

Optimisation of Coal-Bed Methane (CBM) Gas Purification Process

Advanced Modeling Forum

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Daeho Ko



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1. Overview

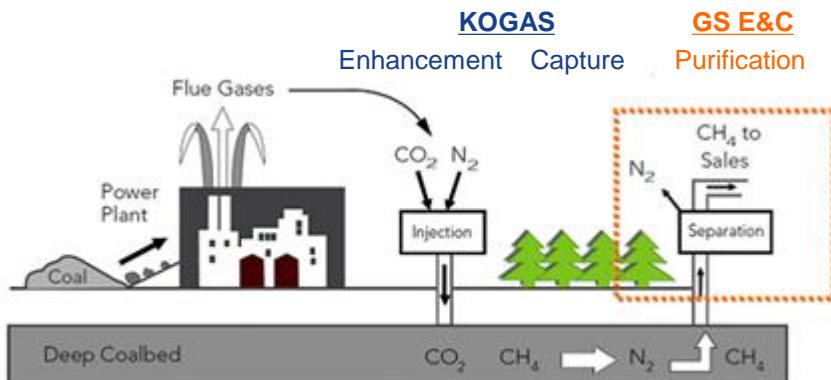
Overview of CBM purification project: Government R&D project in Korea

R&D Project (KEIT of MOTIE in Korea)

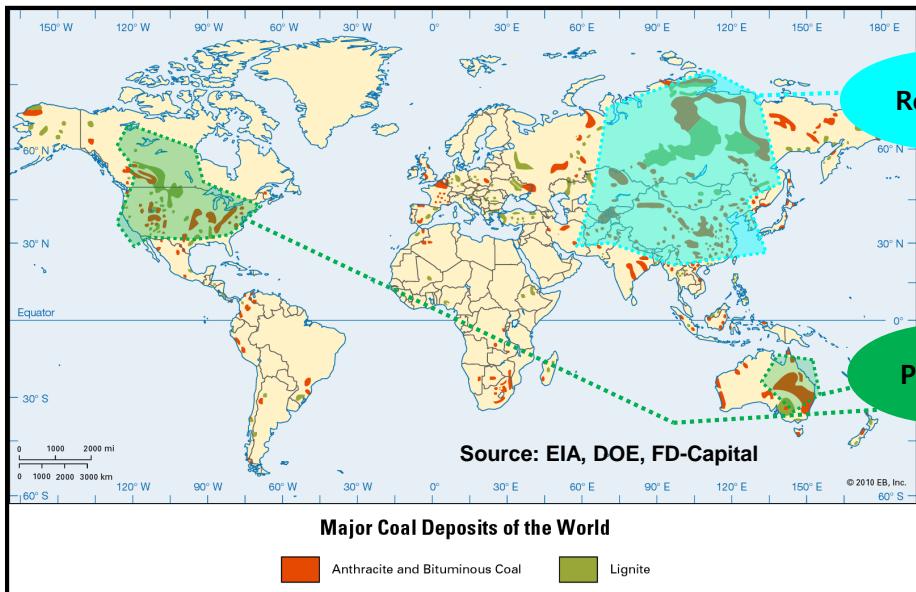
- Development of CoalBed Methane (CBM) Resource Engineering Core Technology

Purposes

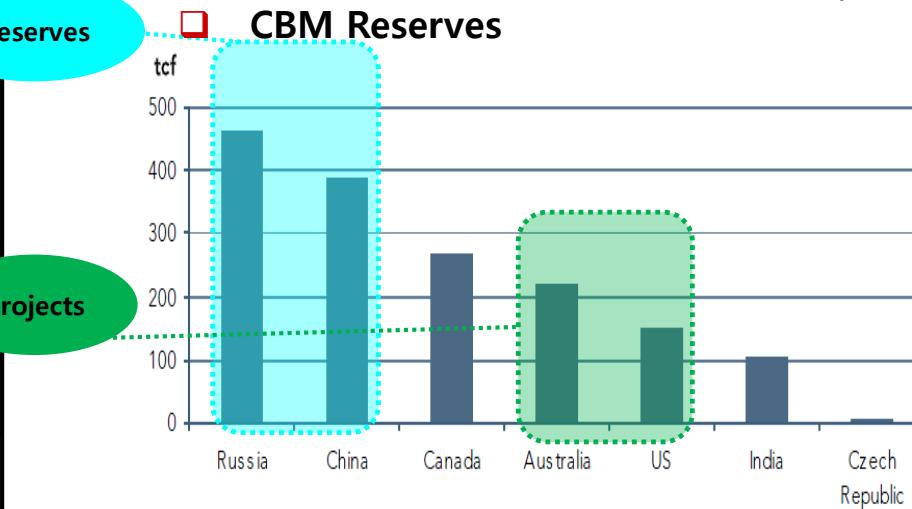
- Development of an energy efficient gas separation system to purify Coal Bed Methane (CBM) gas consisting of mainly methane and other impurities such as carbon dioxide, ethane, and so on
- Pilot Plant construction in the corresponding site



Identified CBM Basin



Source: EIA, DOE, FD-Capital

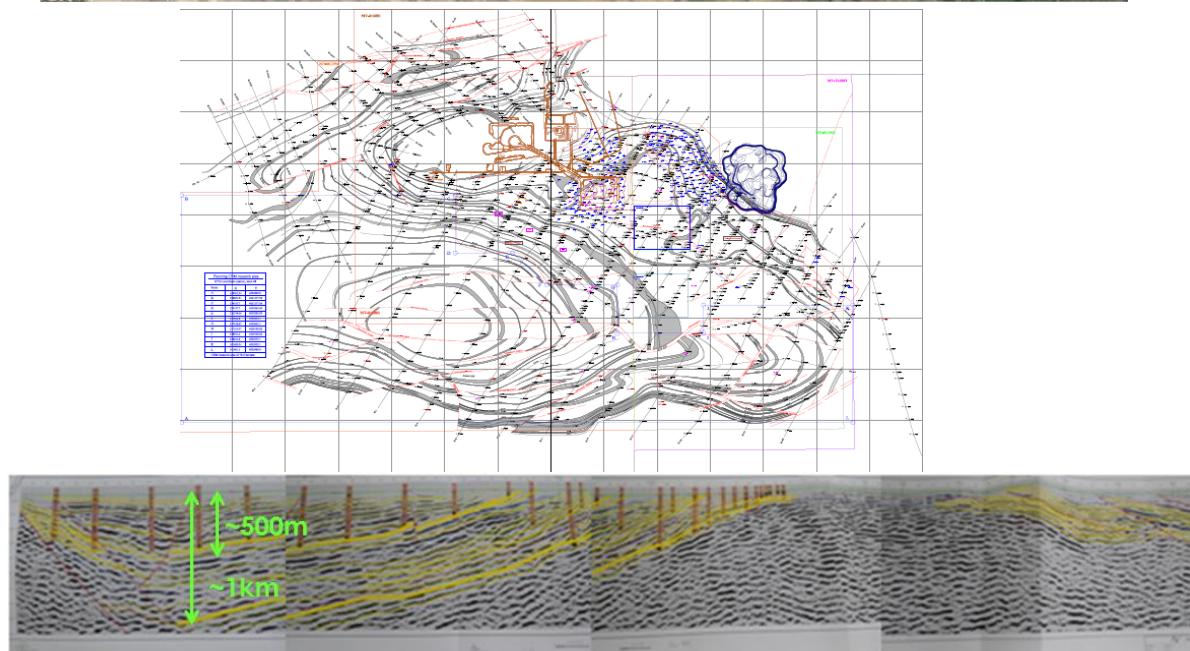


KEIT = Korea Evaluation Institute of Industrial Technology

MOTIE = Ministry of Trade, Industry & Energy

1. Overview

Overview of CBM purification project: CBM Site in Mongolia



1. Overview

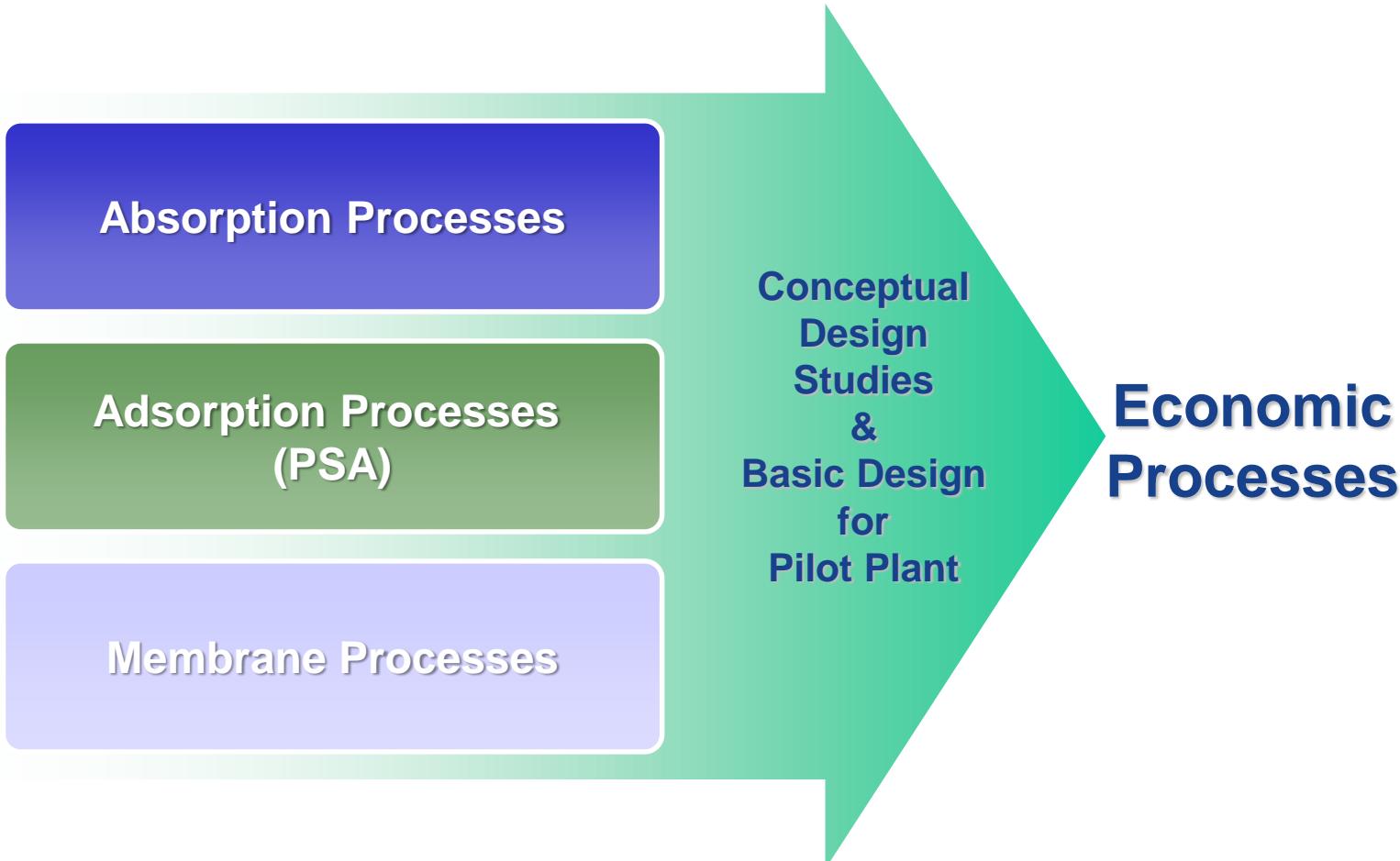
R&D plan (CBM purification technology)

KOGAS has been performing the mining the coal bed methane gas through Mongolian company (ELGEN), and will produce CBM gas on May or June 2015 at Tavan Tolgoi Site in Mongolia.
GS E&C will install PSA pilot plant to purify the CBM gas.

Work Scope	1st (2010.12~2011.05)	2nd (2011.06~2012.05)	3rd (2012.06~2013.05)	4th (2013.06~2014.11)	5th (2014.12~2015.11)	6th (2015.12~2016.11)
● Lab/Bench Scale study (Experiments & Simulation) - Absorption/Adsorption /Membrane - Study of Hybrid systems						
● Conceptual design						
● Basic design of pilot plant (Resizing of the basic design) ● Manufacturing PSA pilot plant ● Transportation to CBM site and construction						
● Pilot plant test & operation						
● Basic design of commercial PSA plant (feed flow: 2,500Nm ³ /h)						

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graph LR; A[1st: 2010.12~2011.05] --> B[2nd: 2011.06~2012.05]; B --> C[3rd: 2012.06~2013.05]; C --> D[4th: 2013.06~2014.11]; D --> E[5th: 2014.12~2015.11]; E --> F[6th: 2015.12~2016.11]; A --> A1[Absorption/Adsorption /Membrane]; A --> A2[Study of Hybrid systems]; A1 --> B; A2 --> B; B --> C; C --> D; D --> E; E --> F; C --> C1[Conceptual design]; C1 --> D; D --> D1[Basic design of pilot plant]; D1 --> D2[Manufacturing PSA pilot plant]; D2 --> D3[Transportation to CBM site and construction]; D3 --> E; E --> E1[Pilot plant test & operation]; E1 --> F; F --> F1[Basic design of commercial PSA plant];
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2. Conceptual design study



2. Conceptual design study

□ Work Done at GE E&C

- Simulation and Experiments of Purification Processes in Bench Scale Unit
- Brief Performance Comparison of Gas Separation/Purification Processes
- Process Design of Pilot Plant to remove sour gas (CO_2) included in CBM
 - ✓ Case Studies of purification processes
 - ✓ Finalization of Concept Design for pilot plant which will be installed in CBM site in Mongolia

2. Conceptual design study

Brief Comparison of Processes

❑ Performance and Scale

Processes	Scale	Performance
Amine absorption	Large	○
Adsorption (PSA)	Medium~Large	○
Membrane	Small	△

Since the technologies for scale up and performance improvements of PSA and Membrane have been developed, The improved large size processes of membrane and PSA have been introduced in industries recently.

❑ Size and Cost (Feed flow rate ~ 600Nm³/hr)

Processes	Pilot Plant Size	Pilot Plant Cost	Things to note	Candidate Processes for Pilot Plant Basic Design
Absorption	10m*15m*15m	Higher than \$1.9MM	Large Scale & Excellent Performance / expensive absorption cost	X
Adsorption (PSA)	10m*15m*10m	About \$0.94MM	Mid-Large Scale & Good performance	○
Membrane	10m*15m*10m	About \$0.94MM	Recently started to be commercialized in large scale	○

Considering the cost, size, and ease of transportation to remote CBM site, Membrane and PSA processes are selected for the conceptual design studies.

