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1	Techno-economic evaluation of post-combustion carbon capture based on chemical
2	absorption for the thermal cracking furnace in ethylene manufacturing
3	
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13	
14	Abstract:
15	As the core equipment of ethylene production plant, thermal cracking furnace generates a large amount of CO ₂
16	emissions. To reduce the CO ₂ emissions, post-combustion carbon capture based on monoethanolamine (MEA)
17	solvent is used to capture CO ₂ from the thermal cracking furnace. The computational fluid dynamics (CFD)
18	method was used to simulate the operation of a 60kt/a thermal cracking furnace to obtain the flow rate and
19	composition of the flue gas. A carbon capture plant model was carried out using Aspen Plus® and validated using
20	the Technology Centre Mongstad (TCM) pilot plant data. Scale-up of the capture plant model was carried out to
21	match the flue gas flow rate of the thermal cracking furnace. Two integration cases of the carbon capture plant and

the industrial thermal cracking unit were carried out. The results show that the excess heat of the gasoline fractionator can be used to provide heat for the carbon capture plant without affecting ethylene production. The economic evaluation was conducted based on the two case studies. Results show that the cost of CO_2 capture can be reduced from \$80.03/tonne without heat integration to \$70.41/tonne with heat integration of gasoline fractionators with carbon capture plant. When considering the impact of carbon credits on capture costs, the cost will be further reduced to \$50.41/tonne.

Keywords: Thermal cracking furnace; solvent-based post-combustion carbon capture; computational fluid dynamics; heat integration;
 economic evaluation

30

31 1. Introduction

32 1.1. Background

Due to the development of world industry, greenhouse gas emissions have been on the increase. CO_2 is the main greenhouse gas. In 2019, CO_2 emissions from fossil fuel burning reached 88.6% of the total greenhouse gas emissions [1]. Due to this, CO_2 emissions have attracted widespread attention. As the largest carbon emitter worldwide, China accounts for 28.8% of the world's total energy carbon emissions [2]. Therefore, it is urgent for China to reduce CO_2 emissions if it is to meet its target of achieving carbon neutrality by 2060.

Ethylene is one of the most extensively used chemical products in the world. In 2020, the worldwide ethylene production capacity reached 197 million tonnes/year [3]. China is the second-largest producer of ethylene in the world [4]. During the cracking of naphtha to ethylene, 1.73 tonnes of CO₂ is emitted for each tonne of ethylene produced [5]. The industrial thermal cracking furnace is the core equipment of the ethylene industry. It generates

Nomenclature		\vec{r}	position vector
a^{I} total interfacial area for mass transfer, m ²		R	universal gas constant
a_p	special area of the packing, m^2/m^3	R_i	net rate of production of species <i>i</i> by chemical reaction, kgmol/m ³ /s
a_v	total area of packing per unit volume, m^2/m^3	ŝ	direction vector
a_{ω}	surface area of wetted packing per unit volume of packing, m ² /m ³	<i>š</i> '	scattering direction vector
A	empirical constants, 4.0	S	slant height of a corrugation, m
A_t	cross-sectional area of the column, m ²	Т	temperature, °C
В	empirical constants, 0.5	Ui, Uj, Ul	velocity component in the <i>i</i> th, <i>j</i> th or <i>I</i> th direction, m/s
C_l	a dimensionless constant which depends on the packing size	Vcc	value of carbon credit, \$/tonne
$C_{l\varepsilon}$	standard $k - \varepsilon$ model constant, 1.44	$V_{G,fl}$	flooding velocity, m/s
$C_{2\varepsilon}$	standard k - ε model constant, 1.92	V_G	superficial gas velocity, m/s
C_c	CO ₂ capture cost, \$/tonne	x_i, x_j, x_l	coordinate direction in the <i>i</i> th, <i>j</i> th or <i>I</i> th direction,
C_{cc}	CO2 capture cost with carbon credit, \$/tonne	Y_P	mass fraction of any product species, P
C_{cm}	mass flow of the captured CO2, kg/s	Y_R	mass fraction of a particular reactant, R
$C_{j,r}$	molar concentration of species j in reaction r , kgmol/m ³	Greek lette	ers
d_p	effective diameter of packing, m	α	absorption coefficient, 1/m
D	diameter, m	A Rich	rich loading, mol CO ₂ /mol MEA
D_{Ag}	gas phase diffusivity of CO2	O Lean	lean loading, mol CO2/mol MEA
D_{Al}	liquid phase diffusivity of CO ₂	3	Ddissipation rate of turbulent kinetic energy, m^{2}/s^{3}
E_a	average annual capital cost, \$	θ	angel with horizontal of falling film or corrugation channel
F_p	packing factor, m ⁻¹	μ	viscosity of gas molecules, kg/m s
F_t	correction factor for total holdup due to efficitive wetted area	μg	gas dynamic viscosity (Pa s)
$g_{e\!f\!f}$	effective gravity, m/s ²	μı	Liquid dynamic viscosity (Pa s)
G	gas mass flow rate, kg/s	$\mu_s{}^l$	superficial velocity for the liquid, m/s
G_k	generation of turbulent kinetic energy, J/m ³ /s	ρ	gas density, kg/m ³
h_L	volumetric liquid holdup, m ³	$ ho_G$	gas density, kg/m ³
h_p	height of the packed section, m	$ ho_{L}, ho_{t}^{l}$	liquid density, kg/m ³
h_t	fractional holdup	Г	net effect of third bodies on the reaction rate
Ι	radiation intensity, J/m ² /s	v	kinematic viscosity, m ² /s
k	turbulent kinetic energy, m ² /s ²	$v'_{i,r}$	stoichiometric coefficient for reactant i ir reaction r
k _{f,r}	forward rate constant for reaction r	$v''_{i,r}$	stoichiometric coefficient for product i ir reaction r
kg	gas film mass transfer coefficient, m/s	$\eta'_{j,r}$	rate exponent for reactant species j in reaction r
kı	liquid film mass transfer coefficient, m/s	$\eta''_{j,r}$	rate exponent for product species j in reaction r

K_{eq}	equilibrium constant, -	σ	Stefan-Boltzmann constant, $5.672 \times 10^{-8} W/m^2 K^4$	
L	solvent mass flow rate, kg/s	σ_S	scattering coefficient, 1/m	
MMEA	molar mass of MEA, kg/kmol	σ_k	standard k - ε model constant, 1.0	
$M_{w,i}$	molecular weight of species <i>i</i> , kg/kgmol	$\sigma_{arepsilon}$	standard k - ε model constant, 1.3	
n	refractive index	φco2	percentage of CO ₂ captured	
Ν	number of chemical special in the system	Φ	phase function	
OM_a	average annual operating cost, \$	ω_{MEA}	MEA concentration, wt%	
ΔP_{fl}	flooding pressure drop, in H2O/ft	Ω'	solid angle	

large amounts of CO₂ with concentrations of 7-10 mol% in the flue gas. Therefore, a significant measure to reduce
 CO₂ emissions from the ethylene plants is to capture the CO₂ produced by the thermal cracking furnace.

46 Several approaches such as oxy-fuel combustion, pre-combustion, and post-combustion can be used for CO₂ 47 capture [6]. Post-combustion capture technology can be used to capture CO_2 from the flue gas released from large 48 stationary sources such as ethylene or power plants without making radical changes to existing plants. The 49 difficulties accompanying its implementation are lower compared to the other capture approaches. Although CO₂ 50 separation technologies such as adsorption, membrane and cryogenic separation are used for post-combustion 51 capture, The liquid absorption-based CO₂ capture is the most matured technology and the most widely used in 52 commercial applications. The MEA based post-combustion CO_2 capture also has high CO_2 capture efficiency 53 (>90%) and CO₂ high purity (>99%) [7]. The adsorption method has low energy consumption and high reliability, however, the adsorption capacity and selectivity of the adsorbent are low[8], particularly at low adsorption 54 55 pressures. The working environment of the membrane separation method is relatively strict, and it lacks stability 56 in a complex environment. Further to this, it is still in the research and development stage. Because MEA has high 57 absorption and separation characteristics for CO_2 , it is suitable for treating flue gas with low CO_2 partial pressure[9]. 58 Therefore, the post-combustion carbon capture (PCC) process with MEA solvent is adopted in this research.

