum
- 24 • Lean/rich heat exchanger
- 25 • Lean cooling heat exchanger
- 26 • Lean pump
- 27 • Rich pump

- 1 • CO₂ compression unit (may need more than one unit), each unit requires a compressor, cooling
2 heat-exchanger, and a knock-out drum (with a demister)

3 For each of the mentioned systems, we need their governing design and operational functions. We
4 start first with flue gas blower. The baseline flue gas flowrate is F_b^{FG} . Therefore, the Sol-PCC
5 process can be designed based on the flue gas flow rate of F^{FG} expressed by,

$$6 \quad F^{FG} \leq F_b^{FG} \quad (13)$$

7 Flue gas with a flowrate of F^{FG} enters the blower(s). As the available blowers have minimum and
8 maximum size ranges, there might be a need for one or more blower(s). We define integer variable
9 x^B as the number of blower with inlet flowrate of F^B expressed by,

$$10 \quad F_{min}^B \leq F^B \leq F_{max}^B \quad (14)$$

11 and

$$12 \quad x^B F^B = F^{FG} \quad (15)$$

13 The energy used for the compression of F^B from pressure of P^{FG} to absorber inlet pressure P_{in}^{Abs} ,
14 as given by,

$$15 \quad E^B = \frac{F^B z^{FG} R T^{FG}}{\eta^B M^{FG}} \frac{k^{FG}}{k^{FG}-1} \left[\left(\frac{P_{in}^{FG,Abs}}{P^{FG,B}} \right)^{\frac{k^{FG}-1}{k^{FG}}} - 1 \right] \quad (16)$$

16 where, η^B is the blower efficiency, R is gas constant, and M^{FG} is flue gas molecular weight. z^{FG}
17 and k^{FG} are average flue gas compressibility factor and polytropic constant, respectively, for the
18 operating conditions of the blower. The flue gas, after blower, enters absorber column with
19 pressure and temperature of $P_{in}^{FG,Abs}$ and $T_{in}^{FG,Abs}$. Undoubtedly, absorber and desorber design
20 account for the major CAPEX and OPEX of a Sol-PCC system. These two units are also one of
21 the most complex systems due to their reactive-separation processes. The detailed rate-based
22 models of packed-bed absorber and desorber are given elsewhere (Khalilpour and Abbas, 2014a)
23 and a summary of the governing equations are provided as a supplementary document. Here, we
24 keep the focus on discussion about general sizing constraints. The critical step in absorber
25 operation and sizing is the diameter and height of the packing concerning the operating conditions
26 of the inlet gas and lean solvent. Generally, there are limitations for absorber diameter and height

1 due to operability issues. As such, the optimal process synthesis may require one or more absorber
 2 column(s). We define integer variable x^{Abs} as the number of absorber columns with inlet flowrate
 3 of F_{in}^{Abs} , where expressed by,

$$4 \quad x^{Abs} F_{in}^{Abs} = F^{FG} \quad (17)$$

5 The height of the absorber column has a constant relation with the packing height
 6 ($H^{Abs} = \alpha_5 H_{pack}^{Abs}$). The manufacturer constraints on column diameter and packing heights are
 7 given by,

$$8 \quad H_{min}^{Abs,pack} \leq H_{pack}^{Abs} \leq H_{max}^{Abs,pack} \quad (18)$$

$$9 \quad D_{min}^{Abs} \leq D^{Abs} \leq D_{max}^{Abs} \quad (19)$$

10 The demister area (A^{Dem}) and packing volumes (V^{pack}) for each absorber columns are therefore
 11 given calculated using D^{Abs} and H_{pack}^{Abs} .

12 The flue gas leaves the absorber with $F_{out}^{FG,Abs}$ and $T_{out}^{FG,Abs}$ and $P_{out}^{FG,Abs}$ and a composition defined
 13 from of the model is provided in the supplementary document. The flue gas is vented to the
 14 atmosphere. The lean solvent entering the top of absorber at the condition $F_{in}^{L,Abs}$, $T_{in}^{L,Abs}$, $P_{in}^{L,Abs}$
 15 and $\alpha_{in}^{L,Abs}$ leaves the column with $F_{out}^{R,Abs}$, $T_{out}^{R,Abs}$, $P_{out}^{R,Abs}$ and $\alpha_{out}^{R,Abs}$. The now-rich solvent is
 16 pumped to the pressure of the desorber column (plus the pressure drop within the lean-rich heat
 17 exchanger). Occasionally, solvent makeup (F^{MU}) is also injected to this flow to compensate for
 18 losses. The power needed for solvent pumping is $E^{R.P}$. If this power is higher than the maximum
 19 capacity of chosen pumps, more than one pump will be needed. We define integer variable $x^{R.P}$
 20 as the number of rich pumps with inlet flowrate of $F^{R.P}$ expressed by,