2. Conceptual design study

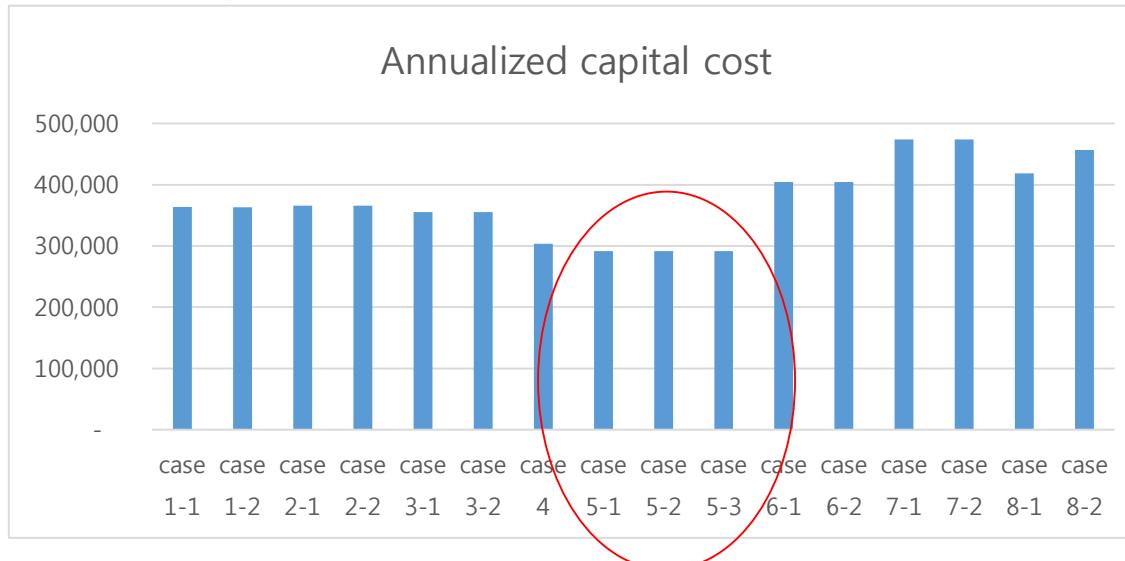
List of the candidate processes for brief comparison



Scenario Index	Adsorbent	1st PSA adsorption pressure (bara)	1st PSA purge pressure (bara)	1st Membrane permeate pressure (bara)	2nd Membrane permeate pressure (bara)	2nd PSA adsorption pressure (bara)	2nd PSA purge pressure (bara)
Hybrid Membrane & PSA with Recycle (1)							
CD1.1	Zeolite	1	0.02	1	0.1		
CD1.2	CMS	10	1	1	0.1		
Hybrid Membrane & PSA with Recycle (2)							
CD2.1	Zeolite	1	0.02	1	0.1		
CD2.2	CMS	10	1	1	0.1		
Hybrid membrane & PSA without Recycle							
CD3.1	Zeolite	1	0.02	1	0.1		
CD3.2	CMS	10	1	1	0.1		
Membrane Only with Recycle							
CD4				1	0.1		
PSA Only							
CD5.1	Zeolite	1	0.02				
CD5.2	CMS	10	1				
CD5.3	CMS	10	0.1				
Hybrid PSA & Membrane with Recycle (3)							
CD6.1	Zeolite	1	0.02	0.1	0.1		
CD6.2	CMS	10	1	0.1	0.1		
Hybrid PSA & Membrane with Recycle (4)							
CD7.1	CMS/Zeolite	10	1	0.1		1	0.02
CD7.2	CMS	10	1	0.1		10	1
Hybrid PSA & Membrane with Recycle (5): Low CH4 composition in feed stream							
CD8.1	CMS			1	0.1	10	1
CD8.2	CMS			1	0.1	10	1

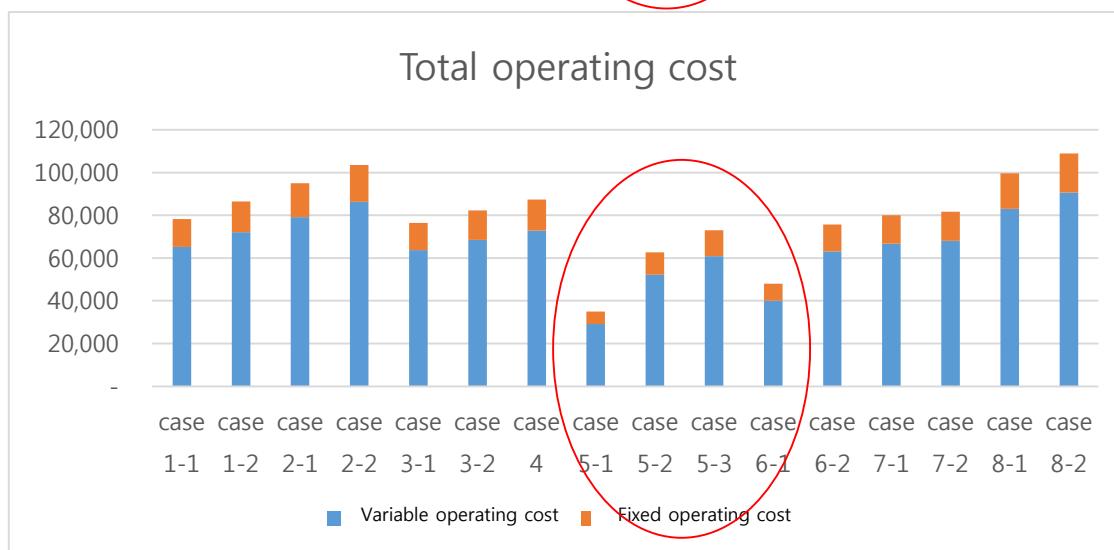
2. Conceptual design study

Economic analysis



Annualized capital cost
= initial investment cost
× capital charge factor

Capital charge factor
= interest rate
× life time of plant



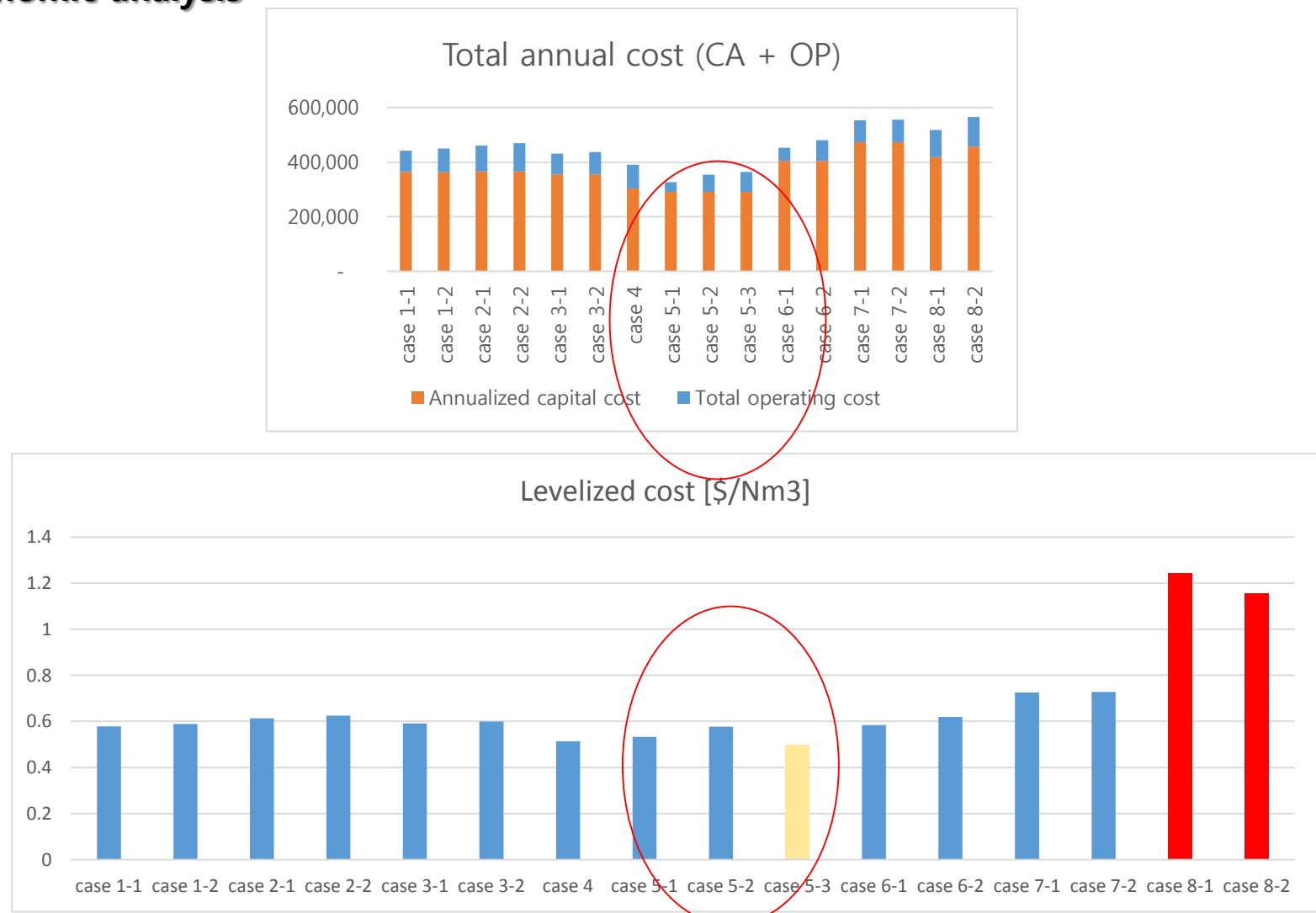
Total operating cost
= fixed operating cost
+ variable operating cost

Fixed operating cost
= maintenance & administration fee
+ property tax + depreciation fee
+ ...
= 3%~5% of initial investment cost

Variable operating cost
= electricity cost + material cost
+ fuel cost +...
Here, only electricity cost is included.

2. Conceptual design study

Economic analysis



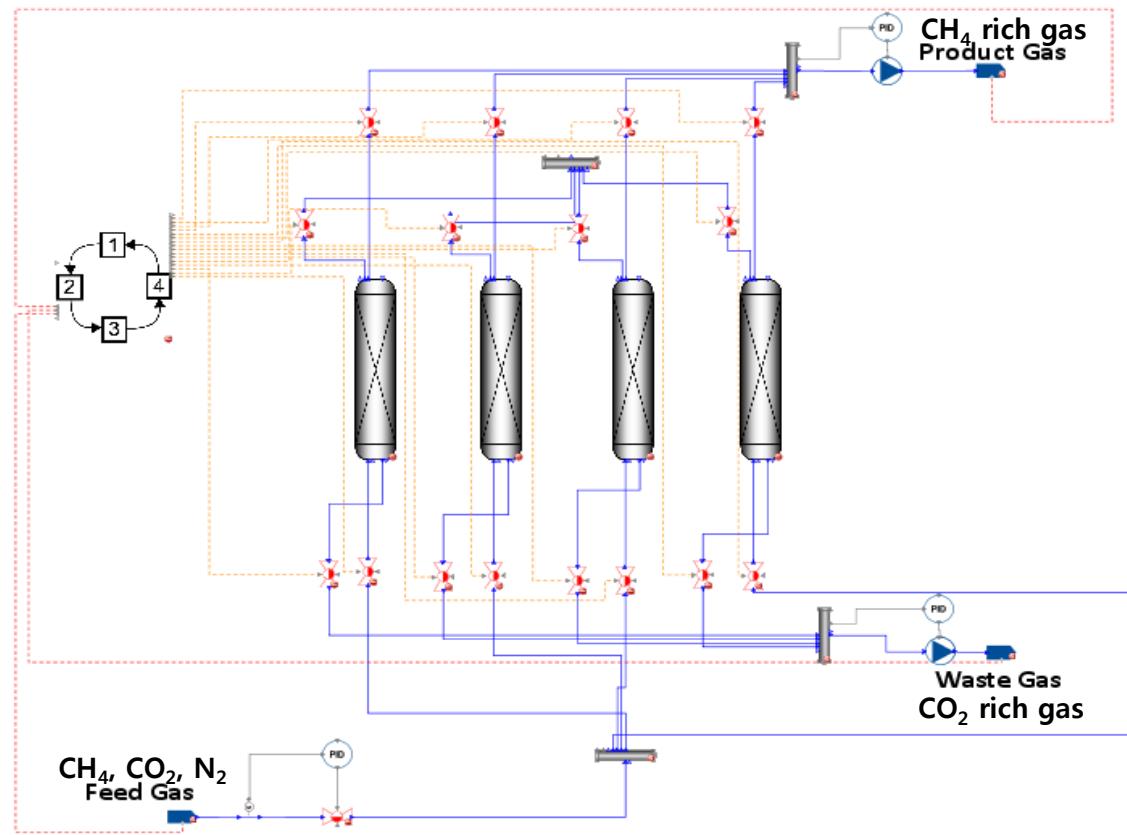
3. Dynamic Modeling of PSA Process

Work Done

1. Isotherm parameter estimation through lab scale experiments
2. PSA simulation model development for CBM purification
3. Basic design of PSA pilot plant
4. Scale up/down design of PSA process
5. Simulation and optimization of PSA through gPROMS modeling

PSA process

CBM feed composition	89.5% CH ₄ 8.18% CO ₂ 2.32% N ₂
Adsorption/desorption pressure	10 barg / -0.9 barg
Number of adsorption beds	Four
Operating step	Twelve
Adsorbent	CMS 3K



Pressure Swing Adsorption (PSA)

PSA is a technology used to separate some gas species from a mixture of gases under pressure according to the species' molecular characteristics and affinity for an adsorbent material. It operates at near-ambient temperatures and differs significantly from cryogenic distillation techniques of gas separation. Specific adsorptive materials (e.g., zeolites, activated carbon, molecular sieves, etc.) are used as a trap, preferentially adsorbing the target gas species at high pressure. The process then swings to low pressure to desorb the adsorbed material.
(Reference: http://en.wikipedia.org/wiki/Pressure_swings_adsorption)

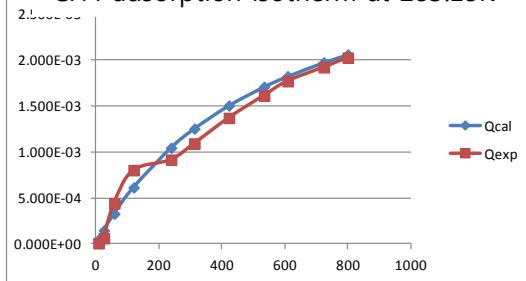
CMS type of adsorbent is selected for PSA systems, because zeolite types are vulnerable to humidity.