59 1.2. Previous research

60 There are many studies on the simulation of the thermal cracking furnace. Zhou and Yang [10] established and 61 optimized a convection section calculation model of the ethylene cracking furnace, which can calculate the 62 temperature and heat duty of the convection section tube row. For the fire side, Hottel and Sarofim [11] presented 63 the zone method initially applied to simulate the radiative heat transfer process [12, 13]. In the past few decades, 64 because of the development of computational fluid dynamics (CFD) and the sharp rise in computing power, CFD 65 has become a favorite tool to simulate the thermal cracking furnace. Many CFD simulation studies have 66 investigated the flow, combustion, radiative heat transfer processes, and the NOx and CO emissions of the furnaces 67 [14-18]. For the process gas side, during the last decades, the research on the modeling of cracking reactions has 68 developed from molecular reaction models [19, 20] to free radical reaction models [21-24], which has made 69 tremendous progress. Findings from these studies, showed that CFD can simulate and correctly predict the detailed 70 concentration of each component of the flue gas from the furnace, including the concentration of CO produced by 71 partial incomplete combustion. This makes the concentration of the components obtained by CFD calculation to 72 be more accurate compared to other simulation tools such as Aspen Plus® which only considers rapid reaction and 73 is unable to simulate partial incomplete reaction. In this paper, the cracking furnace is simulated using the CFD 74 method. 75 Over the past few decades, many researchers have investigated solvent-based PCC technology. Zhang et al. [25] 76 developed a rigorous carbon capture plant model and validated the model using pilot plant data from the University 77 of Texas at Austin. Their results indicated that the high heat duty of the reboiler in the stripper could hinder the 78 widespread large-scale implementation of the liquid absorbent-based PCC process. To reduce the reboiler duty, 79 Freguia and Rochelle [26] conducted sensitivity analyses of the process variables in the CO₂ capture process to

80 analyze the impact of operating conditions on the steam requirement. Wang et al. [6] pointed out that proper process

81 integration could reduce the energy consumption of the PCC process. Tatarczuk et al. [27] used an inter-heated 82 stripper to modify the process of split flow. The pilot trials showed that while the CO_2 capture efficiency was 83 increased by 8-12%, the regeneration duty was reduced by 8-11%.

84 The integration of PCC with coal-fired power plants (CFPP) has been widely studied [28-31]. Liu et al. [32] 85 developed steady-state models for MEA-based PCC process and supercritical CFPP and set up different integration 86 cases to study the performance of thermal integration. Wei et al. [33] developed an integrated model of an industrial 87 fluid catalytic cracking unit and a PCC plant with MEA solvent. They investigated the effect of different heat 88 integration cases on energy consumption. Wu et al. [34] presented a coordinated control strategy for integrating 89 the combined-cycle gas turbine power plant with solvent-based PCC process and considered the influence of 90 disturbances. Chen et al. [35] accomplished an economic optimization for CFPP integrated with PCC process. The 91 overall plant revenue increased using the proposed scheduling. Xi et al. [36] presented a parametric optimization in terms of absorber/stripper size and operating conditions for solvent-based PCC process, where flexible operation 92 93 of the CFPP was considered.

For CO_2 capture from the ethylene industry, Weikl and Schmidt [37] presented a techno-economic study of CO_2 capture from the ethylene production plant. They compared the CO_2 capture performance between the oxyfuelcombustion and post-combustion process in the cracking furnace. Zhao et al.[38] selected ethylene as the research object to study the low-carbon roadmap of chemical production. The emission reduction potential of different ethylene production routes was compared. So far, no study has put forward a detailed integration model of a carbon capture plant with an ethylene production plant.

100 1.3. Motivation and novelty

101 Previous researches have focused on integrating solvent-based PCC plants with refineries and power plants to

reduce CO_2 emissions. However, considering the importance of ethylene manufacturing in the global economy and the accompanying huge carbon emissions, it is imperative to intensify efforts at cutting down CO_2 emissions from this process by integrating it with solvent-based PCC plant. As with the integration of solvent-based PCC plant with power plants and refineries, the energy consumption and the cost of the solvent-based PCC plant integrated with ethylene plant needs to be quantified. In addition to this, various integration schemes that could lead to a reduction in the energy consumption and cost of the process needs to be explored.

To this end, this study evaluates the energy consumption and costs of the solvent-based PCC plant integrated with an ethylene plant based on two integration methods namely No Heat Integration and Heat Integration of Gasoline Fractionators in thermal cracking. The no heat integration method involves the use of purchased lowpressure steam for solvent regeneration when the ethylene plant is integrated with the PCC plant. The heat integration of gasoline fractionator on the other hand involves the use of hot oil to generate the saturated steam that is used for solvent regeneration.

Additionally, economic evaluation of the two proposed integration methods is conducted to evaluate their capacity and cost to reduce CO₂ emissions.

116 The specific novelties of this work can be summarized as follow:

(1) Detailed scale-up of the solvent-based PCC plant based on a flue gas from a commercial thermal cracking
furnace is carried out for the first time.

(2) Assessments of the energy consumption of the solvent-based PCC plant integrated with an ethylene plant
 based on the no heat integration strategy and a novel heat integration of the gasoline fractionators in thermal
 cracking.

122 (3) A detailed economic assessment of the solvent-based PCC plant based on the two integration strategies is

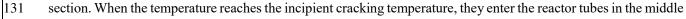
123 performed using the equipment costs, operating costs, and carbon credits as performance indicators.

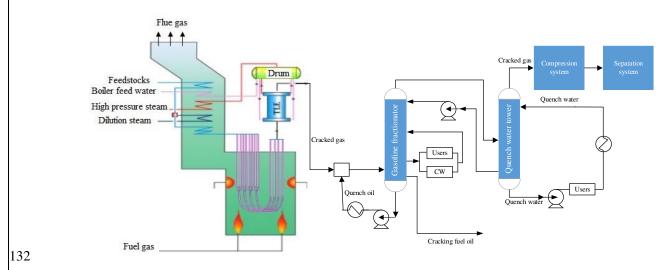
124 2. Process description and model development for the thermal cracking unit

125 2.1. Description of the thermal cracking unit

The thermal cracking unit processes various petroleum hydrocarbon feedstocks such as naphtha and propane into ethylene and propylene under high-temperature conditions. The thermal cracking furnace is the core of a thermal cracking unit. Fig.1 shows a typical industrial thermal cracking unit.

In a thermal cracking furnace, the convection section serves to recover the heat of flue gas, preheat, and vaporize the hydrocarbon feedstock. The hydrocarbon feedstock and dilution steam are heated in the tubes of the convection





133

Fig. 1. Typical arrangement of an industrial thermal cracking unit.

of the radiation section, where the cracking reactions occur. Fuel gas combustion in the radiation section outside the reactor tubes provides the heat required for the cracking reactions. The burners are arranged at the bottom of the firebox and/or on both sides of the side walls. Fuel gas and air enter the firebox through the burners. The released heat is mainly transferred to the medium in the reactor coils by radiation and convection [16]. The quench system includes steam drum and transfer line heat exchanger (TLE). After cracking quickly, the process gas leaves 139 the reactor coils to TLE and is rapidly cooled by heat exchange with the saturated water from the steam drum. The 140 cracking gas from TLE flows into the main pipe and is sent to the gasoline fractionator after oil quenching. In the 141 gasoline fractionator, quench oil is used to cool the cracking gas further and recover the heat of the cracking gas. 142 The heat of the pan oil in the middle of the gasoline fractionator is recovered by low-grade heat users and the 143 circulating water (CW). The users include heat exchangers and materials that need to be heated. After oil washing, 144 the cracked gas enters the quench water tower for further cooling. The quench water after heat exchange with the 145 cracked gas is used to provide heat to the low-level heat users. The cooled cracked gas enters the compression 146 system and separation system for further processing.

147 2.2. Model development for the thermal cracking unit

As described above, the thermal cracking unit consists mainly of the radiation and convection sections. Therefore, to develop an accurate model of the thermal cracking unit, detailed and complete models of the radiation section and the convection section are required. In the current work, the convection section and radiation section of a 60kt/a industrial thermal cracking furnace are simulated using the CFD method. More detailed and elaborate descriptions of the models and governing equations used for the convection section have been presented in Hu et al. [39] and those used for the radiation section are available in Hu et al. [16]. For the sake of brevity and clarity, they are briefly described in the following subsections.

155 2.2.1. Radiation section

A coupled simulation of the radiation section of the thermal cracking unit was carried out using the models for
the turbulence flow, combustion, radiative heat transfer and thermal cracking reaction processes. The turbulence
flow model is based on the standard k-ε two equations presented in Eq. (1) and Eq. (2) [16].

159
$$k - equation: \quad \frac{\partial}{\partial x_i} (\rho k U_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon \tag{1}$$

$$60 \qquad \varepsilon - equation: \quad \frac{\partial}{\partial x_i} (\rho k \varepsilon U_i) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_{\varepsilon}} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \frac{\varepsilon}{k} (C_{1\varepsilon} G_k - C_{2\varepsilon} \rho \varepsilon) \tag{2}$$

161 The fuel gas combustion is described using the finite-rate/eddy-dissipation model [16]. This model computes 162 the chemical source terms using the Arrhenius expressions. In other words, the net production of chemical species 163 *i* due to reaction can be expressed as the sum of the Arrhenius reaction sources over the reactions N_R as follows:

164
$$R_{i} = M_{w,i} \sum_{r=1}^{N_{R}} \hat{R}_{i,r}$$
(3)

165 $\hat{R}_{i,r}$ is the Arrhenius molar rate of creation/destruction of species *i* in reaction r. It is calculated using Eq. (4).