$$21 \quad x^{Abs} F_{in}^{L,Abs} = x^{R.P} F^{R.P} \quad (20)$$

22 The energy consumption of each pump, given by,

$$23 \quad E^{R.P} = \frac{F^{R.P} (P_{in}^{R,Des} + \Delta P^{L,R,HX} - P_{out}^{L,Abs})}{\eta^{R.P}} \quad (21)$$

24 The rich solvent after passing through the rich-lean heat exchanger enters the desorber column(s)
 25 at $T_{in}^{R,Des}$, $P_{in}^{R,Des}$, $T_{in}^{R,Des}$ and $\alpha_{in}^{R,Des}$. The desorber has a complex physico-chemical rate-based heat
 26 and mass transfer. The detailed model is provided in the supplementary document. We define

1 integer variable x^{Des} as the number of desorber columns with inlet rich flowrate of $F_{in}^{R,Des}$, where
 2 expressed by,

$$3 \quad x^{Des} F_{in}^{R,Des} = x^{R,P} F^{R,P} \quad (22)$$

4 The height of the desorber column has a constant relation with the packing height
 5 ($H^{Des} = \alpha_{Des} H_{pack}^{Des}$). The manufacturer constraints on column and packing heights are given by,

$$6 \quad H_{min}^{Des,pack} \leq H_{pack}^{Abs} \leq H_{max}^{Des,pack} \quad (23)$$

$$7 \quad D_{min}^{Des} \leq D^{Des} \leq D_{max}^{Des} \quad (24)$$

8 The demister area and packing volumes for each absorber columns are then given by,

$$9 \quad A^{Dem,Des} = \pi(D^{Des})^2 \quad (25)$$

$$10 \quad V^{pack,Des} = \pi(D^{Des})^2 H_{pack}^{Des} / 4 \quad (26)$$

11 The outlet gas with high CO₂ concentration goes to a heat exchanger to be water-cooled. The
 12 condensed water returns to knock-out drum and recycles to the column for water-washing the
 13 exiting gas. The almost-regenerated solvent from the bottom goes to a reboiler where it is heated
 14 to the saturation temperature and becomes a two-phase stream. The vapor phase flows upward to
 15 the column as stripping gas. The liquid phase, now-called lean solvent, leaves the reboiler with
 16 $F_{out}^{L,Des}$, $T_{out}^{L,Des}$, $P_{out}^{L,Des}$ and $\alpha_{out}^{L,Des}$. This hot lean stream goes through the lean-rich heat exchanger
 17 (LRHX) and passes its heat to the rich solvent coming from absorber(s).

18 The lean-rich heat exchanger is of shell-and-tube type. The heat exchanger design is based on the
 19 interactivity between heat-exchanger area, fluid flow rate, pressure drop and the temperature
 20 approach. A low-temperature approach requires a larger heat transfer area where the opposite
 21 implies higher thermal duty. Key governing equations are given by,

$$22 \quad Q^R = (x^{Abs} F_{out}^{R,Abs}) C p^{R,LRHX} (T_{in}^{R,Des} - T_{out}^{R,Abs}) \quad (27)$$

$$23 \quad Q^L = (x^{Des} F_{out}^{L,Des}) C p^{L,LRHX} (T_{out}^{L,Des} - T_{out}^{L,LRHX}) \quad (28)$$

24 where, $Q^R = Q^L = U^{LRHX} A^{LRHX} F^{LRHX} LMTD^{LRHX}$, in which the log mean temperature difference
 25 (LMTD) is given by,

$$1 \quad LMTD^{LRHX} = \frac{(T_{out}^{L,Des} - T_{out}^{R,Abs}) - (T_{out}^{L,LRHX} - T_{in}^{R,Des})}{\ln \frac{(T_{out}^{L,Des} - T_{out}^{R,Abs})}{(T_{out}^{L,LRHX} - T_{in}^{R,Des})}} \geq \beta^{LRHX} \quad (29)$$