3. Dynamic Modeling of PSA Process

*Adsorption equilibrium
(Extended Langmuir isotherm)*

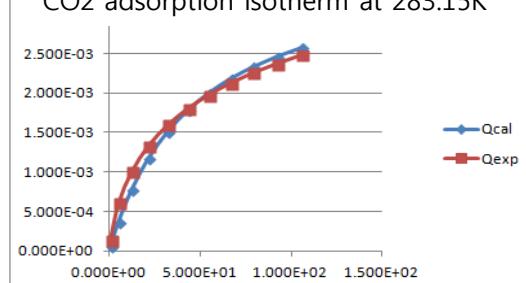
$$q_i^* = \frac{q_{sa,i} b_i P_i}{1 + \sum_{i=1}^n b_i P_i}; q_{sa,i} = q_{sa,i} + \frac{q_{sb,i}}{T}; b_i = b_{0,i} \exp\left(\frac{D_{E,i}}{T}\right)$$

CH4 adsorption isotherm at 283.15K

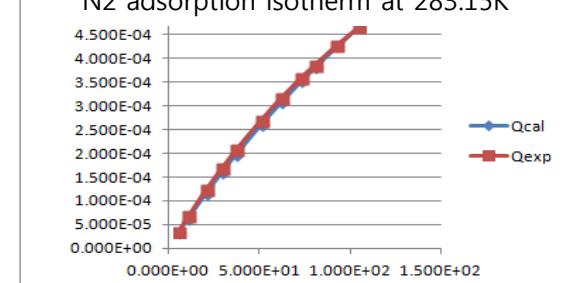


	q _{sa} (mol/g)	q _{sb} (mol-K/g)	b ₀ (1/bar)	D _E (K)	△H (cal/mol)
CH ₄	-0.0018	1.502	0.413302326	-238	974.54
CO ₂	0.0004	0.9374	0.000755814	2250.1	5216.47
N ₂	0.0019	-0.00376	0.000335559	1937.8	3847.03

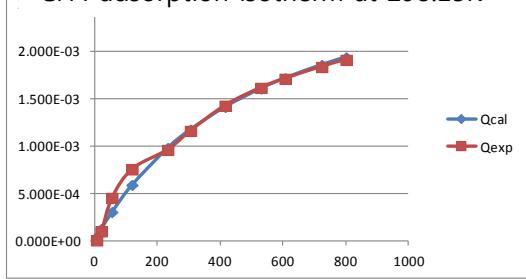
CO₂ adsorption isotherm at 283.15K



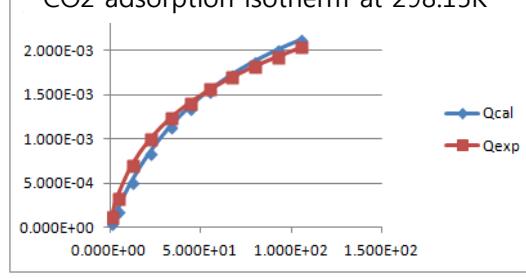
N₂ adsorption isotherm at 283.15K



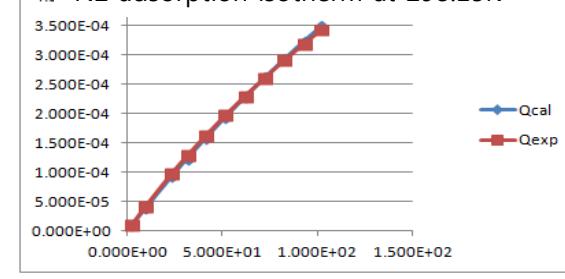
CH4 adsorption isotherm at 298.15K



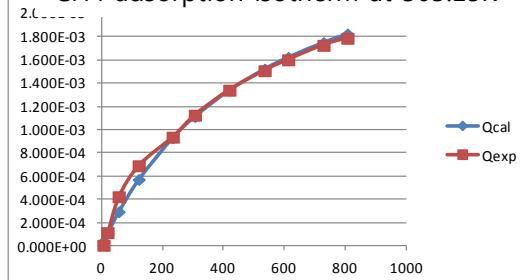
CO₂ adsorption isotherm at 298.15K



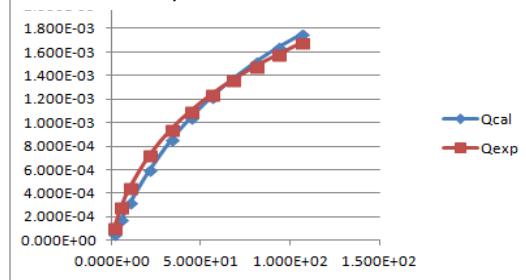
N₂ adsorption isotherm at 298.15K



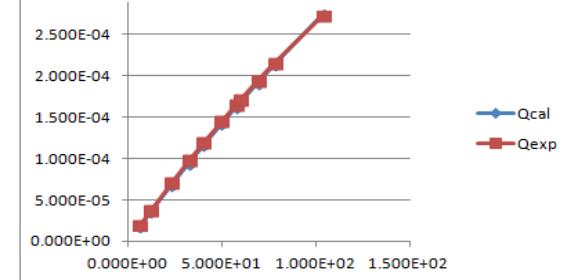
CH4 adsorption isotherm at 303.15K



CO₂ adsorption isotherm at 303.15K



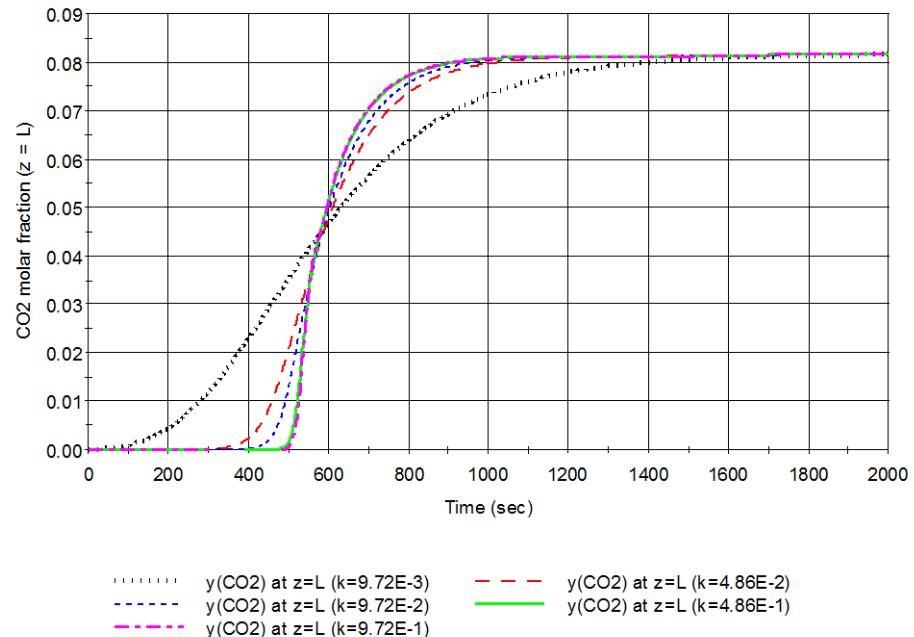
N₂ adsorption isotherm at 303.15K



3. Dynamic Modeling of PSA Process

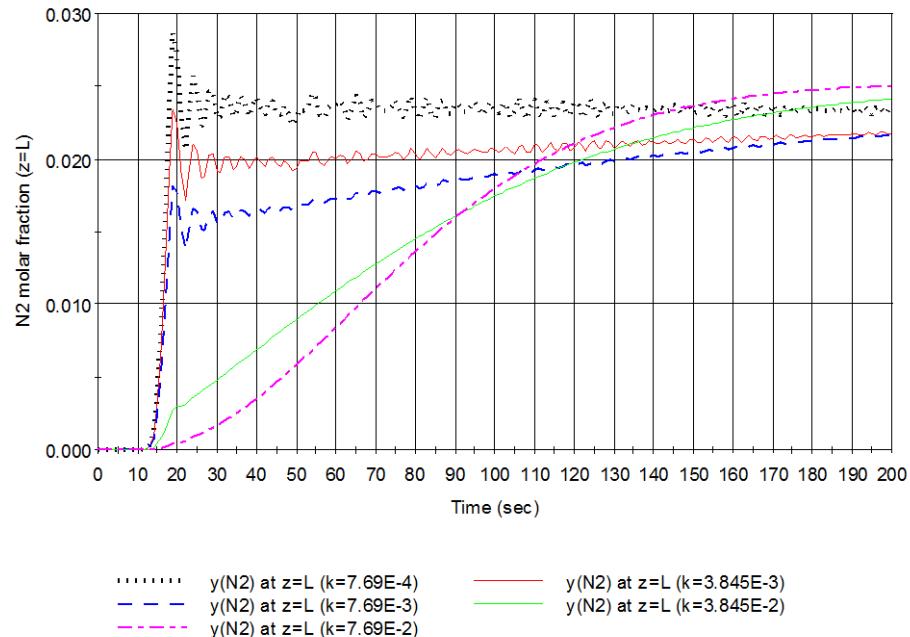
Breakthrough curve behavior

CO₂ breakthrough behavior according to k_{CO_2}



Considering the value of CO₂ measured mass transfer coefficient ($k_{CO_2}=9.72\times 10^{-2}$), the adsorption time can be determined as 140 sec, leading to enough adsorption of CO₂ and high CH₄ purity

N₂ breakthrough behavior according to k_{N_2}



The N₂ breakthrough begins at around 12.5 sec, independently of the mass transfer coefficient values (measured $k_{N_2}=7.69\times 10^{-3}$), N₂ comes out with CH₄ in the purified gas stream.

Mass transfer coefficient measured

$$\begin{aligned} k_{CH_4} &= 5.35 \times 10^{-3} \text{ s}^{-1} \\ k_{CO_2} &= 9.72 \times 10^{-2} \text{ s}^{-1} \\ k_{N_2} &= 7.69 \times 10^{-3} \text{ s}^{-1} \end{aligned}$$

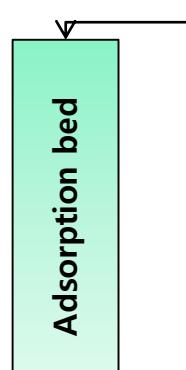
Adsorption rate

$$\frac{\partial q_i}{\partial t} = k_i (q_i^* - q_i)$$

3. Dynamic Modeling of PSA Process

Modeling of 4 Bed 12 Operating Step PSA through One Bed Simulation instead of the Four Bed simulation

Boundary conditions are calculated at the each interacting bed of the corresponding step



Four Bed Twelve Operating Step Sequence & Time

STEP NO.	1	2	3	4	5	6	7	8	9	10	11	12
TIME(sec)	10	120	10	10	120	10	10	120	10	10	120	10
Bed 1	AD	AD	AD	EQ1	RE	EQ2	BD	PU	EQ2	EQ1	PR	PR
Bed 2	BD	PU	EQ2	EQ1	PR	PR	AD	AD	AD	EQ1	RE	EQ2
Bed 3	EQ1	PR	PR	AD	AD	AD	EQ1	RE	EQ2	BD	PU	EQ2
Bed 4	EQ1	RE	EQ2	BD	PU	EQ2	EQ1	PR	PR	AD	AD	AD

- AD : adsorption
- EQ : pressure equalization
- RE : repose
- BD : blow down
- PU : purge
- PR : pressurization



3. Dynamic Modeling of PSA Process

Verification of Simulation Model (4 Bed 12 Operating Step PSA)

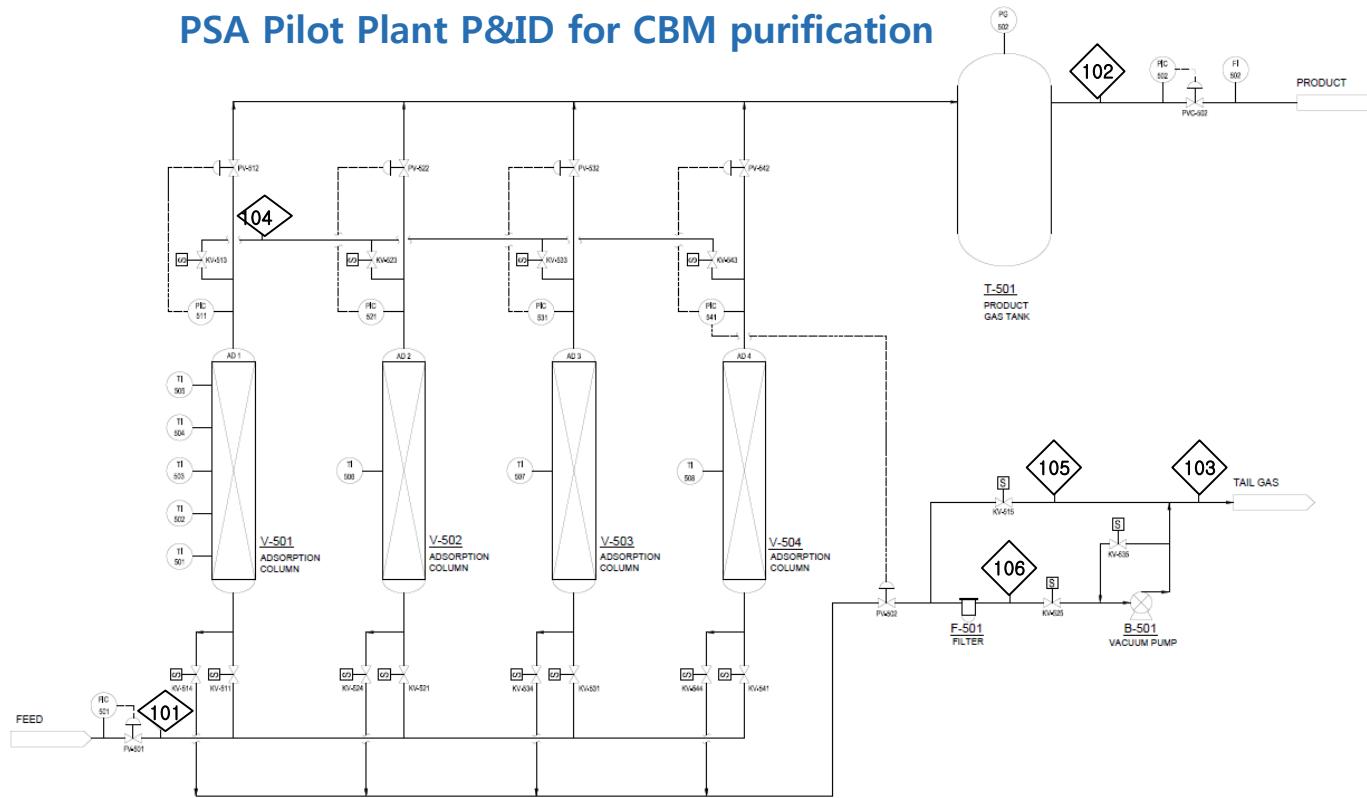
Feed Flow = 100Nm ³ /h		Variables	Basic Design*	Simulation	RME (%)
100Nm ³ /h	Inner Bed Diameter (m)	0.289	CH4 Purity (%)	97.00	96.97
	Packing Bed Height (m)	1.55	CH4 Recovery (%)	92.00	92.03
	Adsorption Pressure (bara)	11	Product Flow (Nm ³ /s)	2.36E-02	2.37E-02
	BlowDown Pressure (bara)	1	Waste Flow (Nm ³ /s)	4.20E-03	4.34E-03
	Purge Pressure (bara)	0.1	Feed Composition: CH4 89.5%, CO2 8.18%, N2 2.32%		
Feed Flow = 0.68Nm ³ /h		Variables	Experiment C1*	Simulation	RME (%)
200 times scale up	Inner Bed Diameter (m)	0.0254	CH4 Purity (%)	96.16	96.00
	Packing Bed Height (m)	1	CH4 Recovery (%)	93.96	93.78
	Adsorption Pressure (bara)	11	Product Flow (Nm ³ /s)	1.65E-04	1.65E-04
	BlowDown Pressure (bara)	1	Waste Flow (Nm ³ /s)	2.39E-05	2.35E-05
	Purge Pressure (bara)	0.259	Feed Composition: CH4 89.5%, CO2 8.18%, N2 2.32%		
Feed Flow = 0.56Nm ³ /h		Variables	Experiment C2*	Simulation	RME (%)
0.5Nm ³ /h	Inner Bed Diameter (m)	0.0254	CH4 Purity (%)	97.12	96.92
	Packing Bed Height (m)	1	CH4 Recovery (%)	92.83	92.78
	Adsorption Pressure (bara)	11	Product Flow (Nm ³ /s)	1.32E-04	1.33E-04
	BlowDown Pressure (bara)	1	Waste Flow (Nm ³ /s)	2.24E-05	2.19E-05
	Purge Pressure (bara)	0.174	Feed Composition: CH4 89.5%, CO2 8.18%, N2 2.32%		
Feed Flow = 0.44Nm ³ /h		Variables	Experiment C3*	Simulation	RME (%)
0.5Nm ³ /h	Inner Bed Diameter (m)	0.0254	CH4 Purity (%)	97.48	97.14
	Packing Bed Height (m)	1	CH4 Recovery (%)	91.19	91.15
	Adsorption Pressure (bara)	11	Product Flow (Nm ³ /s)	1.03E-04	1.03E-04
	BlowDown Pressure (bara)	1.081	Waste Flow (Nm ³ /s)	2.02E-05	1.93E-05
	Purge Pressure (bara)	0.176	Feed Composition: CH4 89.5%, CO2 8.18%, N2 2.32%		