166

169

$$\widehat{R}_{i,r} = \Gamma(v_{i,r}^{"} - v_{i,r}^{'}) \left(k_{f,r} \prod_{j=1}^{N} [C_{j,r}]^{(\eta_{j,r}^{'} + \eta_{j,r}^{'})} \right)$$
(4)

167 The net rate of specie *i* production due to reaction $r(R_{i,r})$ is given by the limiting value of the two expressions 168 in Eq. (5) and Eq. (6).

$$R_{i,r} = \nu_{i,r}' M_{w,i} A \rho \frac{\varepsilon}{k} min\left(\frac{Y_R}{\nu_{R,r}' M_{w,j}}\right)$$
(5)

170
$$R_{i,r} = v_{i,r}' M_{w,i} A B \rho \frac{\varepsilon}{k} \frac{\sum p Y_p}{\sum_j^N v_{j,r}^{"} M_{w,j}}$$
(6)

171 The Discrete Ordinates (DO) model presented in Eq.(7) is used to calculate radiative heat transfer of the furnace172 [16]

173
$$\nabla(I(\vec{r},\vec{s})\vec{s}) + (\alpha + \sigma_s)I(\vec{r},\vec{s}) = \alpha n^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r},\vec{s}')\Phi(\vec{s}.\vec{s}')d\Omega'$$
(7)

The cracking process in the reactor coils of the radiation section is simulated using the one- dimensional reactormodel COILSIM1D [39, 40].

176 2.2.2. Convection section

The model of the convection section consists of the models of the convection chamber and the tubes. The
turbulence flow in the convection chamber is modeled using the k-ε models described in Eq. (1) and Eq. (2).
Likewise, the radiative heat transfer is modeled with the DO model described in Eq. (7). In the tubes of convection

180	section, the renormalization group (RNG) k- ϵ model and the volume of fluid (VOF) model [39] are used to simulate
181	the turbulence flow, and the liquid-vapor two phases flow, respectively. A summary of the geometry and operating
182	conditions of the thermal cracking unit is shown in Table 1, and a comparison between simulation results and
183	industrial data is shown in Table 2.

Table 1 Summary of the thermal cracking geometry and operating conditions

	Radiation section	n specifications			
Length (x direction) (m)	10.368	Length (y direction) (m)	3.55		
Length (z direction) (m)	14.27				
Number of bottom burners	24	Number of side burners	64		
	Convection chamb	per specifications			
Length (x direction) (m)	10.368	Length (y direction) (m)	2.26		
Length (z direction) (m)	13.385				
Number of tube sections	8	Number of total tubes	432		
Firing condition					
Fuel gas flow rate in bottom (kg/h)	2682	Fuel gas flow rate in side (kg/h)	1788		
Excess air (V%)	1.1				
	Fuel composi	tion (mol%)			
CH4	93.55	H_2	6.08		
C2H4	0.14	C ₂ H ₆	0.083		
C3H8	0.062	C4H10	0.065		
Cs	0.020				
	Material p	roperties			
Emissivity of the furnace wall	0.75	Emissivity of tube skin	0.85		

	Feedstock composition (wt%)		
n-Paraffins	30.16	i-Paraffins	41.56
Olefins	1.37	Naphthenes	16.13
Aromatics	10.78		

185 According to the relative error percentage between the simulation results and the industrial data, it can be seen
186 that the model accurately simulates the operation of the industrial ethylene cracking furnace. The simulated results

187 of the outlet temperature and flue gas compositions from the thermal cracking unit are reported in Table 3.

188

Table 2 Comparison between simulation results and industrial data

Simulation results	Industry data	Relative error %
1179	1191	1.01
0.50	0.50	0
62.56	62.70	0.22
41.02	40.14	2.19
32.19	33.86	4.93
	1179 0.50 62.56 41.02	1179 1191 0.50 0.50 62.56 62.70 41.02 40.14

189

Table 3 Simulated flue gas components and temperature

Variable	Value
Outlet temperature (°C)	115.50
Outlet pressure (kPa)	101.3026
Flow rate (kg/s)	24.72
Mole composition	
O ₂ (mol%)	3.87
H ₂ O (mol%)	15.60
CO ₂ (mol%)	7.69
N ₂ (mol%)	72.84

190 3. Process description and model development and model validation of the CO₂

191 capture plant

192 3.1. CO₂ capture plant description

193 The reference capture process used is the standard process shown in Fig.2 [26]. The flue gas entering the 194 abaorber from the cracking furnace contains components such as Oxygen, water, carbon dioxide and nitrogen (as 195 shown in Table 3). It is assumed that particulates, NOx and SOx have been removed from the flue gas prior to 196 entering the absorber. The temperature of the flue gas is cooled with heat exchanger before and after being 197 pressurized in the blower to aid the absorption process . The flue gas is cooled to between 30-40 °C before entering 198 the absorber. . The flue gas enters the bottom of the absorber while the lean solvent enters the absorber from the 199 top. In the countercurrent process, the CO_2 is absorbed, and the treated flue gas is discharged from the top of the 200 absorber. The treated flue gas contains an amount of water and MEA. After recovering the water and MEA from 201 the washing column, the pure gas is discharged into air. The rich solvent leaves the absorber from the bottom and 202 is pumped into the stripper for regeneration after being heated by a cross-heat exchanger. After regeneration, the 203 solvent is returned to the absorber from the bottom of the stripper. The high-purity CO₂ released from the top of 204 the stripper is compressed and stored.

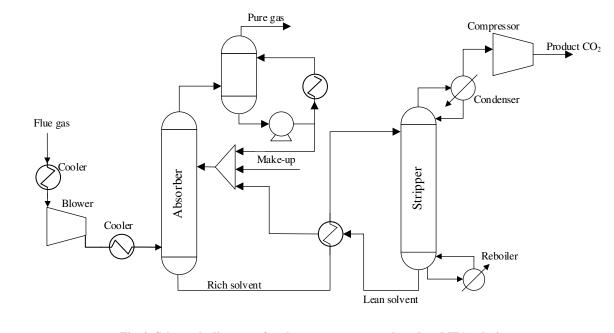


Fig. 2. Schematic diagram of carbon capture process based on MEA solution

207 3.2. Model development of CO_2 capture plant

The CO_2 capture model was developed using Aspen plus V11[®]. The RadFrac block was used to model the absorber and stripper. The liquid phase properties are calculated by the Electrolyte Non-Random-Two-Liquid (ELECNRTL) model and the gas phase properties are calculated with the Redlich-Kwong (RK) equation of state [41]. In this paper, the kinetic model proposed by Aboudehir et al. [42] and Aspentech [43] were used. The equilibrium and rate-controlled reactions describing the absorption of CO_2 by MEA are as follows:

The equilibrium reactions:

214

216

224

226

$$2H_20 \leftrightarrow H_30^+ + 0H^- \tag{8}$$

215
$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{2-}$$
 (9)

 $MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+$ (10)

217 The rate-controlled reactions:

- $218 \qquad \qquad CO_2 + OH^- \to HCO_3^- \tag{11}$
- $HCO_3^- \to CO_2 + OH^- \tag{12}$

220
$$MEA + CO_2 + H_2O \to MEACOO^- + H_3O^+$$
 (13)

221
$$MEACOO^- + H_3O^+ \to MEA + CO_2 + H_2O$$
 (14)

222 The equilibrium constant K_{eq} of reactions (8)-(10) was determined based on molar concentration using the

expression in Eq. (15):

$$\ln(K_{eq}) = A + \frac{B}{T} + C \cdot \ln(T) + D \cdot T$$
(15)

225 The kinetic expression of reactions (11)-(14) is:

$$r = kT^{n} \exp\left(-\frac{E}{RT}\right) \prod_{i=1}^{N} C_{i}^{a_{i}}$$
(16)

227 The values of the parameters for the equilibrium reactions and rate-controlled reactions are shown in Table 4.

228 For the absorber and stripper in the CO₂ capture model, the same packing type and size as the pilot plant are used.

229 The parameters of the pilot plant will be described in section 3.3.

230 The gas-film and liquid-film mass transfer coefficients are obtained from the widely used correlations provided231 by Onda et al.[44]:

232
$$\frac{k_g RT}{a_v D_{Ag}} = C_1 \left(\frac{G}{a_v \mu_g}\right)^{0.7} \left(\frac{\mu_g}{\rho_g D_{Ag}}\right)^{1/3} \left(a_v d_p\right)^{-2.0}$$
(17)

233

236

234
$$k_l \left(\frac{\rho_l}{\mu_l g}\right)^{1/3} = 0.0051 \left(\frac{L}{a_\omega \mu_l}\right)^{2/3} \left(\frac{\mu_l}{\rho_l D_{Al}}\right)^{-0.5} \left(a_\nu d_p\right)^{0.4}$$
(18)

$$a^{I} = a_{p}A_{t}h_{p} \tag{19}$$

237 The liquid holdup in structured packing is provided by Bravo et al.[46]:

$$h_L = h_t h_p A_t \tag{20}$$

239
$$h_t = \left(4\frac{F_t}{S}\right)^{2/3} \left(\frac{3\mu^L u_s^L}{\rho_t^L g_{eff}\varepsilon\sin\theta}\right)^{1/3}$$
(21)

240

Table 4 Coefficients of equilibrium constants and kinetic parameters [41]