2 where β^{LRHX} is a minimum acceptable temperature approach. Given the limitation of heat
 3 exchanger sizes, one or more heat exchangers might be needed; hence, we define an integer
 4 variable x^{LRHX} as the number of lean-rich heat exchanger size, as expressed by,

$$5 \quad A_{min}^{LRHX} \leq A_x^{LRHX} \leq A_{max}^{LRHX} \quad (30)$$

6 and,

$$7 \quad A^{LRHX} = x^{LRHX} A_x^{LRHX} \quad (31)$$

8 These constraints will identify the exit temperature of the lean solvent, $T_{out}^{L,LRHX}$. Evidently, this
 9 temperature is greater than the inlet temperature of the absorber, further cooling is required before
 10 the lean solvent enters the top of the absorber columns. The duty of lean cooling heat exchanger
 11 (LCHX) is given by,

$$12 \quad Q^{LCHX} = (x^{Des} F_{out}^{L,Des}) C p^{L,LCHX} (T_{out}^{L,LRHX} - T_{in}^{L,Abs}) \quad (32)$$

13 The cooling water enters and leaves at $T_{in}^{L,cw}$ and $T_{out}^{L,cw}$. Therefore, we have,

$$14 \quad Q^{LCHX} = U^{LCHX} A^{LCHX} F^{LCHX} LMTD^{LCHX} \quad (33)$$

15 where,

$$16 \quad LMTD^{LCHX} = \frac{(T_{out}^{L,LRHX} - T_{in}^{L,cw}) - (T_{in}^{L,Abs} - T_{out}^{L,cw})}{\ln \frac{(T_{out}^{L,LRHX} - T_{in}^{L,cw})}{(T_{in}^{L,Abs} - T_{out}^{L,cw})}} \geq \beta^{LCHX} \quad (34)$$

17 and β^{LCHX} is a minimum acceptable temperature approach. Given the limitations concerning heat
 18 exchanger sizes, one or more heat exchangers might be needed, we define an integer variable
 19 x^{LCHX} as the number of lean cooling heat exchanger size, as expressed by,

$$20 \quad A_{min}^{LCHX} \leq A_x^{LCHX} \leq A_{max}^{LCHX} \quad (35)$$

21 and

$$22 \quad A^{LCHX} = x^{LCHX} A_x^{LCHX} \quad (36)$$

23 The gas exiting the top of the stripper is mainly CO₂ and water. It is therefore cooled to remove
 24 the major water fraction. The two-phase cooled stream goes to a reflux drum (with a demister) in

1 which the liquid stream is returned to the desorber and the gas stream (mainly CO₂) goes for the
 2 compression/liquefaction unit. Depending on the ultimate destination of CO₂, one or more stages
 3 of compression is required to increase the pressure of the gas from pressure at desorber exit, P^{Des} ,
 4 to export pressure, P^{exp} . A network of compressors is required since the compression ratio ($P^{exp}/$
 5 P^{Des}) exceeds the ability of a single compressor (having a compressibility factor less than 4). It is
 6 proven that the optimal compression ratio that minimizes total work is such that each stage has an
 7 identical ratio (Finlayson, 2006). This can be generalized for a network of x^{com} stages of
 8 compressors, as expressed by,

$$9 \quad \frac{P_1}{P_{Des}} = \frac{P_2}{P_1} = \dots = \frac{P_{x^{comp}}}{P_{x^{comp}-1}} = \left(\frac{P_{x^{comp}}}{P_{Des}} \right)^{1/x^{comp}} \quad (39)$$

10 Each compression unit is composed of one scrubber, one compressor, and a so-called intercooler
 11 heat exchanger after each compressor to decrease the elevated gas temperature and volume. The
 12 compressor works to increase the pressure of gas from p_{i-1} to p_i , as given by,

$$13 \quad E_i^{Cmp} = \frac{p_i n_i}{\rho_i (n_i - 1)} \left[\left(\frac{p_i}{p_{i-1}} \right)^{\frac{n_i - 1}{n_i}} - 1 \right] \quad (37)$$