* Basic design and experiments were performed by GENS Engineering (PSA design company) in Korea

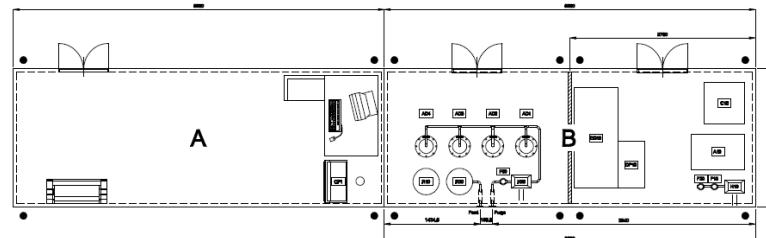
RME =Relative Mean Error = $(\phi_{Exp} - \phi_{Cal})/\phi_{Cal} \times 100\%$

4. Optimization of PSA for Scale up & down Design

PSA Pilot Plant P&ID for CBM purification



PSA Pilot Plant Layout for CBM purification



Length = 11,160mm, Width = 2,050mm, Height = 2,300mm

4. Optimization of PSA for Scale up & down Design

Re-design*: feed flow $100\text{Nm}^3/\text{h} \rightarrow 10\text{Nm}^3/\text{h}$

Material balance for PSA pilot plant (feed flow: $10\text{Nm}^3/\text{h}$)

Stream No.	101 Feed stream	102 Product stream	103 Waste stream	104 Pressure equalization stream	105 Blow down stream	106 Purge stream
Phase	Vapor	Vapor	Vapor	Vapor	Vapor	Vapor
Molar Fraction (mole %)	CH ₄	0.895	0.97	0.4738		
	CO ₂	0.082	0.0072	0.5023		
	N ₂	0.023	0.0228	0.0244		
Vol. flow rate (Nm ³ /h)	10	8.5	1.5	1.45	0.4	1.1
Temperature (°C)	20	20	20	20	20	20
Pressure (kg/cm ² G)	10	10	-0.9	10→6.5	0.1	-0.9
				6.5→3		

Four Bed Twelve Operating Step Sequence & Time

STEP NO.	1	2	3	4	5	6	7	8	9	10	11	12
TIME(sec)	10	120	10	10	120	10	10	120	10	10	120	10
Bed 1	AD	AD	AD	EQ1	RE	EQ2	BD	PU	EQ2	EQ1	PR	PR
Bed 2	BD	PU	EQ2	EQ1	PR	PR	AD	AD	AD	EQ1	RE	EQ2
Bed 3	EQ1	PR	PR	AD	AD	AD	EQ1	RE	EQ2	BD	PU	EQ2
Bed 4	EQ1	RE	EQ2	BD	PU	EQ2	EQ1	PR	PR	AD	AD	AD

- AD : adsorption
- EQ : pressure equalization
- RE : repose
- BD : blow down
- PU : purge
- PR : pressurization

Design Basis	
1. Inner diameter of adsorption bed	0.15m
2. Packing Height of Adsorption bed	1.12m
3. Material of bed	Carbon steel
4. Design Capacity	$10\text{Nm}^3/\text{h}$ (Feed flow)
5. Feed temperature	Ambient temperature
6. Product flow rate	$8.5\text{Nm}^3/\text{h}$
7. CH ₄ Purity	Above 97%
8. CH ₄ Recovery	85~90%

* The PSA Optimization method of Ko et. al (2005) is adopted to perform the Re-Sizing of the PSA plant

4. Optimisation of PSA for Scale up & down Design

PSA optimisation* model (feed flow: 10Nm³/h)

$$\text{Min. obj} = 10^5 \times \varepsilon - \text{Purity}_{CH_4} - \text{Recovery}_{CH_4}$$

Subject to

		Case 1		Case 2		Case 3	
Variables	Unit	LB	UB	LB	UB	LB	UB
CH ₄ Purity	-	0.97	1.00	0.975	1.00	0.975	1.00
CH ₄ Recovery	-	0.90	1.00	0.80	1.00	0.75	1.00
L	m	1.0	1.3	1.0	1.3	1.12	1.12
R _{bed}	m	0.0	1.0	0.0	1.0	0.0	1.0
L/u _{feed}	Sec	0.75	2.7	0.75	2.7	0.75	2.7
T _{i,j,t=0}	K	290	340	290	340	290	340
q _{CH4,j,t=0}	mol/g	0	10	0	10	0	10
q _{CO2,j,t=0}	mol/g	0	1	0	1	0	1
q _{N2,j,t=0}	mol/g	0	1	0	1	0	1
y _{i,j,t=0}	-	0	1	0	1	0	1
△φ _j	K, mol/g, or -	-ε	ε	-ε	ε	-ε	ε
△φ _j	$\Delta\phi_j = \phi_{j,t=0} - \phi_{j,t=t_{cycle}}$, Here, φ stands for T, q, and y						

Step times are fixed as shown in following Table

Step No.	1	2	3	4	5	6	7	8	9	10	11	12
Time(sec)	10	120	10	10	120	10	10	120	10	10	120	10
Step	AD	AD	AD	EQ1	RE	EQ2	BD	PU	EQ2	EQ1	PR	PR

Optimal result

	Case 1	Case 2	Case 3
CH ₄ Purity	0.9744	0.97545	0.97603
CH ₄ Recovery	0.9104	0.85868	0.78598
L	1.1193	1.00113	1.12
R _{bed}	0.05148	0.06624	0.0755
L/u _{feed}	1.22447	1.81348	2.63549

Case 3 is the selected design for pilot plant to obtain the high purity of CH₄.

Constraints to determine cyclic steady state (CSS).

What is CSS?

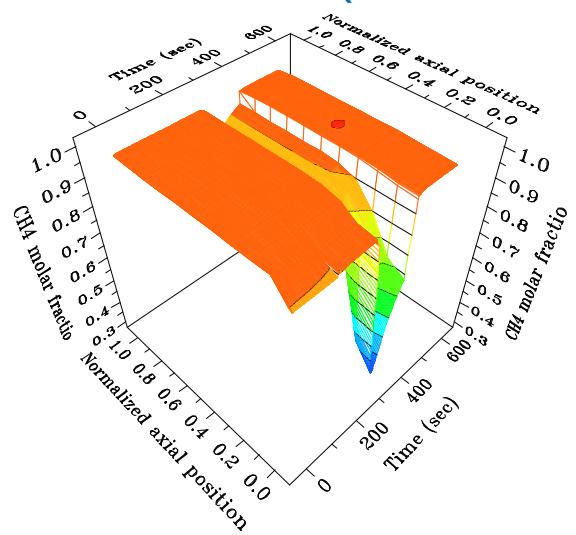


* The PSA Optimization method of Ko et. al (2005) is adopted to perform the Re-design of the PSA plant

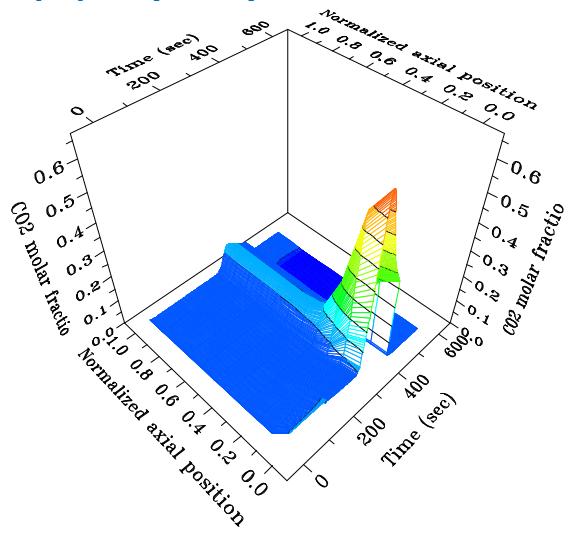


4. Optimisation of PSA for Scale up & down Design

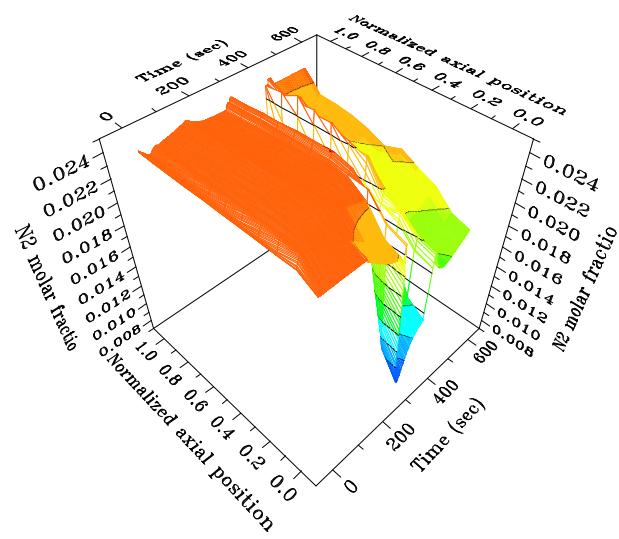
PSA simulation (feed flow: 10Nm³/h) of pilot plant