ABCDEq.(8)132.889-13455.9-22.4770Eq.(9)216.049-12431.7-35.4820Eq.(10)-3.038-7008.360-0.00313KE (cal/mol)Eq.(11)4.32e+1313,249Eq.(12)2.38e+1729,451Eq.(13)9.77e+109855.8						
Eq.(9) 216.049 -12431.7 -35.482 0 Eq.(10) -3.038 -7008.36 0 -0.00313 K E (cal/mol) Eq.(11) 4.32e+13 13,249 Eq.(12) 2.38e+17 29,451		А	В	С	D	
Eq.(10) -3.038 -7008.36 0 -0.00313 K E (cal/mol) Eq.(11) 4.32e+13 13,249 Eq.(12) 2.38e+17 29,451	Eq.(8)	132.889	-13455.9	-22.477	0	
K E (cal/mol) Eq.(11) 4.32e+13 13,249 Eq.(12) 2.38e+17 29,451	Eq.(9)	216.049	-12431.7	-35.482	0	
Eq.(11) 4.32e+13 13,249 Eq.(12) 2.38e+17 29,451	Eq.(10)	-3.038	-7008.36	0	-0.00313	
Eq.(12) 2.38e+17 29,451		К			E (cal/mol)	
	Eq.(11)		4.32e+13	13,249		
Eq.(13) 9.77e+10 9855.8	Eq.(12)) 2.38e+17		29,451		
	Eq.(13)	(13) 9.77e+10			9855.8	

Eq.(14)	2.18e + 18	14138.4

241 3.3. Model validation of the CO₂ capture plant

The CO₂ Technology Centre Mongstad (TCM) located in Bergen is the largest test facility for CO₂ capture 242 243 technology globally. The TCM pilot plant is designed to be flexible and can test different configurations. The capture plant can treat flue gas from residual fluid catalytic crackers with a CO₂ content of approximately 13-14 244 vol%. It can also treat flue gas with 3.5vol% CO₂ from the combined heat and power (CHP) plant. When processing 245 246 the flue gas from the CHP plant, the primary equipment data of the TCM carbon capture plant is listed in Table 5. 247 The CHP plant has a flue gas flow rate of 60000 Sm³/h and can capture 80 tonnes of CO_2 per day[47]. There is an 248 absorption column equivalent to a diameter of 3 m for the CO₂ absorption into MEA solvent, and the packing 249 height is up to 24 m. The performance of the carbon capture plant was tested in 2014 and 2015 with 30wt% MEA 250 as solvent [48, 49]. Table 6 provides the main process information of the CO₂ capture plant during the averaged 251 base-case test period. The detailed gas composition data is from Øi and Fagerheim[50].

252

Table 5 Column specifications of the absorber and stripper in the TCM carbon capture pilot plant

	Absorber	Stripper
Geometry	Rectangular	Cylindrical
Cross-sectional area (m ²)	7.1	1.33
Packing type	Koch Glitsch Flexipac 2X	Koch Glitsch Flexipac 2X
Packing height (m)	24	8

The model is validated with the test data from the TCM pilot plant. The simulation results of CO_2 loading and capture level under two different feed conditions were compared with the data of pilot plants in 2014 and 2015. The CO_2 loading in MEA solvent and the percentage CO_2 capture level is calculated using Eq. (22) and Eq. (23) [33].

257
$$= \frac{[CO_2] \ loading \ (mol \ CO_2/mol \ MEA)}{[MEA] + [MCO_3^-] + [MEACOO^-]}$$
(22)

258
$$Capture \ level = \left(\frac{y_{CO_2in} - y_{CO_2out}}{y_{CO_2in}}\right) \times 100\%$$
(23)

Table 7 shows the comparison between the results of experimental measurement and simulation. From the percentage relative error (PRE) of the simulation results and experimental data, it can be obtained that the model

- can simulate the pilot plant well.
- 262

Table 6 Baseline process conditions from TCM CO₂ capture plant [48, 49]

Parameter	2014 Baseline data	2015 Baseline data
Flue gas flow rate (Sm ³ /h)	46970	59430
Lean solvent flow (kg/h)	54900	57434
L/G ratio (kg/kg)	1.17	0.97
Flue gas temperature (°C)	25	29.8
Flue gas pressure (bar)	1.063	1.01
CO ₂ (vol%)	3.7	3.7
O ₂ (vol%)	13.6	14.6
N ₂ (vol%)	79.75	78
H2O (vol%)	2.95	3.7
Lean solvent temperature (°C)	36.5	37
Lean solvent pressure (bar)	1.0313	1.0313
Lean MEA concentration (wt%)	30	31
Lean solvent density (kg/m ³)	1067	1073
Lean CO ₂ loading (mol CO ₂ /mol MEA)	0.23	0.2
Rich CO ₂ loading (mol CO ₂ /mol MEA)	0.48	0.48

TCM Reboiler duty (GJ/t CO ₂)	4.14	3.62	
TCM plant CO ₂ capture level (%)	93.5	83.4	

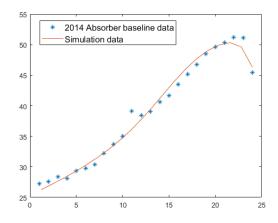
263	Fig.3. and Fig.4. represent the temperature profiles of the liquid phase in the absorber and stripper, respectively.
264	Since there is no temperature profile of the stripper in the 2014 baseline case, only the temperature profile of the
265	absorber is validated[48, 49]. The average deviation of the simulated temperature of the absorber in the 2014
266	baseline case is 0.2°C. The average deviation of the simulated temperature of the absorber and stripper in the 2015
267	baseline case is 4.4°C and 1.8°C, respectively. By comparison, the model prediction deviation of the 2015 baseline
268	case is higher than that of 2014. However, the deviation of the predicted temperature from the data of the TCM
269	pilot plant is still low. The comparison results show that the model can reasonably simulate the operation of
270	absorber and stripper.

271

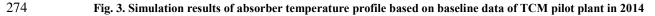
Table 7 Results from model validation

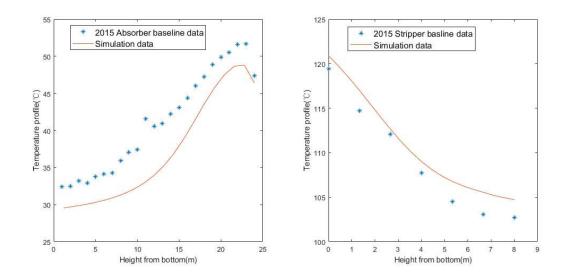
2014 Baseline	2015 Baseline
0.23	0.20
0.234	0.21
1.74	5.00
0.48	0.48
0.489	0.483
1.88	0.63
4.14	3.62
4.02	3.57
2.9	1.4
93.5	83.4
	0.23 0.234 1.74 0.48 0.489 1.88 4.14 4.02 2.9

CO ₂ capture level of the model (%)	90	80.2
PRE of CO ₂ capture level (%)	3.74	3.84

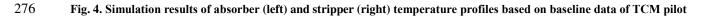


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277

plant in 2015

278 4. Integration of the thermal cracking unit with PCC process

- 279 4.1. Model scale-up
- 280 In order to integrate the thermal cracking unit with PCC process, the validated CO₂ capture plant model needs

to be scaled up to the size capable of handling the flue gas from the industrial thermal cracking unit. The scale-up

allows the lean solvent flow rate and the dimensions of the absorber and the stripper to be determined.

283 In commercial-scale PCC process research, the generalized Pressure Drop Correlation (GPDC) method is

usually used to scale up the validated pilot-scale model. The pressure drop of the column needs to be assumed

285 when using the GPDC method, which may result in an inaccurate prediction of the column diameter. Otitoju et

- al.[51] proposed a method to predict packed column diameter without assuming pressure drop. This new method
- 287 is adopted in this paper to estimate the diameter of the absorber and stripper.

288 Kister et al. [52] correlated the pressure drop when the initial overflow occurs in the packed columns with the

289 packing factor F_P , as shown in Eq.(24):

$$\Delta P_{fl} = 0.115 F_P^{0.7} \tag{24}$$

291 This equation is particularly suitable for packing with F_P between 10 and 60 ft⁻¹. When F_P exceeds

 $292 \quad 60 \text{ ft}^{-1}$, this equation should not be used.

293 The flooding velocity in Eq. (25) is calculated as follows[51]:

294

$$V_{G,fl} = 0.3048 \left[\left(\frac{\rho_G}{\rho_L - \rho_G} \right)^{-0.5} v^{-0.05} F_P^{-0.5} \left\{ A \left(log \left(\frac{L}{G} \sqrt{\frac{\rho_G}{\rho_L}} \right) \right)^2 + B \left(log \left(\frac{L}{G} \sqrt{\frac{\rho_G}{\rho_L}} \right) \right) + C \right\} \right]$$
(25)

Table 8 summarizes the equation that determines the parameters A, B, C in Eq.(25) and their application scope.

296

290

Table 8 Expressions for parameters in Eq.(25).