14 where, n is polytropic index. The gas temperature rises after each compression stage as given by,

$$15 \quad \Delta T = \frac{(T_{i-1} + 273.15)}{\eta_{is}} \left[\left(\frac{p_i}{p_{i-1}} \right)^{\frac{n_i - 1}{n_i}} - 1 \right] \quad (38)$$

16 Given the cooling water inlet and outlet temperatures, the inter-cooling compressor area is
 17 computed. With the cooling gas pressure and temperature, the scrubbers' volume is calculated.
 18 With the compressor unit, all auxiliary equipment is sized. All knock-out drums are sized based
 19 on the governing equations given in Ludwig's Handbook (Coker, 2011). Having described all unit
 20 operations, the total module cost $C_{TM} = \sum C_{BM}$ in Eq. (6) could be given in more details by,

$$21 \quad C_{TM} = \sum C_{BM} = x^{Abs} C_{BM}^{Abs} + x^{Abs.Dem} C_{BM}^{Abs.Dem} + x^{Des} C_{BM}^{Des} + x^{Des.Dem} C_{BM}^{Des.Dem} +
 22 \quad x^{Des.Reb} C_{BM}^{Des.Reb} + x^{Des.CHX} C_{BM}^{Des.CHX} + x^{Des.Ref} C_{BM}^{Des.Ref} + x^{Blow} C_{BM}^{Blow} + x^{R.P} C_{BM}^{R.P} +
 23 \quad x^{LRHX} C_{BM}^{LRHX} + x^{LCHX} C_{BM}^{LCHX} + x^{R.P} C_{BM}^{R.P} + \sum_{i=1}^{x^{Com}} (C_{BM,i}^{Comp} + C_{BM,i}^{IntCHX} + C_{BM,i}^{Scrub}) \quad (39)$$

1 The $\sum VOM$ in Eq. (9) is also obtained by summation of all variable operating cost, as given by,

$$2$$
$$3 \quad VOM_y = TPY \sum VOM = TPY [EEP_y (x^B E^B + x^{R.P} E^{R.P} + \sum_{i=1}^{x^{Com}} E_i^{Com}) +$$
$$4 \quad HEP_y (x^{Des} Q^{Reb}) + CEP_y (x^{LCHX} Q^{LCHX} + x^{Des} Q^{Des.CHX} + \sum_{i=1}^{x^{Com}} Q_i^{IntCHX}) + SP_y F^{MU}] \quad (40)$$
$$5$$

6 This completes our sizing formulation.

7

8 **3.3. Problem execution**

9 The structure of this problem solution is illustrated in Figure 2. Given the complex nature of
10 absorber and desorbed processes, we have found heuristic algorithms (such as evolutionary
11 algorithms) the most reliable solution approach. Once, the input parameters are supplied (A in
12 Figure 2), the program initiates with the selection of a set of random values for the direct variables
13 (No 1-9 in Table 1 or section B in Figure 2). With this, the process design initiates; the
14 specifications of absorber (sections C-D in Figure 2) and desorber (sections E-F in Figure 2) are
15 found based on the set of equations supplied in the supplementary file. The specifications of other
16 equipment (sections G in Figure 2) are found using Eqs. (13-40). The program then calculates the
17 objective function values using relevant Eqs. (1-12) and (39-40). Having obtained the objective
18 value, a new set of random values are generated for the direct variables (B in Figure 2), and the
19 execution is repeated until the program converges in the optimal value. In this study, we have used
20 Matlab[®] 2014b, though any open-source or proprietary programming software environment can
21 be employed.

22

23 **4. Case study**

24 A 300 MW coal-fired power plant in Australia typically burns pulverized black coal with 25% ash,
25 8% moisture, and dry-ash-free (DAF) with the chemical composition of 83.3% carbon, 5.4%
26 hydrogen, 1.9% nitrogen, 0.6% sulfur, and 8.8% oxygen. The power plant emits 12260 mol/s
27 (353.3 kg/s) of flue gas when operating at its full capacity. The flue gas composition is 13.0 vol%
28 (19.8 wt%) CO₂, 70.37% N₂, 13.52% H₂O, 3.11% O₂ and ppm levels of SO_x and NO_x. The SO_x
29 and NO_x are removed from the flue gas before venting or entering the PCC process. When
30 operated in the full capacity, the plant emits 2.2 million tonnes of CO₂ per annum. The company
31 desires to investigate the feasibility of investment in a Sol-PCC process which can annually capture
32 $\geq 75\%$ of its CO₂ emission when operating at a capacity factor of 85%. The preferred solvent is