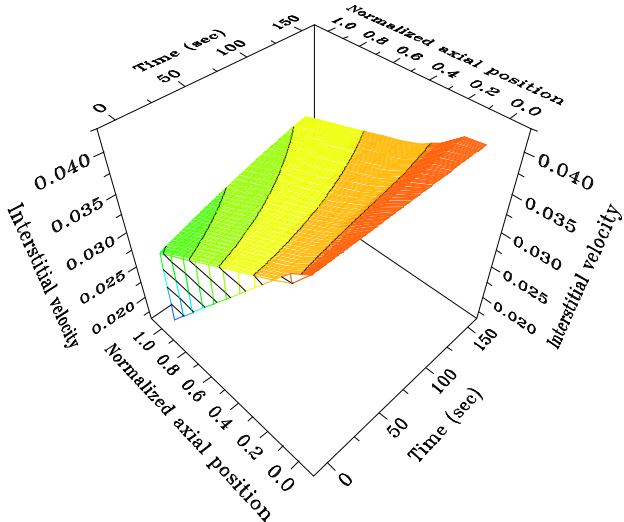
CH4 molar fraction at CSS



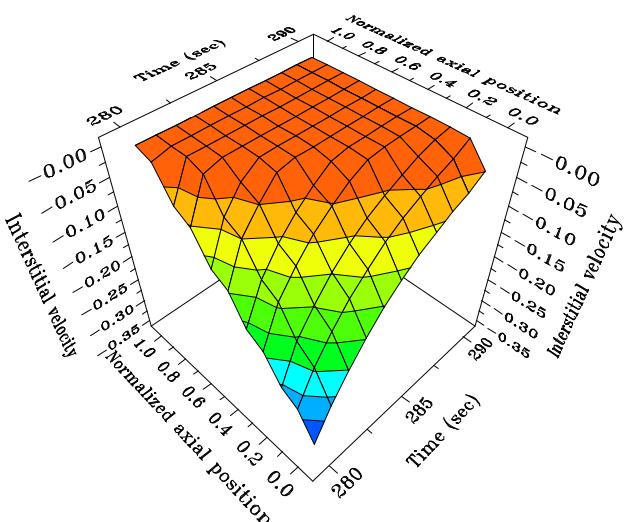
CO2 molar fraction at CSS



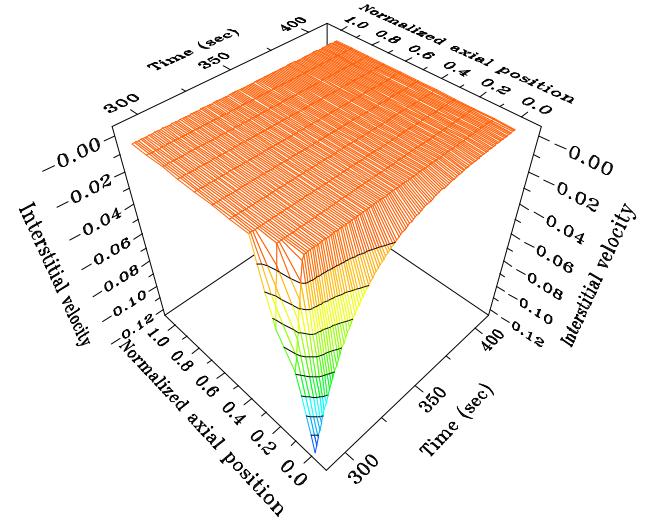
N2 molar fraction at CSS



Velocity of adsorption step at CSS



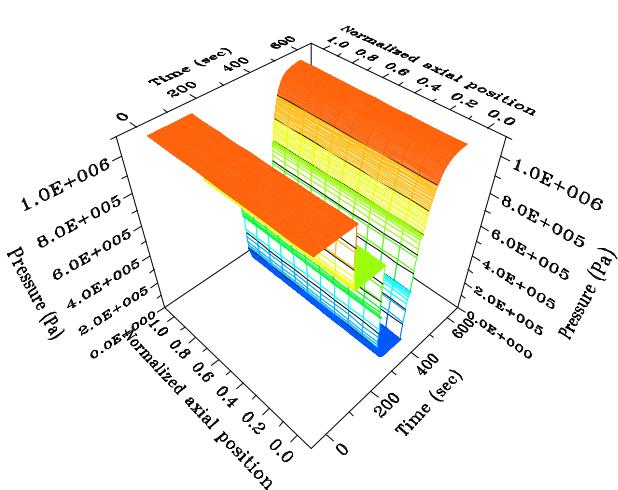
Velocity of blowdown step at CSS



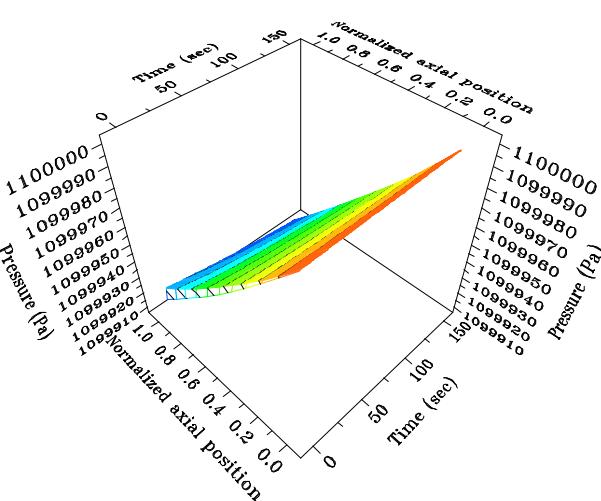
Velocity of purge step at CSS

4. Optimisation of PSA for Scale up & down Design

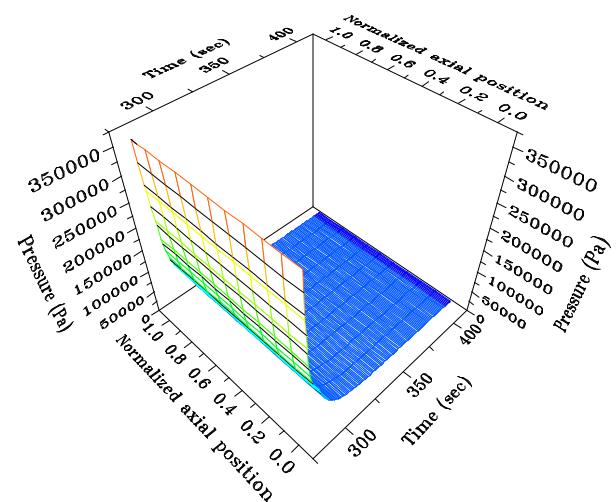
PSA simulation (feed flow: 10Nm³/h) of pilot plant



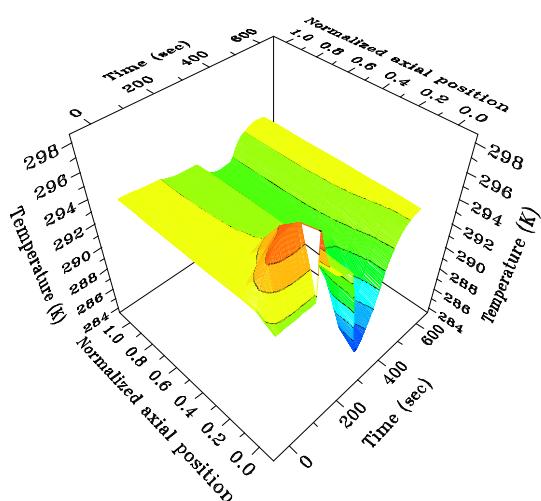
Pressure at CSS



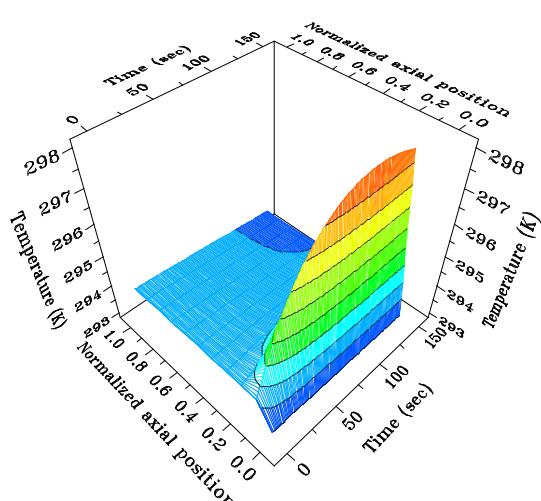
Pressure of adsorption step at CSS



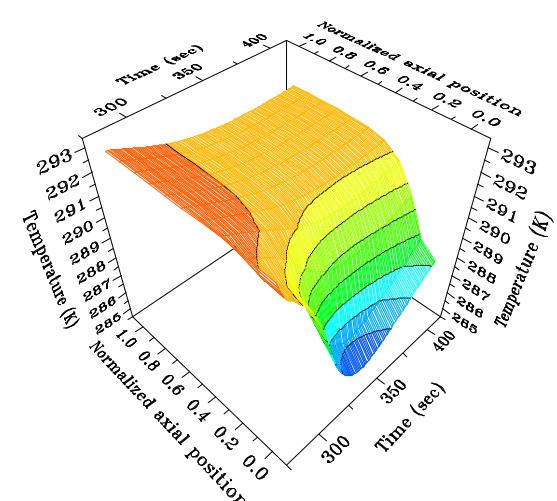
Pressure of blowdown & purge step at CSS



Temperature at CSS



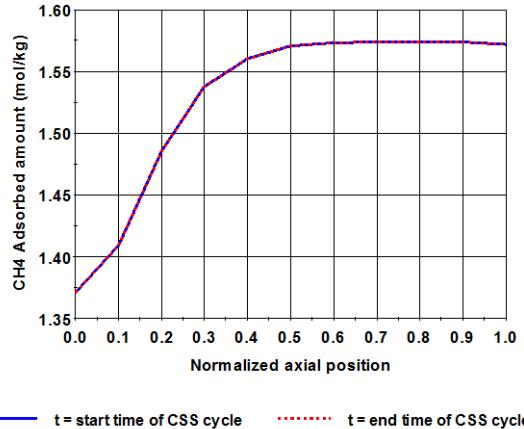
Temperature of adsorption step at CSS



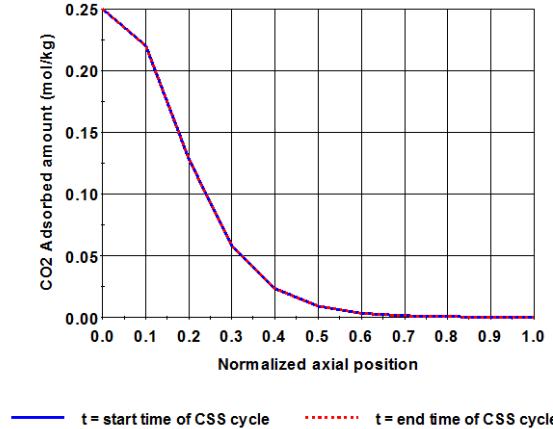
Temperature of blowdown & purge step at CSS

4. Optimisation of PSA for Scale up & down Design

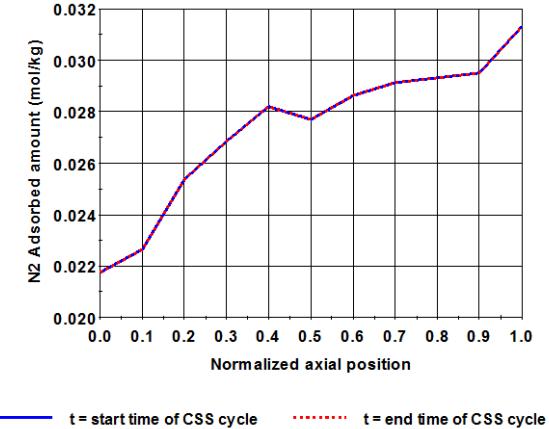
PSA simulation (feed flow: 10Nm³/h) of pilot plant: CSS check



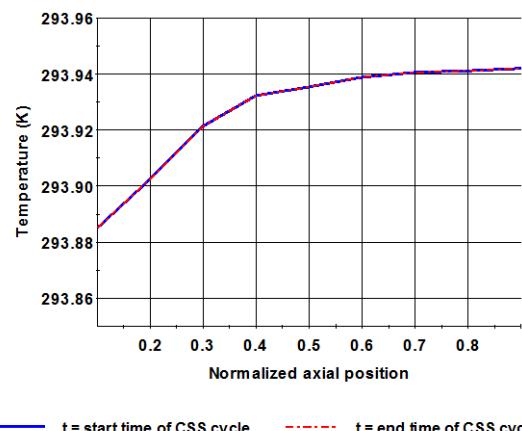
Adsorbed amount of CH₄ at CSS



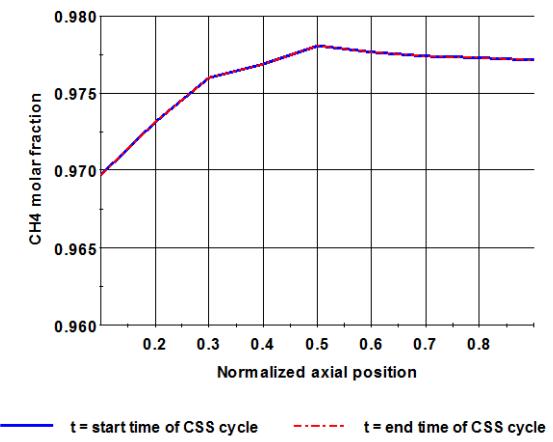
Adsorbed amount of CO₂ at CSS



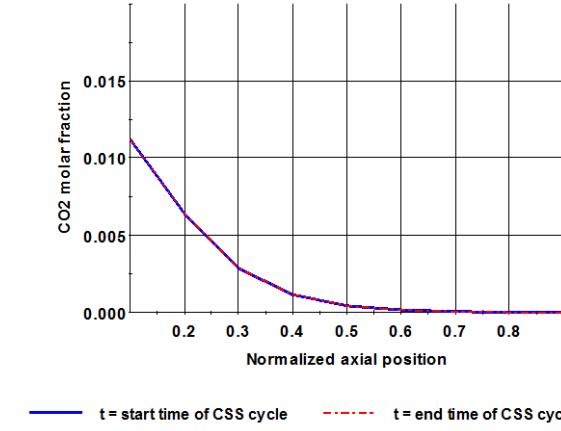
Adsorbed amount of N₂ at CSS



Temperature at CSS



CH₄ molar fraction at CSS



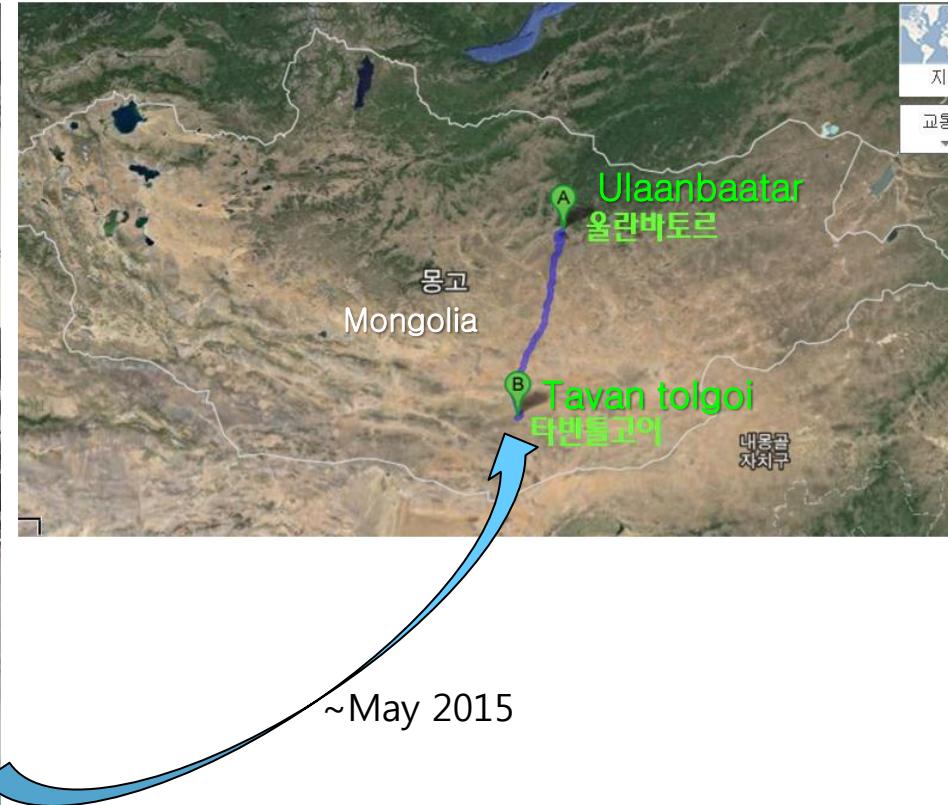
CO₂ molar fraction at CSS

4. Optimization of PSA for Scale up & down Design

Photo of PSA pilot plant (10Nm³/h)



CBM Site in Mongolia



4. Optimisation of PSA for Scale up & down Design

PSA optimisation model

$$\text{Min. } obj = 10^5 \times \varepsilon$$

Feed flow (Nm ³ /h)		200		500		1000		2500		5000	
Variables	Unit	LB	UB								
CH_4 Purity	-	0.97	1.00	0.97	1.00	0.97	1.00	0.97	1.00	0.97	1.00
CH_4 Recovery	-	0.90	1.00	0.90	1.00	0.90	1.00	0.90	1.00	0.90	1.00
L	m	2.12	2.12	2.2	2.2	1.95	1.95	2.16	2.16	2.125	2.125
R_{bed}	m	0	1	0	1	0	1	0	1	0	1
L/u_{feed}	sec	0.75	2.63	0.75	2.63	0.75	2.63	0.75	2.63	0.75	2.63
Adsorbent amount per feed flow	kg/(Nm ³ /h)	0.7	0.72	0.7	0.72	0.7	0.72	0.7	0.72	0.7	0.72
$T_{i,j,t=0}$	K	290	340	290	340	290	340	290	340	290	340
$q_{CH4,j,t=0}$	mol/g	0	10	0	10	0	10	0	10	0	10
$q_{CO2,j,t=0}, q_{N2,j,t=0}$	mol/g	0	1	0	1	0	1	0	1	0	1
$y_{i,j,t=0}$	-	0	1	0	1	0	1	0	1	0	1
$\Delta\phi_j$	$K, mol/g, or -$	$-\varepsilon$	ε								
$\Delta\phi_j = \phi_{j,t=0} - \phi_{j,t=t_{cycle}}$, Here, ϕ stands for T, q , and y											

4. Optimisation of PSA for Scale up & down Design

Optimal result

Feed flow (Nm ³ /h)	Inner Diameter (m)		Adsorbent amount (kg)		CH ₄ Purity		CH ₄ Recovery	
	PSA Vendor	GS E&C	PSA Vendor	GS E&C	PSA Vendor	GS E&C	PSA Vendor	GS E&C
200	0.3428	0.350247	138	144	0.97	0.971106	0.90	0.909797
500	0.5308	0.543626	344	360	0.97	0.971216	0.90	0.910607
1000	0.8	0.8166	691	720	0.97	0.971366	0.90	0.910791
2500	1.2	1.21405	1725	1762.8	0.97	0.971402	0.90	0.912999
5000	1.7	1.73253	3375	3531.8	0.97	0.971518	0.90	0.912653

Conclusion

❑ Work Done

- Conceptual design study for CBM purification processes through
 - comparing various gas separation/purification processes and
 - brief economic analysis of the candidate processes
- Basic design of the selected process (VPSA) through conceptual design study
- Construction and validation of PSA simulation model by using gPROMS
- Scale up/down design (Re-sizing of adsorption bed) of PSA through optimisation by using gPROMS

❑ Work To Do

- PSA pilot plant designed in this study will be transported into CBM site (Tavan tolgoi in Mongolia) and installed by the end of May in 2015.
- Pilot Plant commissioning and operation for the demonstration of CBM purification leading to energy utilization of CBM
- Basic design of commercial size PSA plant (feed flow: 2500Nm³/h)

Any Question?