Parameters	Expression	Range of application	
А	$0.07 \ln(\Delta P_{\rm fl})$ -0.11	$0.5 \leq \Delta P_{fl} \leq 5.0 \text{ in}H_2O/\text{ft}$	
В	-0.25ln(ΔPfl)-0.89	$0.5 \leq \Delta P_{fl} \leq 1.0 \text{ inH}_2\text{O/ft}$	
В	-0.89	$1.0 \leq \Delta P_{fl} \leq 5.0 \text{ inH}_2\text{O/ft}$	
С	$0.12\ln(\Delta P_{\rm fl})+0.71$	$0.5 \leq \Delta P_{fl} \leq 5.0 \text{ inH}_2\text{O/ft}$	

297 These parameters are determined by the pressure drop of the flooding point, calculated by Eq.(24). Once the

298 physical quantities such as velocity, density, and viscosity of each phase are known, the flooding velocity in the 299 packed column can be calculated. It is generally assumed that the packed column is operated at 60-80% flooding 300 velocity [53]. Taking the intermediate value that the column is operated at 70% flooding velocity. The superficial 301 gas velocity is defined:

$$V_G = 0.7 V_{G,fl}$$
 (26)

At 70% flooding velocity, the column diameter is defined:

$$D = \sqrt{\frac{4G}{\pi V_G \rho_G}}$$
(27)

The flow rate and compositions of the flue gas are provided in Table 3. Assuming the absorption capacity is 0.2 mol $_{CO2}$ /mol $_{MEA}$, it can be estimated how much solvent is needed to fulfill 90% capture level in the absorber with 307 30 wt% MEA.

The flow rate of lean solvent is calculated using the expression shown in Eq. (28).

309

$$L_{lean} = \frac{G x_{CO_2} \varphi_{CO_2}}{(\alpha_{rich} - \alpha_{lean})} * \frac{M_{MEA}}{44 * \omega_{MEA}}$$
(28)

For the stripper, the total solvent flow rate equals the sum of the rich solvent flow rate and the reflux flow rate. The gas flow is equal to the boiling rate to maintain the CO_2 loading in the lean solvent at 0.23 mol $_{CO2}$ / mol $_{MEA}$. Thus, the solvent flow rate of the absorber and stripper are calculated to be 62.58 kg/s and 66.14 kg/s, respectively. The vapour flow rate is 7.6 kg/s.

The diameters of the absorber and stripper can be calculated using Eq.(25)-(27). The absorber and stripper are packed with Flexipac 2X with the F_P of 49.8 m⁻¹ (15.179 ft⁻¹) in the TCM pilot plant model. The estimated solvent flow rates and the packing factor in the previous calculation are input to Eq.(25) and Eq.(26). Thus, the superficial gas velocities of the absorber and stripper are calculated to be 1.55 m/s and 1.53 m/s, respectively. Therefore, according to Eq.(27), the diameters of the absorber and stripper are 3.80 m and 2.50 m, respectively. Table 9 shows 319 the calculated data and results of the absorber and the stripper.

	Absorber	Stainman
	Absorber	Stripper
Gas flow (kg/s)	24.72	7.60
Liquid flow (kg/s)	62.58	66.14
Packing type	Flexipac 2X	Flexipac 2X
$\rho_G(\mathrm{kg/m^3})$	1.42	1.02
$ ho_L (\mathrm{kg}/\mathrm{m}^3)$	1033.00	1038.00
F_p (ft ⁻¹)	15.18	15.18
$v (m^2/s)$	0.002	0.0007
A	-0.13	-0.13
В	-0.83	-0.83
C	0.68	0.68
Column diameter (m)	3.80	2.50
Packing height (m)	24.00	10.00

Table 9 Capture plant equipment design

4.2. Steady-state integration case studies 321

322 4.2.1. Case 1: No heat integration of PCC plant into the thermal cracking furnace

323 The temperature of the flue gas at the outlet of the thermal cracking furnace is relatively high, reaching 115.50°C. 324 Before entering the absorber, the flue gas is pretreated to improve the absorption efficiency. The flue gas 325 temperature is cooled to 37°C using cooling water. This is the same as the flue gas temperature in the TCM pilot 326 plant.

327	In the solvent-based carbon capture plant, while CO ₂ is absorbed into the MEA solvent, part of the water and
328	MEA will be released from the top of the absorber together with the treated flue gas. After the treated flue gas
329	passes through the wash column, part of the water and MEA are recovered. But the evaporated water and MEA
330	make the PCC process fail to achieve water/MEA balance. To compensate for the material loss, make-up water

331	and make-up MEA are added to the carbon capture plant. The flow rate of make-up water and make-up MEA is
332	calculated based on the flow rate of those components in the released treated gas. High concentrations of CO_2 can
333	be obtained from the top of the stripper. The captured CO_2 needs to be compressed and dehydrated to reach the
334	requirements for storage and transportation. Three-stage compression is used to compress the captured CO ₂ , and
335	an intermediate cooler and dehydration module are set. After compression, the pressure of CO_2 is 23 bar and the
336	temperature is 240.15K (-33°C). Fig.5 shows a closed-loop model of the carbon capture plant developed using
337	Aspen Plus [®] .
220	

The components and flow rate of the flue gas shown in Table 3 are used as input into the CO_2 capture model. The dimensions of absorber and stripper in Table 9 are also input into the model. The lean solvent used for the absorption contains a CO_2 loading of 0.23 mol $_{CO2}$ /mol $_{MEA}$ and an MEA concentration of 30 wt%. The specifications of the large-scale carbon capture plant are listed in Table 10.

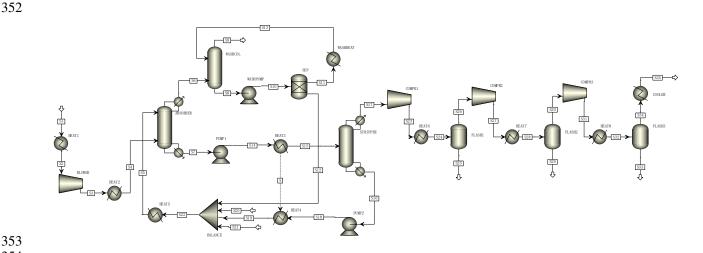
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Table 10 The specifications of the large-scale capture plant.

	Case 1
Flue gas flow rate (kg/s)	24.72
CO ₂ content of flue gas(mol%)	7.69
Capture level (%)	90.00
Mass flow rate of CO ₂ captured (kg/s)	2.71
L/G ratio (kg/kg)	2.53
Lean loading (mol CO ₂ /mol MEA)	0.23
Rich loading (mol CO2/mol MEA)	0.53
Reboiler duty (MW)	10.34
Specific reboiler duty (GJ/tonne CO2)	3.82

From the carbon capture plant result, it can be obtained that the reboiler duty is 10.34 MW when 90% capture is achieved. The specific reboiler duty of the carbon capture plant is 3.82 GJ/tonne CO₂. Usman et.al[54] studied the comparative potential of different power generation systems. For the natural gas combined cycle (NGCC)

- 346 power plant with exhaust gas recirculation, when the molar fraction of CO_2 in flue gas is 6.53%, the specific reboiler duty is 3.84GJ/tonne CO₂. This result is close to the specific reboiler duty in case 1. 347
- 348 The stripper reboiler is the largest energy consumer in the carbon capture plant [55]. Although medium and high-pressure steam are produced in an ethylene plant. These steam flows are fully allocated therefore leaving no 349 350 surplus steam to heat the reboiler. For the no heat integration case study, the heat required by the reboiler of the 351 PCC process is provided by a low-pressure steam of 130°C, which is purchased at the cost of 0.0019 \$/MJ.



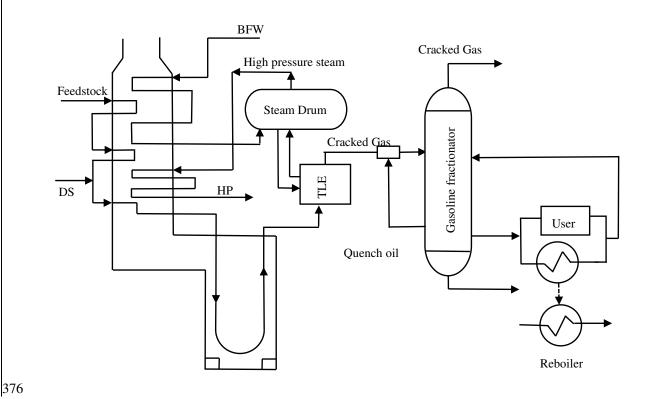
- 353 354
- 355

Fig. 5. The closed-loop model of case 1 developed using Aspen Plus®

356 4.2.2. Case 2: Heat integration of gasoline fractionator to the CO₂ capture process

357 In this case study, the excess heat of the gasoline fractionator is supplied to the CO_2 capture process for solvent 358 regeneration. The primary function of the gasoline fractionator is to cool the cracking gas and initially separate the 359 gasoline components, diesel components, and fuel oil in the cracking gas. After the cracking gas from TLE is cooled to about 220-230°C using quench oil in the quencher, it enters the gasoline fractionator. When naphtha is 360 361 used for cracking, the temperature at the bottom of the gasoline fractionator is 180-190°C [56]. The quench oil 362 from the bottom of the gasoline fractionator is sent to the dilution steam system as a heat source to generate dilution 363 steam. The heat of the cracking gas is recovered. The cracking gas is cooled by quench oil in the gasoline fractionator. When the temperature is reduced to 109°C, the cracking gas leaves from the top of gasoline fractionator and enters the quench water tower for further cooling. As shown in fig.1, (in the pan oil section of the gasoline fractionator), the pan oil is used for heating , including heat exchangers and the materials that need to be heated. The excess heat is recovered with circulating water. This excess heat can be used to heat the reboiler of the stripper.