1 MEA due to the minimum commercial risks. The optimum operating temperature of an MEA
 2 absorber is commonly in a range of 40-60 °C; hence, the temperature of flue gas requires to be
 3 adjusted to the range of absorber operating conditions before entering the absorber. The
 4 physicochemical properties (viscosities, densities, thermal conductivities, surface tensions, the
 5 heat of reaction, diffusivities, specific heat, mass, and heat transfer coefficients) of the MEA
 6 solvents used in this modeling/design work are explained and presented in (Khalilpour and Abbas,
 7 2014b). The techno-economic parameters for equipment bare module cost calculations are given
 8 in Table 3. The maximum allowable column diameter and packing heights are 12 m and 25 m,
 9 respectively. The captured CO₂ is aimed to be compressed to 100 bars, cooled to 50 °C; and
 10 subsequently exported for the planned applications (sequestration, utilization, etc.).

11 **Table 3:** The optimal operational and design variables with two objective functions (Turton et al., 2008).

Equipment	$\log_{10} C_p^0$ $= K_1 + K_2 \log_{10} X$ $+ K_3 [\log_{10} X]^2$			F_P			$F_{BM} = B_1 + B_2 F_M F_P$		
	K_1	K_2	K_3	C_1	C_2	C_3	B_1	B_2	F_M
Blower (Centrifugal Radial Fan)	3.54	-0.35	0.45	0.00	0.21	-0.03	2.74 (CS)		
Columns (vertical vessel)	3.50	0.45	0.11	$F_P = \frac{PD}{2[850 - 0.6P]} + 0.00315$ 0.0063			2.25	1.82	3.10 (SS)
Packing (ceramic) absorber/desorber	3.07	0.97	0.01	-	-	-	4.20		
Demister (absorber, desorber, knock-out drums)	3.24	0.48	0.34	$F_{BM} = 1.00$ (SS)					
Rich solvent pump (Centrifugal)	3.39	0.05	0.15	-0.39	0.40	-0.00	1.89	1.35	2.30 (SS)
Compressor (centrifugal)	2.29	1.36	-0.10	$F_{BM} = 5.80$ (SS)					
Compressor electric drive	2.46	1.42	-0.18	$F_{BM} = 1.50$					
Reflux drum horizontal	3.56	0.38	0.09	$F_P = \frac{PD}{2[850 - 0.6P]} + 0.00315$ 0.0063			1.49	1.52	2.3 (SS)
Shell and Tube HX	4.32	-0.30	0.16	0.04	-0.11	0.08	1.63	1.66	2.73 (SS/SS)
Kettle reboiler	4.47	-0.53	0.40	0.04	-0.11	0.08	1.63	1.66	2.73 (SS/SS)

CEPCI: 397; SS: Stainless steel; CS: Carbon steel; HX: heat exchanger; P: pressure; D: diameter

12
 13 The fixed and variable operating cost parameters are given in Table 4. The Chemical Engineering
 14 Plant Cost Index (CEPCI) is used to convert the economic values to 2016 dollar (index: 541.7). It
 15 is noteworthy to clarify that we use electricity price to calculate the reboiler energy. This is because
 16 the steam which is used to heat the reboiler is extracted from power plant turbines aimed for
 17 electricity generation. In this study, we have assumed that one Joule of reboiler energy equals to
 18 0.19 Joule of electricity, i.e., $HEP = 0.19EEP$ (Khalilpour and Abbas, 2011). The minimum
 19 acceptable temperature approach is 3 °C for the kettle reboiler and 5 °C for all other heat
 20 exchangers.

1 The company desires to assess two different scenarios. In scenario (i), the objective is to design
 2 the plant with minimum possible total capital investment. In scenario (ii), the objective is to design
 3 the plant to minimize the levelized costs per unit weight of captured CO₂. The planning horizon is
 4 25 years with a constant discount rate of 10%, and an inflation rate of 3%.

5 **Table 4:** Economic parameters (annual basis unless otherwise the unit is mentioned).