Email: daeho.ko@gsconst.co.kr

Appendix

A1. Candidate processes for conceptual design study

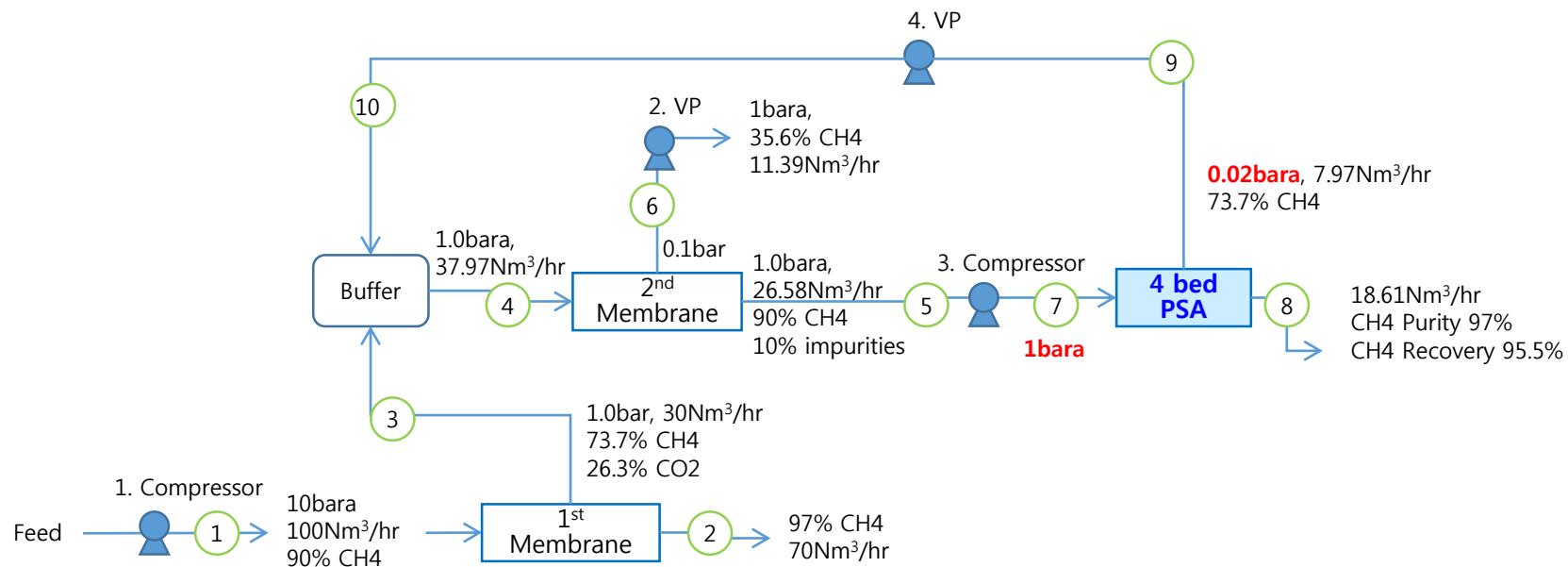
A2. Operation step of four bed PSA process

A3. Definition of cyclic steady state (CSS)

A4. PSA optimisation approach at CSS

A1. Candidate processes for conceptual design study

CD1.1: Hybrid Membrane & PSA(Zeolite) (Feed 100Lube/hr) w/ recycle

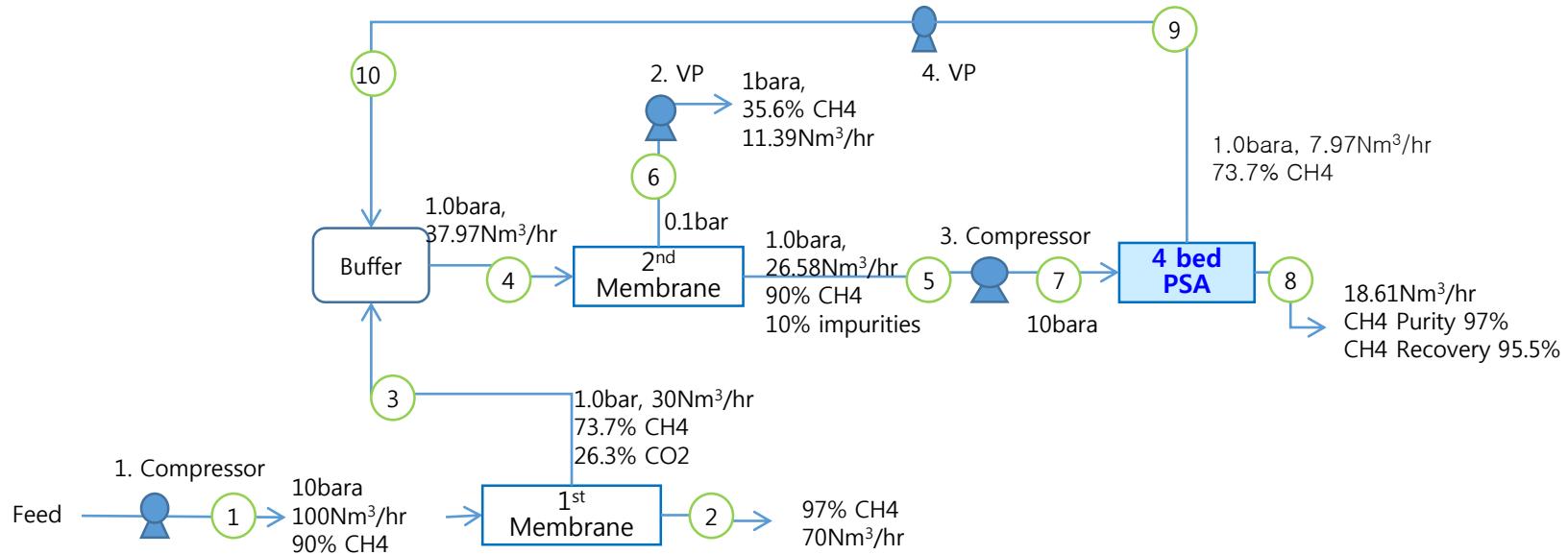


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Mem. 1	Feed	1	10	25	100.00	90.00	10.00
	Retentate	2	10	25	68.57	97.00	3.00
	Permeate	3	1	25	31.43	73.67	26.33
Mem. 2	Feed*	4	1	25	39.39	73.67	26.33
	Retentate	5	1	25	26.56	90.00	10.00
	Permeate	6	0.1	25	12.83	35.56	64.44
PSA	Feed	7	1	25	26.56	90.00	10.00
	Product	8	1	25	18.60	97.00	3.00
	Purge	9	0.02	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
1	100.00	9.49
2	12.83	1.28
3	26.56	0.00
4	7.96	1.64
Total Power [kW]		12.41
Total Power per product flow rate [kW/(Nm³/hr)]		0.14

A1. Candidate processes for conceptual design study

CD1.2: Hybrid Membrane & PSA(CMS) (Feed 100Lube/hr) w/ recycle

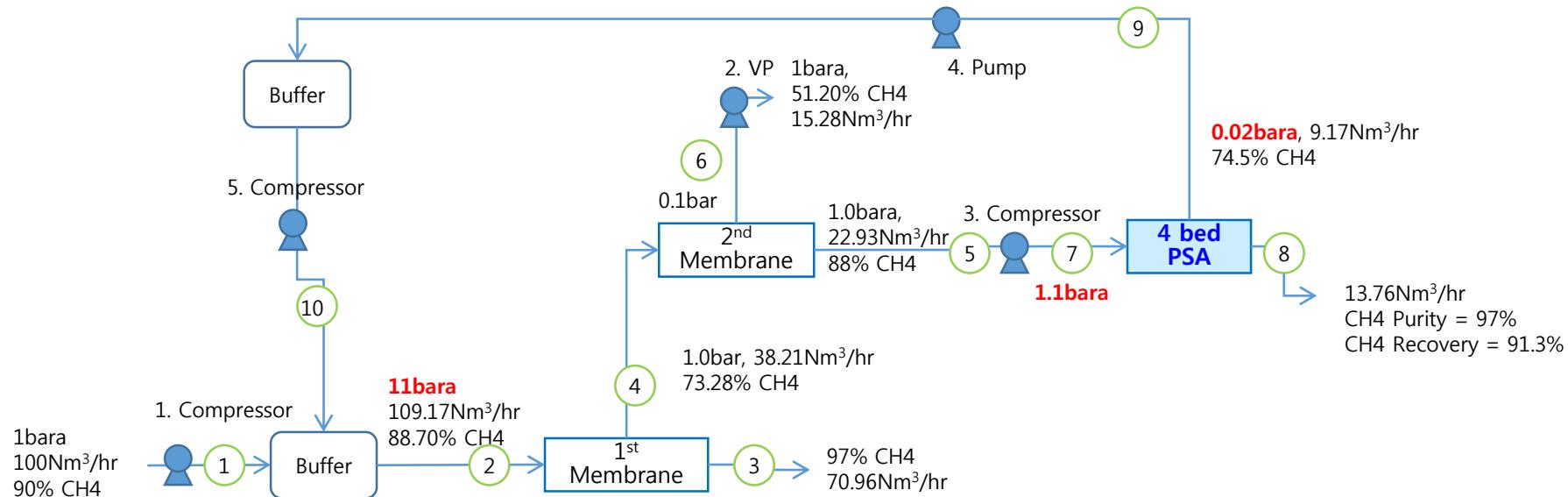


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO2 Conc. (mol.%)
Mem. 1	Feed	1	10	25	100.00	90.00	10.00
	Retentate	2	10	25	68.57	97.00	3.00
	Permeate	3	1	25	31.43	73.67	26.33
Mem. 2	Feed*	4	1	25	39.39	73.67	26.33
	Retentate	5	1	25	26.56	90.00	10.00
	Permeate	6	0.1	25	12.83	35.56	64.44
PSA	Feed	7	10	25	26.56	90.00	10.00
	Product	8	1	25	18.60	97.00	3.00
	Purge	9	1	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.49
2	12.83	1.28
3	26.56	2.95
4	7.96	0.00
Total Power [kW]		13.72
Total Power per product flow rate [kW/(Nm³/hr)]		0.16

A1. Candidate processes for conceptual design study

CD2.1: Hybrid Membrane & PSA (Zeolite) (Feed 100Lube/hr) w/ recycle

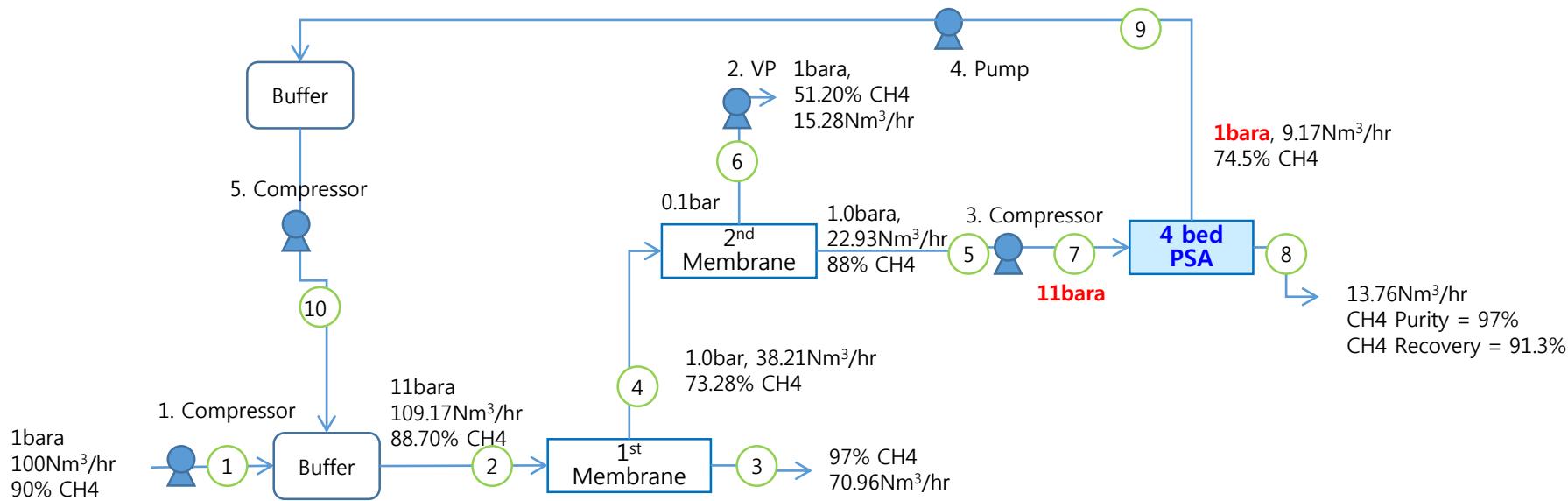


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO2 Conc. (mol.%)
Feed	Feed	1	1	25	100.00	90.00	10.00
Mem. 1	Feed	2	11	25	106.43	88.70	11.30
Mem. 1	Retentate	3	11	25	69.34	97.00	3.00
Mem. 1	Permeate	4	1	25	37.09	73.28	26.72
Mem. 2	Feed*	4	1	25	37.09	73.28	26.72
Mem. 2	Retentate	5	1	25	22.90	88.00	12.00
Mem. 2	Permeate	6	0.1	25	14.19	51.20	48.80
PSA	Feed	7	1.1	25	22.90	88.00	12.00
PSA	Product	8	1	25	16.47	97.00	3.00
PSA	Purge	9	0.02	25	6.43	74.50	25.50
	Recycled	10	10	25	6.43	74.50	25.50