To improve the energy recovery of the quench oil system, a stream of hot oil is extracted from the middle of gasoline fractionator to recover heat. A stream of 150°C hot oil is drawn off from the middle of the gasoline fractionator to heat the process water and generate saturated steam with a pressure of 2.7 bar. This saturated steam is used as a heat source for the stripper reboiler in the carbon capture plant. The hot oil is cooled and returned to the gasoline fractionator. The schematic diagram of heat integration of the gasoline fractionator in thermal cracking unit with the reboiler of the CO₂ capture process is shown in Fig. 6. The closed-loop model of case 2 developed using Aspen Plus[®] is shown in Fig. 7.



377 Fig.6. The heat integration of gasoline fractionator in thermal cracking unit with the reboiler of the

CO₂ capture process

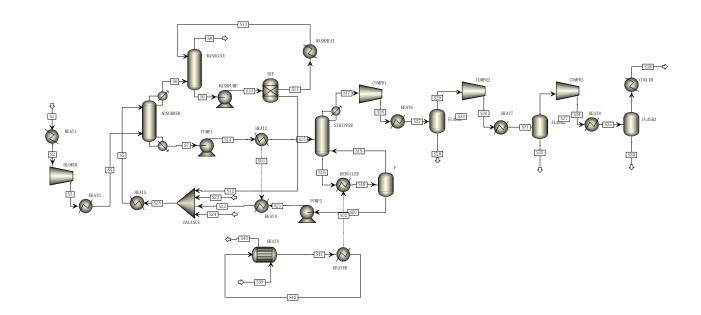






Fig.7. The closed-loop model of case 2 developed using Aspen Plus®

Distillate composition in the cracking gas stream is complex, including heavy cracking gasoline, cracking diesel, 382 383 and cracking fuel oil. Given this, the method of ordinary paraffin substitution is used to determine the feed components in the simulation. In the gasoline fractionator process, n-decane (NBP=174°C), n-tetradecane 384 (NBP=254°C), and n-docosane (NBP=355°C) are used to describe heavy cracking gasoline, cracking diesel, 385 386 cracking fuel oil, respectively. The physical property method selected is the Soave Redlich Kwong (SRK) equation 387 of state, which is used to simulate the stream of the gasoline fractionator. The performance of the CO_2 capture process using excess heat of the gasoline fractionator is shown in Table 11. The 150°C hot oil from the gasoline 388 389 fractionator is used to heat process water and cooled to 139°C before being returned to the gasoline fractionator. 390 In this case, the gasoline fractionator is integrated with the carbon capture process. The hot oil from the gasoline 391 fractionator can directly heat the circulating reboiler condensate into 2.7 bar saturated steam that is then used for

378

392 solvent regeneration. This approach reduced the energy consumption for solvent regeneration by Case 2 by about 393 3% compared to Case 1. This shows that by using the excess heat of the gasoline fractionator, the energy 394 consumption of the PCC process can be reduced. Case 2 also eliminates the cost of purchasing steam and has 395 potential to reduce the cost of condensate treating equipment.

3	Q	6
\mathcal{I}	,	v

Table 11 Performance of CO₂ capture process using the excess heat of gasoline fractionator

	Case 2
Capture level (%)	90.00
CO ₂ captured (kg/s)	2.71
Reboiler duty (MW)	10.04
Specific duty (GJ/tonne CO ₂)	3.70
Saturated steam flow rate (kg/s)	4.58
Temperature of hot oil before heating water (°C)	150
Temperature of hot oil after heating water (°C)	139

397 5. Economic analysis

The economic analysis of the PCC process was using the Aspen Capital Cost Estimator (ACCE) V11 and the detailed process flowsheet in Fig.5 and Fig.7. The ACCE V11 is used to calculate the equipment cost, which included the absorber, the stripper, heat exchangers, and pumps (based on 2018 USD). Li et al.[55] compared the detailed cost of the MEA-based carbon capture plant with the equipment cost generated by ACCE, and the difference in the total equipment cost was only 5.2%. Therefore, the ACCE can reasonably estimate the equipment cost of carbon capture plants.

404 The cost of a CO_2 capture plant includes capital expenditure (CAPEX) and operation expenditure (OPEX). The 405 CAPEX is calculated from the direct cost of equipment at the PCC plant. The OPEX consists of fixed O&M cost 406 and variable O&M cost. It is assumed that the fixed O&M cost accounts for 3.5% of the CAPEX of the PCC plant, 407 which is composed of total maintenance cost and labor cost [55]. The variable O&M cost is caused by energy and 408 chemical consumption during operation, including electricity cost, cooling water cost, steam cost, make-up water
409 cost, and make-up MEA cost.

For the two cases, the simulated closed-loop model of the PCC process in Aspen Plus are exported to the ACCE 410 411 platform. The model blocks are then correctly mapped so that the appropriate costing models are applied to 412 calculate the direct equipment cost of the PCC plant. The calculated results by ACCE for the direct equipment cost 413 of the carbon capture plant based on the two cases considered in this study are listed in Table 12. From the direct 414 equipment cost, it can be found that the stripper cost, cross-heat exchanger cost and heat exchanger cost of case 2 are different from case 1. In case 2, the stripper reboiler is heated by saturated steam from the hot oil in the gasoline 415 416 fractionator. Therefore, case 2 requires a cross-heat exchanger and heat exchanger to heat the reboiler. The resulted in a higher direct equipment cost for case 2 compared to case 1. 417

 Table 12 Direct equipment cost of the large-scale PCC plant of case 1 and case 2

Equipment	Case 1 (M\$)	Case 2 (M\$)
Absorber	0.42	0.42
Blower	5.74	5.74
Compressors	2.46	2.46
Lean solvent pump	0.01	0.01
Rich solvent pump	0.15	0.15
Wash pump	0.005	0.005
Wash column	0.33	0.33
Wash heat exchanger	0.03	0.03
Separator	0.02	0.02
Stripper	0.86	0.82
HeatX	N/A	0.13
Heaters	0.27	0.29
Flashes	0.05	0.05
Total direct cost (TDC)	10.345	10.455

419 It is assumed that the life cycle for the carbon capture plant is 20 years, and the operating time is 8000 hours per

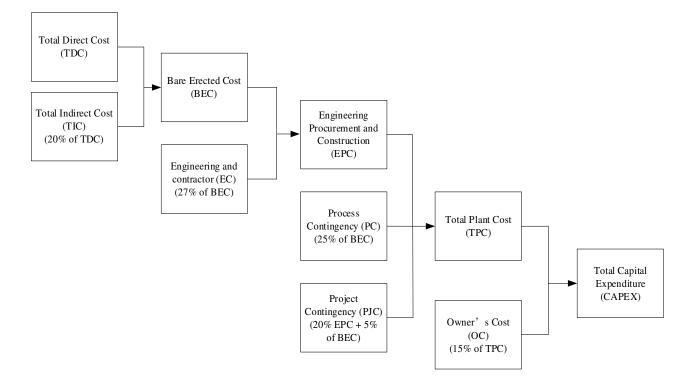
- 420 year. The prices of consumables and utility units in the carbon capture process are provided in Table 13. The factory
- 421 is set up in East China, and the price is from East China[57].
- The approach for determining the capital expenditures (CAPEX) is shown in Fig.8. Otitoju et al.[58] has
 published the indices used for the CAPEX approach. The CAPEX of the large-scale PCC plant of case 1 and case
 2 are provided in Table 14.

425 The total annual cost of a PCC plant is equal to the sum of the annual capital cost (ACC) and the annual operating

426 costs. The ACC can be obtained by annualizing CAPEX. The formula for calculation is as follows:

427
$$ACC = CAPEX\left(\frac{i(1+i)^n}{(1+i)^n - 1}\right)$$
(29)

428 where *n* is the equipment life, n=20; *i* is the interest rate, i=10%.



429

430

Fig.8. The capital expenditures (CAPEX) approach for CO₂ capture plant[58]

431

Table 13 The price of consumables and energy

Description	Value
Electricity (\$/kWh)	0.0762
Low-pressure Steam (\$/MJ)	0.0019
MEA make-up (\$/tonne)	1512.4
Water make-up (\$/tonne)	0.62
Cooling water (\$/tonne)	0.23
Refrigerant - Propane (\$/tonne)	42347.2
Operating time per year (hour)	8000
Exchange rate in 2018 (\$/yuan)	0.15124

432 The CO₂ capture cost is an important economic indicator to evaluate the cost of the PCC process. Without

433 considering the transportation and storage costs of CO_2 , the calculation equation is shown in Eq.(30):

$$C_c = \frac{E_a + OM_a}{C_{cm}}$$
(30)

Table 14 CAPEX of the large-scale PCC plant of case 1 and case 2

	Case 1 (M\$)	Case 2 (M\$)
Total direct cost (TDC)	10.345	10.455
Total indirect cost (TIC)	2.069	2.091
Bare erected cost (BEC)	12.414	12.546
Engineering and contractor (EC)	3.352	3.387
Engineering procurement and construction (EPC)	15.766	15.933
Process contingency (PC)	3.104	3.137
Project contingency (PJC)	3.774	3.814
Total plant cost (TPC)	22.644	22.884
Owner's cost (OC)	3.397	3.433
Total capital expenditure (CAPEX)	26.041	26.317