	Range	Values for this study
Manufacturing cost		
Fixed charge		
Property Insurance	1% of FCI	1
Variable production cost		
Utilities	according to optimisation results	
MEA makeup	1.5kg/tonne-CO ₂ -captured	
Maintenance and repairs	1-10% of FCI	5
Operating labour	3% FCI	3
Supervision	15% of operating a labor	15
Laboratory charges	10-20% of operating a labor	15
Operating supplies	15% of maintenance and repairs	15
Plant overhead cost	50-70% of (maintenance + operating + labour + supervision)	60
General expenses		
Administrative cost	15-25% of (maintenance + operating + labour + supervision)	20
R&D cost	0.5% FCI	0.5
Utilities		
Electricity (110-440V)		49.36 \$2016/MWh (NEM, Australia)
Cooling water (30-45°C)		0.48 \$2016/GJ (Turton et al., 2009)

6
 7 Table 5 shows the results of the optimization for the two required objective functions. The program
 8 can find the optimal values of both technical (design and operational) and economic variables.
 9 Under the CAPEX optimization (scenario i), the program synthesizes a PCC plant with two
 10 absorber columns (Diameter: 10.54 m, packing height: 13.20 m) and one desorber column
 11 (Diameter: 11.27 m, Packing height: 14.60 m). The optimal reboiler duty of the desorber is found
 12 as 4.87 GJ/tonne-CO₂. The minimum CAPEX is evaluated as \$312.36 million. The levelized cost
 13 of CO₂ capture and compression, under this scenario, is found to be 58.07 \$/tonne-CO₂.

14 The carbon capture levelized cost under scenario (ii) is a combination of both CAPEX and OPEX.
 15 The ideal process combination under this scenario is similar to the CAPEX scenario, i.e., two
 16 absorber columns and one desorber column. However, the corresponding values of techno-
 17 economic variables are different in this scenario. Absorber columns have a diameter of 10.52 m

1 and packing height of 18.20 m. The diameter of desorber column is 9.68 m with packing height
 2 being 18.90 m.

3 The absorber and desorber columns are deemed to be larger than those for the previous scenario.
 4 The reason for scenario (i) having shorter absorber and desorber columns lies in the fact that
 5 installation cost is directly linked with column height. The lower, the column height, the lower
 6 will be the ultimate CAPEX. However, lower columns lead to increased operating costs. As
 7 scenario (i), does not include operating costs, the lowest CAPEX is achieved by using short
 8 columns and passing all subsequences on the operating costs. However, the objective function of
 9 scenario (ii) concurrently considers minimization of both CAPEX and OPEX. As such, though it
 10 leads to larger column heights than scenario (i), its reboiler duty is considerably low, (2.5 GJ/tonne-
 11 CO₂ vs 4.87 GJ/tonne-CO₂ in the previous scenario).

12 The CAPEX, under scenario (ii), is around \$12.82 million higher than the previous scenario
 13 (\$325.18 million vs. \$312.36 million). Nonetheless, the minimum levelized cost is found to be
 14 52.82 \$/tonne-CO₂ which is 5.25 \$/tonne-CO₂ lower than the scenario one. The schematic of the
 15 process within the scenario two is illustrated Figure 3. This example demonstrates the design and
 16 operational interactivity, and how the plant design can essentially change with different project's
 17 objectives. It is also highlighting that the optimal design can vary depending on the local economic
 18 input parameters and desires.