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.92
2	14.19	1.72
3	22.90	0.08
4	6.43	3.34
5	6.43	0
Total Power [kW]		15.06
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.18

A1. Candidate processes for conceptual design study

CD2.2: Hybrid Membrane & PSA (CMS) (Feed 100Lube/hr) w/ recycle

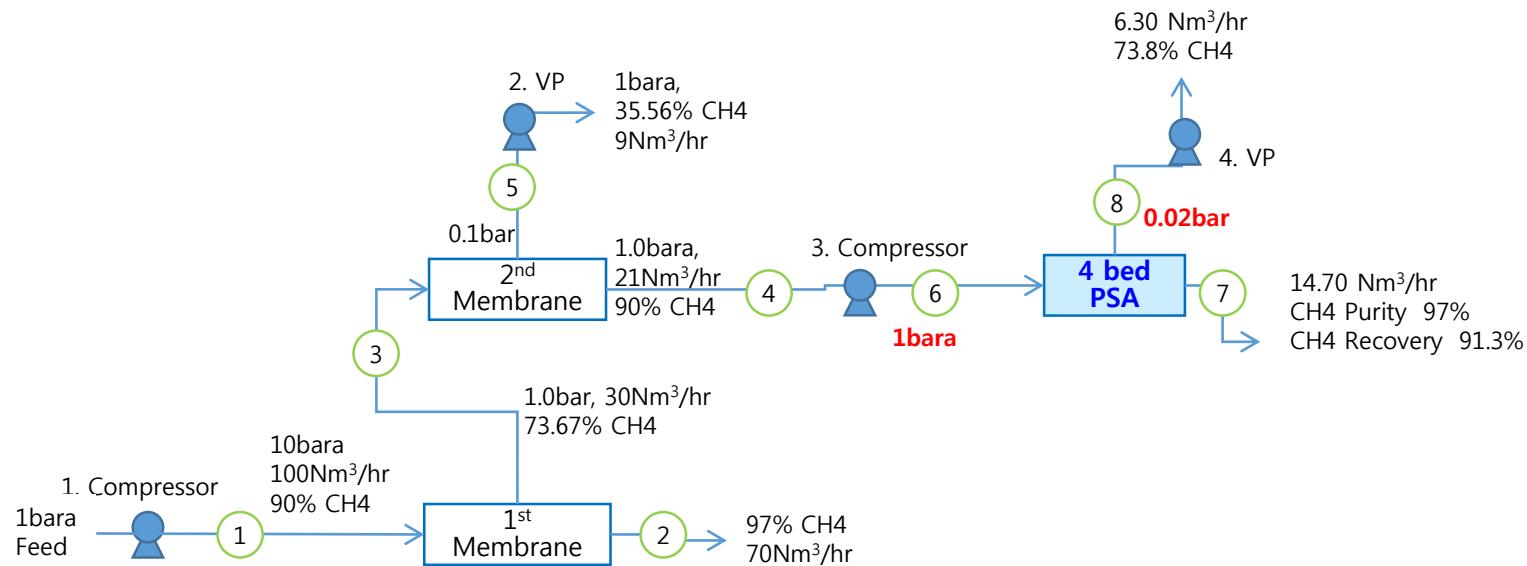


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Feed	Feed	1	1	25	100.00	90.00	10.00
Mem. 1	Feed	2	11	25	106.43	88.70	11.30
Mem. 1	Retentate	3	11	25	69.34	97.00	3.00
Mem. 1	Permeate	4	1	25	37.09	73.28	26.72
Mem. 2	Feed*	4	1	25	37.09	73.28	26.72
Mem. 2	Retentate	5	1	25	22.90	88.00	12.00
Mem. 2	Permeate	6	0.1	25	14.19	51.20	48.80
PSA	Feed	7	11	25	22.90	88.00	12.00
PSA	Product	8	1	25	16.47	97.00	3.00
PSA	Purge	9	1	25	6.43	74.50	25.50
	Recycled	10	11	25	6.43	74.50	25.50

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.92
2	14.19	1.72
3	22.90	2.73
4	6.43	0.94
5	6.43	0
Total Power [kW]		16.41
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.19

A1. Candidate processes for conceptual design study

CD3.1: Hybrid Membrane & PSA (Zeolite) (Feed 100Lube/hr) w/o recycle

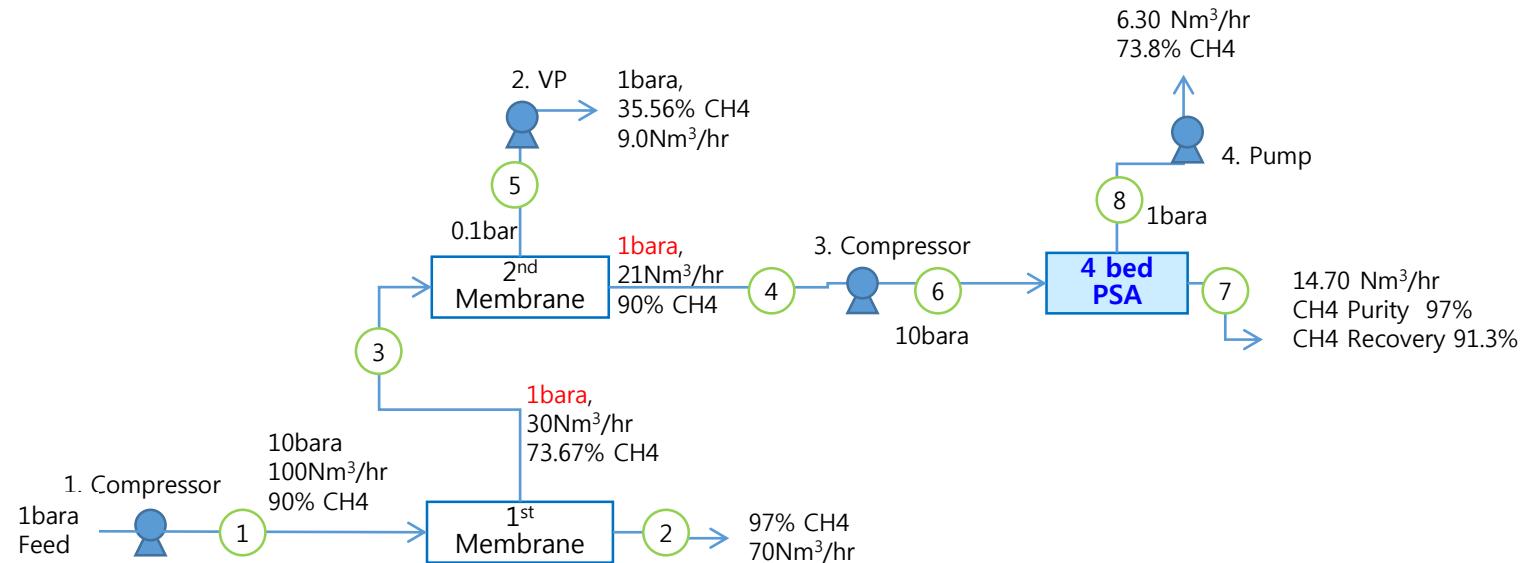


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO2 Conc. (mol.%)
Mem. 1	Feed	1	10	25	100.00	90.00	10.00
Mem. 1	Retentate	2	10	25	68.57	97.00	3.00
Mem. 1	Permeate	3	1	25	31.43	73.67	26.33
Mem. 2	Feed*	3	1	25	31.43	73.67	26.33
Mem. 2	Retentate	4	1	25	20.99	90.00	10.00
Mem. 2	Permeate	5	0.1	25	10.44	35.56	64.44
PSA	Feed	6	1	25	20.99	90.00	10.00
PSA	Product	7	1	25	14.70	97.00	3.00
PSA	Purge	8	0.02	25	6.29	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.94
2	10.44	1.01
3	20.99	0.00
4	6.29	1.17
Total Power [kW]		12.12
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.18

A1. Candidate processes for conceptual design study

CD3.2: Hybrid Membrane & PSA (CMS) (Feed 100Lube/hr) w/o recycle

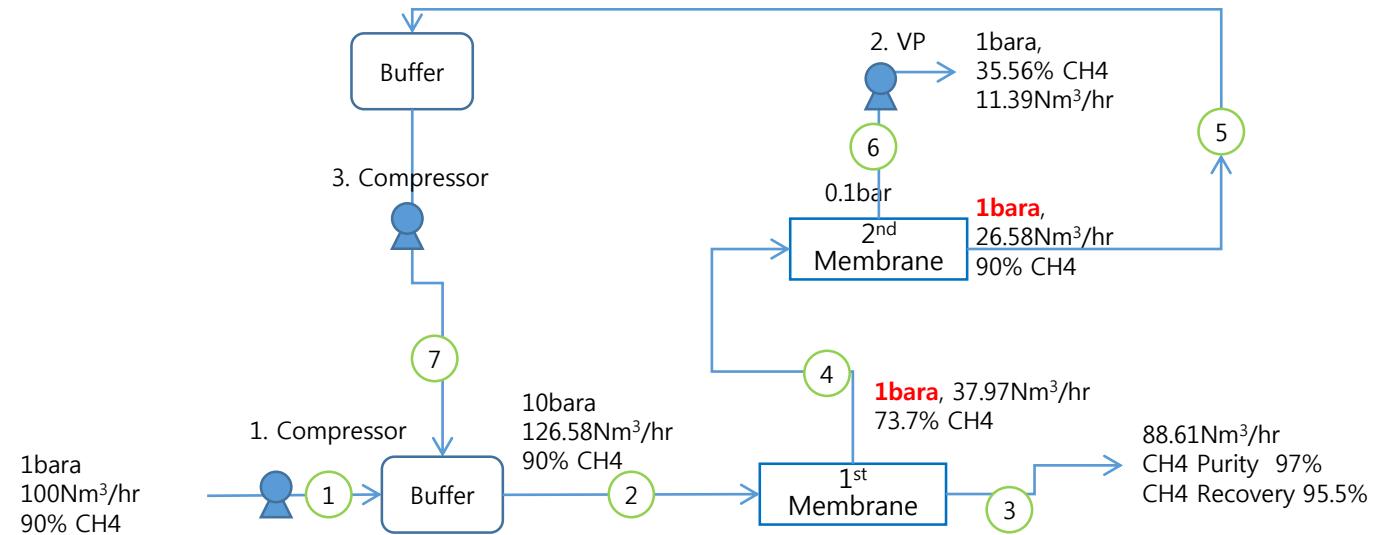


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Mem. 1	Feed	1	10	25	100.00	90.00	10.00
Mem. 1	Retentate	2	10	25	68.57	97.00	3.00
Mem. 1	Permeate	3	1	25	31.43	73.67	26.33
Mem. 2	Feed*	3	1	25	31.43	73.67	26.33
Mem. 2	Retentate	4	1	25	20.99	90.00	10.00
Mem. 2	Permeate	5	0.1	25	10.44	35.56	64.44
PSA	Feed	6	10	25	20.99	90.00	10.00
PSA	Product	7	1	25	14.70	97.00	3.00
PSA	Purge	8	1	25	6.29	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.94
2	10.44	1.01
3	20.99	2.09
4	6.29	0
Total Power [kW]		13.04
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.19

A1. Candidate processes for conceptual design study

CD4: Membrane System Only (Feed 100Lube/hr)

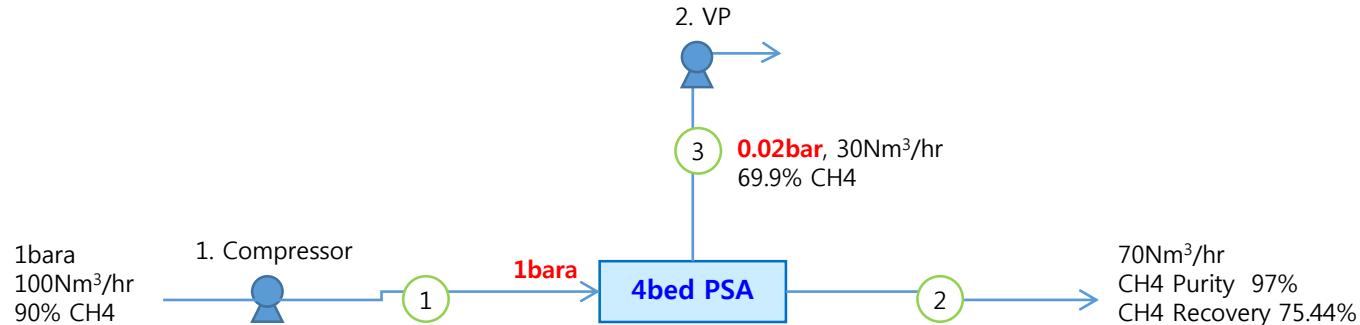


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Feed	Feed	1	1	25	100.00	90.00	10.00
Mem. 1	Feed	2	10	25	126.56	90.00	10.00
Mem. 1	Retentate	3	10	25	86.79	97.00	3.00
Mem. 1	Permeate	4	1	25	39.77	73.67	26.33
Mem. 2	Feed*	4	1	25	39.77	73.67	26.33
Mem. 2	Retentate	5	1	25	26.56	90.00	10.00
Mem. 2	Permeate	6	0.1	25	13.21	35.56	64.44
	Recycled	7	10	25	26.56	90.00	10.00

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.94
2	13.21	1.28
3	26.56	2.64
Total Power [kW]		13.86
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.16

A1. Candidate processes for conceptual design study

CD5.1: VSA System Only (Feed 100Lube/hr) (Zeolite)

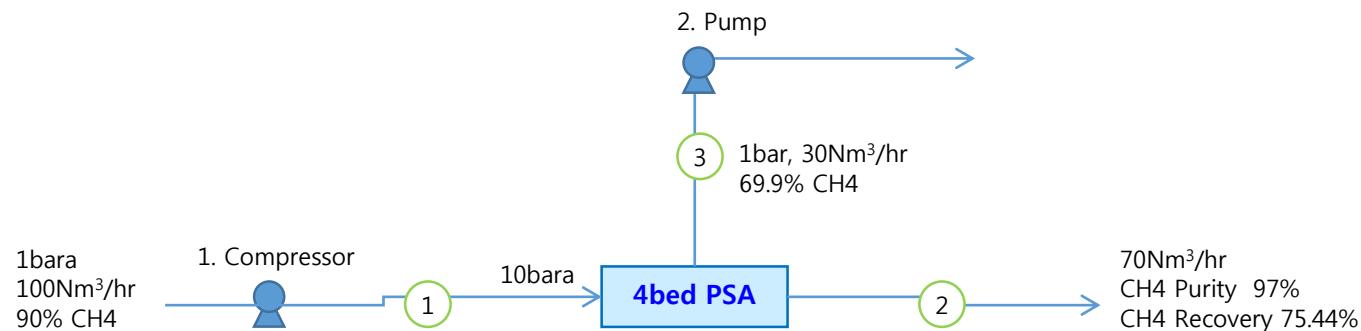


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA	Feed	1	1	25	100.00	90.00	10.00
PSA	Product	2	1	25	70.00	97.00	3.00
PSA	Purge	3	0.02	25	30.00	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
1	100.00	0.00
2	30.00	5.55
Total Power [kW]		5.55
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.08