436 Carbon credit is a permit that allows a company to emit a certain amount of CO₂ or other greenhouse gases.

Industries that cannot reduce CO_2 emissions can purchase credits from other sectors that can reduce more CO_2 emissions than required through carbon credit trading [59]. Recently, the United States and other countries announced carbon credit for the capture and storage of CO_2 . The range of carbon credit obtained from Mokheimer et al. [60] is from 11.7 to 50 USD/t CO_2 . In this paper, 20 USD/t CO_2 is chosen to observe the impact of carbon credit on the cost of carbon capture. When considering carbon credits, the cost of carbon capture is calculated as shown in Eq.(31):

443
$$C_{cc} = \frac{E_a + OM_a}{C_{cm}} - V_{CC}$$
(31)

444 A summary of the economic benefits of the carbon capture plant is listed in Table 15. Among the variable O&M 445 costs, the cost of make-up water is much lower than other consumables. This is because the water and the MEA in 446 the absorbed flue gas are recovered before the flue gas is discharged, as shown in Fig 2. This operation can reduce 447 the amount of make-up water and make-up MEA. At the same time, the price of make-up water is much lower 448 than the price of make-up MEA, thus the cost of make-up water is lower than other consumables. In case 2, the 449 steam required for reboiler heating is generated from the hot oil of the gasoline fractionator. Therefore, the low 450 pressure steam cost of case 2 is lower than that of case 1. The CO_2 capture cost is \$80.03/tonne with purchased 451 steam for heating, while the capture cost is \$70.41/tonne using excess heat of the gasoline fractionator. When 452 considering carbon credits, the CO_2 capture cost of the two integration schemes is 60.03/tonne and 50.41/tonne, 453 respectively.

Table 15 Summary of the economic performance of the large-scale PCC plant of case 1 and case 2

Description		Case 1	Case 2
CAPEX (M\$)		26.041	26.317
ACC (M\$/yr)		3.059	3.091
Fixed O&M cost (M\$/yr)		0.911	0.921
Variable O&M cost	Electricity (M\$/yr)	0.665	0.643

	Cooling water(M\$/yr)	0.464	0.276	
	Low-pressure steam (M\$/yr)	1.139	0.548	
	Refrigerant - Propane(M\$/yr)	0.001	0.001	
	Water make-up (\$/yr)	223.62	93.45	
	MEA make-up (\$/yr)	62.55	59.21	
Total annual cost (M\$/	yr)	6.24	5.49	
CO ₂ capture cost (\$/top	nne CO ₂)	80.03	70.41	
CO ₂ capture cost with	carbon credit (\$/tonne CO ₂)	60.03	50.41	

Kangkang Li et al. [55] studied the technical and economic performance of the post-combustion capture process based on MEA and compared the carbon capture cost with other publications. The carbon capture cost of the published study ranges from 62-95.2 \$/tonne CO₂. By comparing the cost of two carbon capture cases, the cost of the basic integration of PCC into the thermal cracking furnace is within a reasonable range. Furthermore, when the excess heat of the gasoline fractionator is used to heat the reboiler, the CO₂ capture cost can be significantly reduced.

461 **6.** Conclusions

A detailed technical and economic evaluation of a solvent-based PCC plant for a commercial ethylene plant have been performed in this paper based on two integration strategies-namely no heat integration and heat integration of gasoline fractionator. The composition and flow rate of the flue gas in the thermal cracking furnace are obtained by CFD method. The steady-state model of the PCC plant based on MEA solvent is developed and validated with experimental data collected in 2014 and 2015 at the TCM pilot plant. Furthermore, the PCC plant model is scaled up to treat flue gas from a commercial scale thermal cracking unit.

468 The reboiler of the stripper consumes a significant quantity of energy for solvent regeneration in the carbon 469 capture process. To quantify and reduce this energy consumption, we conduct two integration cases to compare 470 the impact of different heat sources on the energy consumption and cost of CO_2 capture. In the first case, the heat to the reboiler is supplied by steam purchased from a nearby industrial zone. In the second case, the hot oil of the gasoline fractionator is used to heat the circulating condensate into saturated steam. Technical and economic analysis show that heat integration of gasoline fractionators in the thermal cracking unit with the CO_2 capture process could reduce the energy consumption and the capture cost. This study has great potential to inspire researchers worldwide towards research on carbon capture for petrochemical industry.

476

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483 Appendix

484 Table A1

485 Results for material and energy flow flowrates in each stream of Fig. 5.

	S 1	S2	S3	S4	S5	S 6	S 7	S 8	S9	S10	S1 1	S12	S1 3	S1 4	S1 5	S1 6	S17	S18	S1 9
T (K)	388 .65	33 8.2	34 8.8	30 3.2	31 0.2	33 2.0	308 .4	328 .4	32 6.9	328 .4	32 8.4	328 .4	31 3	29 9.2	39 5.9	32 2.2	310. 2	310 .2	32 2.3
P (bar)	1.0 1	1.0 1	1.1	1.1	1.0 3	1.0 1	1.0 1	0.9 2	0.9	1.1	1.1	1.1	1.9	15 0	1.1	1.1	1.03	1.0 3	1.0 3
Vap. Frac	1	1	1	1	0	1	0	0	1	0	0	0	1	0	0	0	0	0	0
Mole Flow (kmol/ s)	0.8 9	0.8 9	0.8 9	0.8 9	1.6 9	0.8 3	1.6 9	0.1 7	0.8 2	0.1 7	0.1 7	0.0 06	0.0 64	0.0 64	1.6 9	1.6 9	1.1e -5	0.0 004	1.0 9
Mass Flow (kg/s)	24. 72	24. 72	24. 72	24. 72	41. 32	22. 09	43. 95	3.1 1	21. 98	3.1 1	3	0.1 1	2.7 5	2.7 5	41. 20	41. 20	0.00 065	0.0 068	41 30
Volum e Flow (cum/s)	28. 31	24. 62	23. 38	20. 86	0.0 39	22. 89	0.0 36	0.0 032	24. 87	0.0 032	0.0 03	0.0 002	0.8 7	0.0 04	0.0 42	0.0 39	6.4e -7	6.8 e-6	0. 4
Enth (Gcal/h)	- 47. 8	- 51. 0	- 50. 7	- 55. 9	- 43 2.2	- 31. 20	- 456 .9	- 42. 01	- 30. 1	- 42. 01	- 40. 6	- 1.4 1	- 21. 3	- 22. 0	- 42 0.1	- 42 9.2	- 0.00 2	- 0.0 92	- 43 0.
Mass Flov	v (kg/s)																		
MEA	0	0	0	0	6.7 1	0.0 1	0.6 9	0.0 023	0	0.0 023	0	0.0 003	0	0	6.7 9	6.7 1	0.00 065	0	6. 1
H2O	2.4 96	2.4 96	2.4 96	2.4 96	26. 80	2.5 6	25. 95	3.1 0	2.4 6	3.1 0	3	0.0 98	0.0 45	0.0 45	26. 69	26. 70	0	0.0 068	26 81
CO2	3.0 05	3.0 05	3.0 05	3.0 05	0	0.3 0	0.0 033	0	0.2 9	0	0	0	2.7 07	2.7 07	0	0	0	0	0
H3O+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

486

487 Table A2

OH-

HCO3-

CO3-2

MEAH

MEAC

00-

N2

O2

 $^+$

18.

1.1

18.

1.1

18.

1.1

18.

1.1

0.0

0.0

2.9

4.7

18.

1.1

1.5

1.2

7.9

6.5

0.0

0.0

0.0

18.

1.1

0.0

0.0

0.0

0.0

0.0

0.0

0.0

0.0

0.0

2.9

4.7

0.0

0.0

2.9

4.7

0.0

0.0

2.9

4.7

488 Results for mass fraction and mole flowrate of components in each stream of Fig.5.

	S1	S2	S3	S4	S5	S6	S7	S 8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19
Mass Frac	tion																		
MEA	0	0	0	0	0.162	0.0004	0.016	0.0007	0	0.000 7	0	0.003	0	0	0.16	0.16	1	0	0.16
H2O	0.101	0.101	0.101	0.101	0.649	0.116	0.59	0.995	0.11	0.995	1	0.88	0.01 7	0.01 7	0.65	0.65	0	1	0.65
CO2	0.122	0.122	0.122	0.122	0	0.014	0	0	0.014	0	0	0	0.98 3	0.98 3	0	0	0	0	0
H3O+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
НСО3-	0	0	0	0	0.0004	0	0.034	0.0014	0	0.001 4	0	0.02	0	0	0.002	0.000 5	0	0	0.000 5
CO3-2	0	0	0	0	0.002	0	0.028	0	0	0	0	0.000 8	0	0	0.000 1	0.001 3	0	0	0.001
MEAH+	0	0	0	0	0.072	0	0.18	0.0019	0	0.002	0	0.05	0	0	0.08	0.072	0	0	0.072