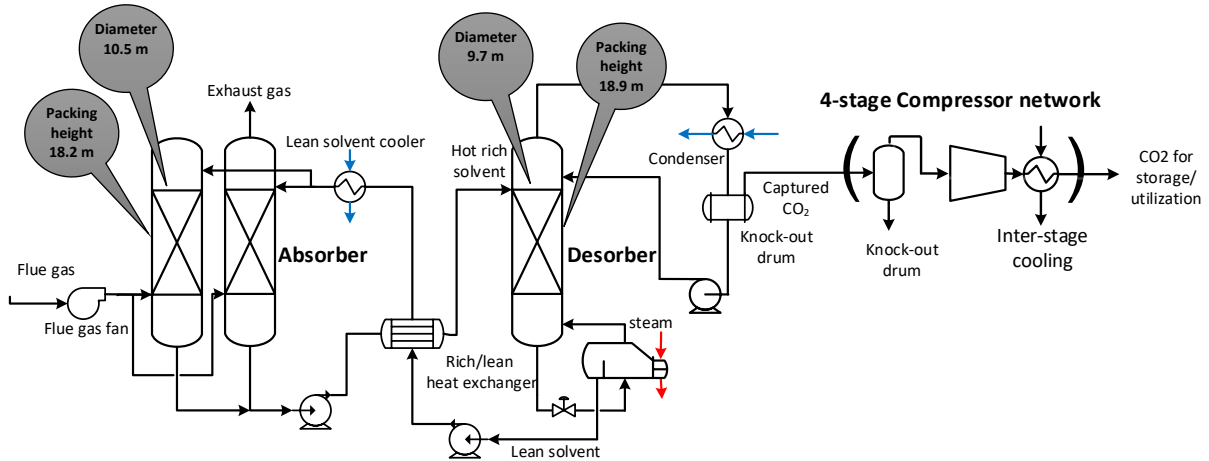
19 **Table 5:** The optimal operational and design variables with two objective functions.

	Objective	Scenario (i): Min. CAPEX	Scenario (ii): Min. levelized capture cost
	Blower (No. units), [flowrate/unit, m ³ /s], [power/unit, MW]	(2), [157.80], [3.02]	(2), [157.80], [3.02]
Technical values	Absorber		
	Number of columns	2	2
	Column diameter (m)	10.54	10.52
	Packing height (m)	13.20	18.20
	Packing type	Berl saddle 50 mm	Berl saddle 50 mm
	Demister size (m ²)	87.20	86.90
	Desorber		
	Number of columns	1	1
	Column diameter (m)	11.27	9.68
	Packing height (m)	14.60	18.90
	Packing type	Berl saddle 50 mm	Berl saddle 50 mm
	Demister area	99.70	73.60
	Condenser area (m ²)	2107.30	1859.90
	Reflux drum Diameter (m), height (m)	4.10, 20.97	3.92, 23.28
	Kettle reboiler area (m ²), and temperature approach (°C)	17023.11, 3.00	8738.76, 3.00
	Compressor and export train		
Number of compressor stages	4	4	
Pressure ratios	2.80	2.80	

Operational values	Compressor 1 capacity (MW)	5.54	5.55
	Compressor 2 capacity (MW)	5.54	5.55
	Compressor 3 capacity (MW)	5.54	5.55
	Compressor 4 capacity (MW)	5.54	5.55
	Knock-out drum 1 Diameter (m), height (m)	-	-
	Knock-out drum 2 Diameter (m), height (m)	2.76, 12.40	2.76, 12.40
	Knock-out drum 3 Diameter (m), height (m)	2.13, 7.08	2.13, 7.08
	Knock-out drum 4 Diameter (m), height (m)	1.62, 3.65	1.62, 3.65
	Inter-stage cooling HX 1 area (m ²)	-	-
	Inter-stage cooling HX 2 area (m ²)	191.32	191.32
	Inter-stage cooling HX 3 area (m ²)	190.25	190.25
	Inter-stage cooling HX 4 area (m ²)	200.76	200.7
	Final cooling HX (export CO ₂ to 50 °C) area (m ²)	239.13	239.13
	Lean/rich Heat-exchanger size (m ²), and temperature approach (°C)	17922.04, 7.00	17840.95, 7.00
	Lean cooler HX area (m ²)	992.77	981.88
	CO ₂ capture efficiency (%) of the PCC plant	90.00	90.00
	Absorber		
	Temperature of the inlet flue gas to absorber (°C)	50.00	50.00
	Temperature of the inlet solvent to absorber (°C)	56.62	56.89
	Temperature of the outlet solvent from absorber (°C)	63.00	63.00
Lean loading	0.25	0.30	
Rich loading	0.40	0.45	
Pressures of absorber columns (kPa)	1.05-1.10	1.02-1.10	
Pressure drop of absorber column(s) (kPa)	5.40	7.75	
L _{mol} /G _{mol}	6.83	6.83	
CO ₂ molar fraction of the emitted flue gas	0.01	0.01	
Desorber			
Temperature of the inlet solvent to desorber (°C)	107.64	107.68	
Temperature of the gas at desorber column exit (°C)	107.94	108.45	
Pressure of desorber columns (kPa)	1.64-1.70	1.62-1.70	
Pressure drop of desorber columns (kPa)	6.46	8.09	
CO ₂ molar fraction of the gas at the top of desorber	0.21	0.39	
L _{mol} /G _{mol}	11.22	19.85	
Reboiler temperature (°C)	127	127	
Reboiler duty (GJ/tonne-CO₂)	4.87	2.5	
Total CO₂ captured annually (million tonnes/y) (% of CO₂ generation)	1.69 (76.8)	1.69 (76.8)	
Economic values			
FOM (\$million/y)	23.33	23.71	
VOM (\$million/y)	40.24	29.58	
Total OPEX (\$million/y)	63.57	53.29	
Total capital investment (\$million)	312.36 (objective)	325.18	
Levelized capture cost (\$/tonne-CO₂)	58.07	52.82 (objective)	