MEACO O-	0	0	0	0	0.114	0	0.15	0.000	7 0		0.000 7	0	0.05	0	0	0.1	1	0.12	0	0		0.12
N2	0.733	0.733	0.733	0.733	0	0.820	0	0	0.8	25	0	0	0	0	0	0	(0	0	0		0
O2	0.044	0.044	0.044	0.044	0	0.050	0	0	0.0	50	0	0	0	0	0	0	(0	0	0		0
Mole Flow	v (kmol/	s)																				
MEA	0	0	0	0	0.110	0.000 5	1 0.006 6	5 00000 3	0.		0	0	0	0	0	0.1	1	0.11	1.1e -5	0		0.11
H2O	0.139	0.139	0.139	0.139	1.488	0.142	0.85	0.006	0.1	4	0.17	0.1 7	0.005	0.00 3	0.00 3	1.4	8	1.48	0	0.0 4	000	1.49
CO2	0.068 3	0.068 3	0.068 3	0.068 3	0	0.006	8 0	0	0.0 8	06	0	0	0	0.06 2	0.06 2	0	(0	0	0		0
H3O+	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	(0	0	0		0
OH-	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	(0	0	0		0
НСО3-	0	0	0	0	0.0002 8	0	0.015	5 0	0		0	0	0	0	0	0.0		0.000 4	0	0		0.000 4
CO3-2	0	0	0	0	0.0013	0	0.012	2 0	0		0	0	0	0	0	0		0.000 9	0	0		0.000 9
MEAH+	0	0	0	0	0.048	0	0.076	6 0.000	0 0		0	0	0	0	0	0.0	47 (0.048	0	0		0.048
MEACO O-	0	0	0	0	0.045	0	0.037	0.000 5	0 0		0	0	0	0	0	0.0	45	0.046	0	0		0.046
N2	0.647	0.647	0.647	0.647	0	0.647	0	0	0.6	5	0	0	0	0	0	0	(0	0	0		0
02	0.034 4	0.034 4	0.034 4	0.034 4	0	0.034	4 0	0	0.0	34	0	0	0	0	0	0		0	0	0		0
Table A3 Results for r	4 4 4 4																					
	S1	S2 S3	S4	S5	S6 S	57 S	8 S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S19	S2	0 9	521	S22	S23
				331.	308. 3	331. 3	31. 306	. 377.	392.	313	299.	394.	394.	394.	394.	320.	310.2	2 31		320.	403.	403

P (bar)	1.01	1.1	1.1	1.03	1.11	1.01	1.11	1.11	2.4	2.4	1.9	1.9	150	1.9	1.9	1.9	1.1	1.1	1.1	1.1	1.1	2.7	2.7
Vap. Frac	1	1	1	0	1	0	1	0	0	0.00 9	0	1	0	0.12	1	0	0	0	0	0	0	0	1
Mole Flow (kmol/s)	0.89	0.89	0.89	1.69	0.82	1.69	0.82	0.00 6	1.69	1.69	1.92	0.06 4	0.06 4	1.92	0.24	1.69	1.69	1.69	1.1e- 05	0.00 04	1.69	0.25	0.25
Mass Flow (kg/s)	24.7 2	24.7 2	24.7 2	41.3 2	21.9 7	43.9 5	21.9 7	0.12	43.9 5	43.9 5	45.6 3	2.75	2.75	45.6 3	4.44	41.2	41.2	41.2	0.000 65	0.00 7	41.3	4.58	4.58
Volume Flow (cum/s)	24.6 2	23.3 8	20.8 6	0.03 9	20.3 7	0.03 6	20.3 7	0.00 01	0.03 8	0.24	0.04 6	0.87	0.00 4	4.05	4.0	0.04 2	0.04 2	0.03 9	6.4e- 07	6.97 e-06	0.03 9	0.00 5	3.11
Enth (Gcal/h)	- 51.0	- 50.7	- 55.9	- 432. 2	- 29.9	- 456. 9	- 29.9 4	-1.49	- 456. 9	- 447. 8	- 478. 0	- 21.3	- 22.0	- 469. 4	- 49.1	- 420. 3	- 420. 3	- 429. 3	- 0.002	- 0.09 4	- 430. 9	- 60.8	- 52.2
Mass Flo	w (kg/s))																					
MEA	0	0	0	6.71	0	0.69	0	0.00 2	0.16	0.99	6.54	0	0	6.83	0.04 5	6.79	6.79	6.71	0.000 65	0	6.72	0	0
H2O	2.49 6	2.49 6	2.49 6	26.8 0	2.46	25.9 5	2.46	0.10 6	26.4	26.5	30.6 4	0.04 2	0.04 2	30.8	4.11	26.6 9	26.6 9	26.6 9	0	0.00 7	26.8 1	4.58	4.58
CO2	3.00 5	3.00 5	3.00 5	0	0.30	0.00 33	0.30	0	0	0.39	0.00 5	2.70 8	2.70 8	0.28	0.28	0	0	0	0	0	0	0	0
H3O+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
НСО3-	0	0	0	0.01 7	0	1.50	0	0	0.98	0.72 3	0.57	0	0	0.09	0	0.09 4	0.09 4	0.02	0	0	0.02	0	0
CO3-2	0	0	0	0.07 9	0	1.23	0	0	0.24	0.02 3	0.08	0	0	0	0	0.00 4	0.00 4	0.06	0	0	0.06	0	0
MEAH+	0	0	0	2.99 5	0	7.99	0	0.00 4	6.97	6.20	3.38	0	0	2.91	0	2.91	2.91	2.97	0	0	2.97	0	0
MEACO O-	0	0	0	4.71 4	0	6.59	0	0.00 5	9.19	9.07	4.42	0	0	4.71	0	4.71	4.71	4.74	0	0	4.75	0	0
N2	18.1	18.1	18.1	0	18.1	0	18.1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

O2	1.10	1.10	1.10	0	1.10	0	1.10	0 0	0	0	0	0	0	0	0	0	0	0		0	0	0
Table A4 Results for	r mass fr	action a	nd mole	e flowrate	e of con	nponents	s in eacl	n stream o	of Fig.7.													
	S 1	S2	S3	S4	S5	S 6	S 7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18	S1 9	S20	S21	5
Mass Fr	action																					
MEA	0	0	0	0.162	0	0.01 6	0	0.016	0.00 4	0.02 3	0.14	0	0	0.1 5	0.01	0.16	0.16	0.16	1	0	0.16	(
H2O	0.10 1	0.10 1	0.10 1	0.649	0.11 2	0.59	0.11	0.903	0.6	0.6	0.67	0.0 17	0.0 17	0.6 7	0.93	0.65	0.65	0.65	0	1	0.65	1
CO2	0.12 2	0.12 2	0.12 2	0	0.01 4	0	0.01 4	0	0	0.00 9	0.00 01	0.9 83	0.9 83	0.0 08	0.06	0	0	0	0	0	0	0
H3O+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	C
OH-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	(
НСО3-	0	0	0	0.000 4	0	0.03 4	0	0	0.02 2	0.01 6	0.01 4	0	0	0.0 02	0	0.00 2	0.00 2	0.00 05	0	0	0.00 05	C
CO3-2	0	0	0	0.002	0	0.02 8	0	0	0.00 4	0.00 2	0.00 2	0	0	0	0	0.00 01	0.00 01	0.00 14	0	0	0.00 1	C
MEAH +	0	0	0	0.072	0	0.18	0	0.032	0.16	0.14	0.07 4	0	0	0.0 7	0	0.08	0.08	0.07	0	0	0.08	C
MEAC OO-	0	0	0	0.114	0	0.15	0	0.044	0.21	0.21	0.1	0	0	0.1	0	0.11	0.11	0.11	0	0	0.11	C
N2	0.73 3	0.73 3	0.73 3	0	0.82 5	0	0.82 5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
02	0.04 4	0.04 4	0.04 4	0	0.05 0	0	0.05 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flo	ow (kmo	l/s)																				

H2O	0.13 9	0.13 9	0.13 9	1.488	0.14 2	0.85	0.14	0.006	1.47	1.47	1.7	0.0 03	0.0 03	1.7 1	0.23	1.48	1.48	1.48	0	0.00 04	1.49	0. 25	0. 25
CO2	0.06 83	0.06 83	0.06 83	0	0.00 68	0	0.00 68	0	0	0.00 9	0.00 01	0.0 62	0.0 62	0.0 06	0.00 6	0	0	0	0	0	0	0	0
H3O+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
НСО3-	0	0	0	0.000 28	0	0.01 5	0	0	0.01 6	0.01 2	0.00 9	0	0	0.0 02	0	0.00 2	0.00 2	0.00 03	0	0	0.00 03	0	0
CO3-2	0	0	0	0.001 3	0	0.01 2	0	0	0.00 4	0.00 04	0.00 1	0	0	0	0	0	0	0	0	0	0.00 1	0	0
MEAH +	0	0	0	0.048	0	0.07 6	0	0.000 06	0.11	0.1	0.05	0	0	0.0 47	0	0.04 7	0.04 7	0.04 8	0	0	0.04 8	0	0
MEAC OO-	0	0	0	0.045	0	0.03 7	0	0.000 05	0.08 8	0.09	0.04	0	0	0.0 45	0	0.04 5	0.04 5	0.04 6	0	0	0.04 6	0	0
N2	0.64 7	0.64 7	0.64 7	0	0.64 7	0	0.65	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
02	0.03 44	0.03 44	0.03 44	0	0.34 4	0	0.03 4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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