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Rich loading	Lean loading	$T_{in}^{FG,Ab}$ (°C)	$T_{in}^{L,Abs}$ (°C)	$T_{out}^{FG,Ab}$ (°C)	$T_{out}^{R,Abs}$ (°C)	$y_{CO_2,out}$	D (m)	Z (m)	P_{out} (bar)	ΔP (kPa)	Q^L (lit/s)	L_{mol} (mol/s)	L_{mol}/G_{mol}	Q (MJ/kg-CO ₂)
Absorber (two units)														
0.45	0.30	50.0	56.9	57.0	63.0	0.01	10.5	18.2	1.1	7.75	956.2	42076.0	6.83	-
Desorber (one unit)														
0.45	0.30	107.7	124	108.5	118.0	0.39	9.7	18.9	1.7	8.09	1912.4	82158.2	19.85	2.5

5

6 **Figure 3:** Schematic of solvent-based PCC process configuration for a 300 MW coal-fired power plant with the list
7 of optimal design and operation values using minimum levelized capture cost as the objective function.

8

9 5. Conclusion

10 In this paper, we developed an equation-based methodology to address the uncertainties and
11 variabilities in the techno-economic assessment of integrated Sol-PCC processes. These
12 technologies are undoubtedly complex due to involving reactive separation. Hence, integrating
13 their physico-chemical models with techno-economic design optimisation algorithms adds further
14 to the project complexity. The method developed here is capable of evaluating feasible design
15 variables compatible with economic objectives. This decision-support tool consists of a
16 comprehensive techno-economic approach for finding the right design and operation values.
17 Techno-economic assessments conducted for a 300 MW coal-fired power plant integrated with a
18 Sol-PCC process used to showcase the interactivity between design and operational parameters for
19 two separate practice scopes of i) minimizing total capital investment, and ii) minimizing levelized
20 capture costs. Comparison of the examined scenarios showed that despite ~5% increase in the total
21 capital investment, the levelized capture costs reduced by ~9% within the case (ii) which
22 influences a significant difference in running expenditure of the plant over its lifecycle. These
23 results further imply that design and operation variables vary based on different techno-economic

1 objectives; while each case might be efficient on its own merits, most likely there is no single
2 optimal design exists which can deliver all different objectives at once.

3 **Glossary**

4 **Abbreviations**

5 CAPEX	capital expenditure (equivalent to total capital investment, TCI)
6 CEPCI	Chemical Engineering Plant Cost Index
7 FOB	free on board
8 MEA	monoethanolamine
9 OPEX	operational expenditure

10

11 **Notations**

12 C_{FCI}	fixed CAPEX
13 C_{BM}	bare module cost
14 C_{TM}	total module cost
15 C_{FCI}	fix capital investment
16 C_{FIT}	freight, insurance, and taxes
17 C_{TCT}	total capital investment (equivalent to CAPEX)
18 CF	annual capacity factor
19 CEP_y	cooling energy price at year y
20 FCF	fixed charge factor
21 FOM_y	fixed operation and maintenance costs during year y
22 EEP_y	pool price electricity at year y
23 HEP_y	heating energy price at year y
24 IRR	initial rate of return
25 LCOP	levelized cost of product
26 NPV	net present value
27 OX_y	OPEX during year y
28 r	discount rate
29 T	length of the planning horizon
30 TPY	number of periods (Δt) within a year
31 VOM_y	variable operation and maintenance costs during year y
32 Δt	time interval

33

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