A1. Candidate processes for conceptual design study

CD5.2: PSA System Only (Feed 100Lube/hr) (CMS)

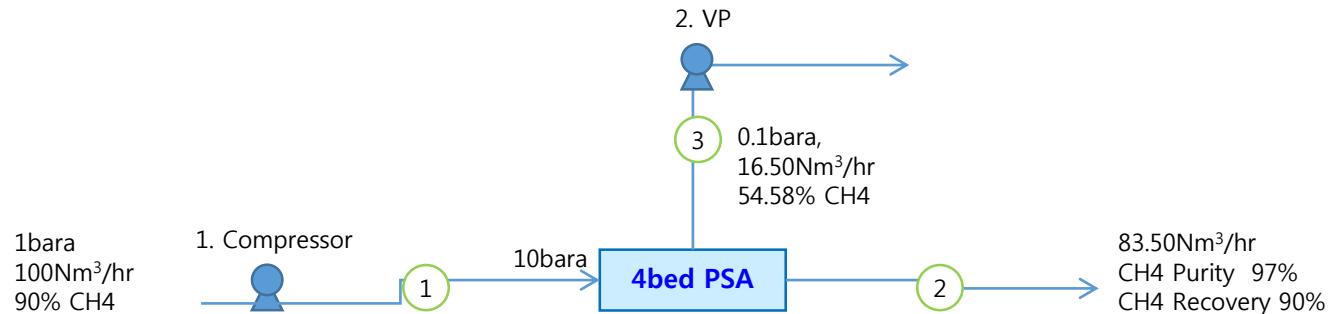


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA	Feed	1	10	25	100.00	90.00	10.00
PSA	Product	2	1	25	70.00	97.00	3.00
PSA	Purge	3	1	25	30.00	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.94
2	30.00	0.00
Total Power [kW]		9.94
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.14

A1. Candidate processes for conceptual design study

CD5.3: VPSA System Only (Feed 100Nm³/hr): CMS, 0.1bar desorption & 10bar adsorption

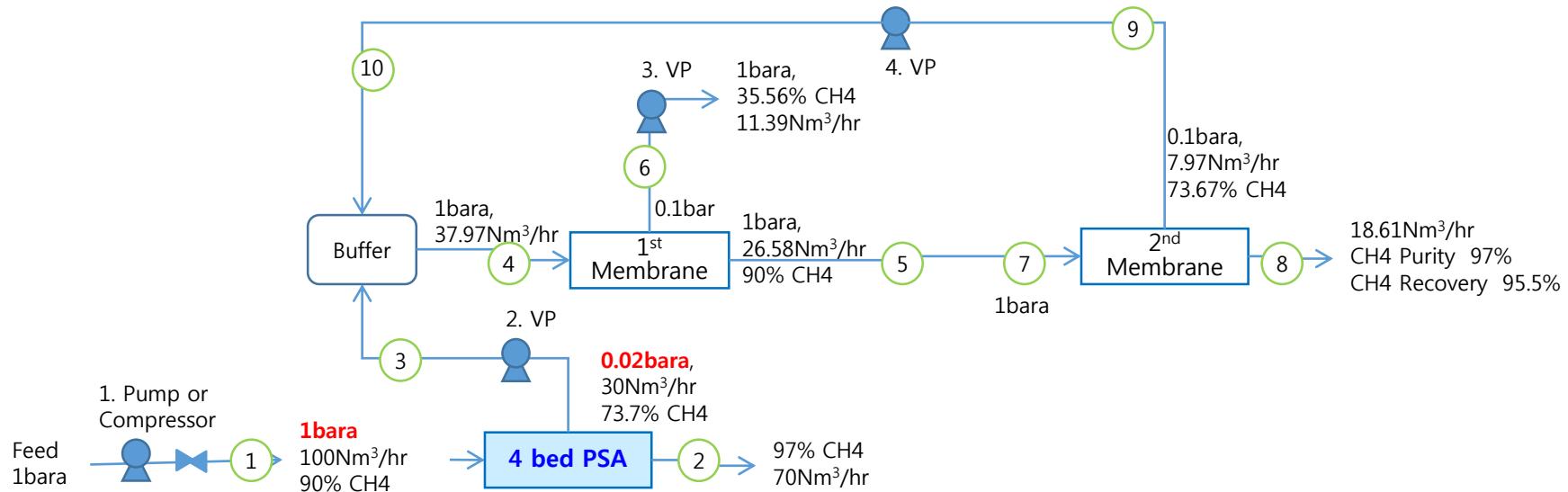


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA	Feed	1	10	25	100.00	90.00	10.00
PSA	Product	2	1	25	83.50	97.00	3.00
PSA	Purge	3	0.1	25	16.50	54.58	45.42

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.94
2	16.50	1.64
Total Power [kW]		11.58
Total Power per product flow rate [kW/(Nm³/hr)]		0.14

A1. Candidate processes for conceptual design study

CD6.1: Hybrid VSA(Zeolite) & Membrane (Feed 100Lube/hr) w/ recycle

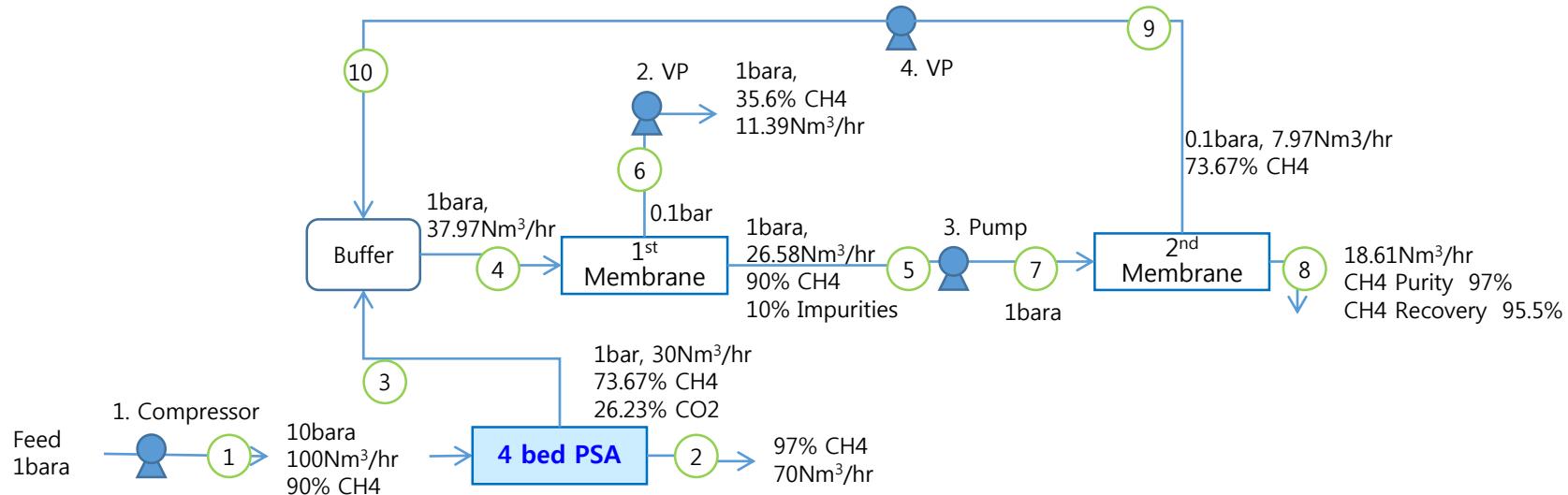


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA	Feed	1	1	25	100.00	90.00	10.00
	Product	2	1	25	69.92	97.00	3.00
	Purge	3	0.02	25	30.08	73.67	26.33
Mem. 1	Feed*	4	1	25	38.04	73.67	26.33
	Retentate	5	1	25	26.56	90.00	10.00
	Permeate	6	0.1	25	11.48	35.56	64.44
Mem. 2	Feed	7	1	25	26.56	90.00	10.00
	Retentate	8	1	25	18.60	97.00	3.00
	Permeate	9	0.1	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate (Nm ³ /hr)	Power (kW)
1	100.00	0
2	30.08	5.55
3	11.48	1.28
4	7.96	0.79
Total Power [kW]		7.62
Total Power per product flow rate [kW/(Nm³/hr)]		0.09

A1. Candidate processes for conceptual design study

CD6.2: Hybrid PSA(CMS) & Membrane (Feed 100Lube/hr) w/ recycle

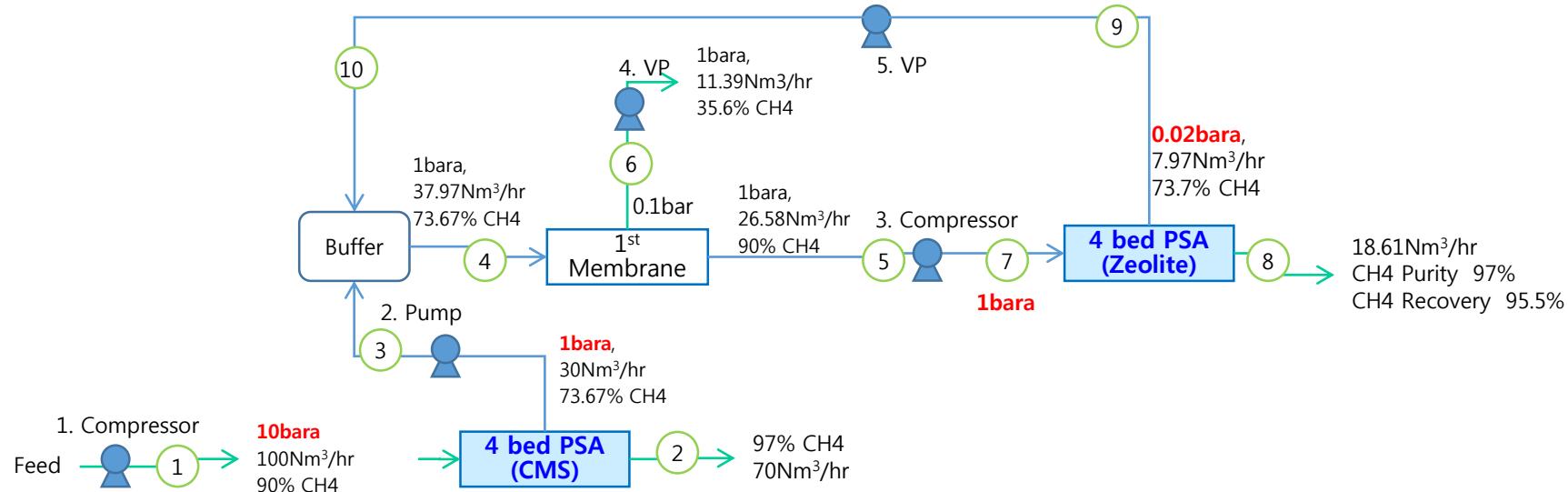


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA	Feed	1	10	25	100.00	90.00	10.00
	Product	2	1	25	69.92	97.00	3.00
	Purge	3	1	25	30.08	73.67	26.33
Mem. 1	Feed*	4	1	25	38.04	73.67	26.33
	Retentate	5	1	25	26.56	90.00	10.00
Mem. 1	Permeate	6	0.1	25	11.48	35.56	64.44
	Feed	7	1	25	26.56	90.00	10.00
Mem. 2	Retentate	8	1	25	18.60	97.00	3.00
	Permeate	9	0.1	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate (Nm ³ /hr)	Power (kW)
1	100.00	9.94
2	11.48	1.28
3	26.56	0
4	7.96	0.79
Total Power [kW]		12.01
Total Power per product flow rate [kW/(Nm³/hr)]		0.14

A1. Candidate processes for conceptual design study

CD7.1. Hybrid VPSA(CMS/Zeolite) & Membrane (Feed 100Lube/hr) w/ recycle

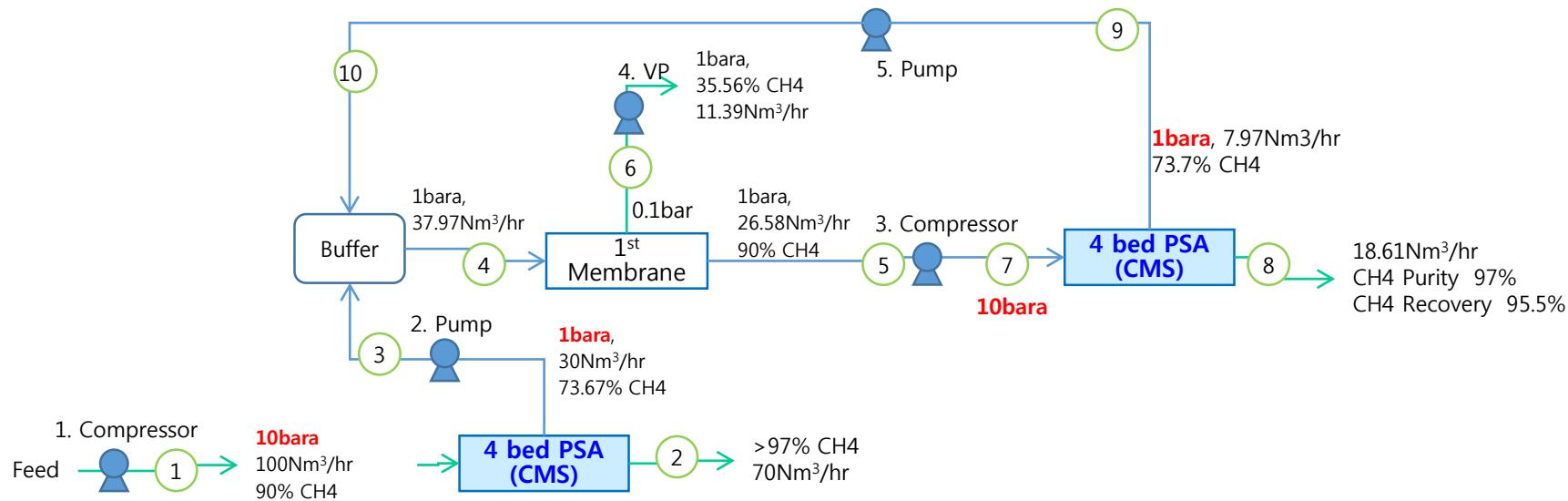


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
PSA 1	Feed	1	10	25	100.00	90.00	10.00
	Product	2	1	25	68.57	97.00	3.00
	Purge	3	1	25	31.43	73.67	26.33
Mem. 1	Feed*	4	1	25	39.39	73.67	26.33
	Retentate	5	1	25	26.57	90.00	10.00
	Permeate	6	0.1	25	12.82	35.56	64.44
PSA 2	Feed	7	1	25	26.57	90.00	10.00
	Product	8	1	25	18.61	97.00	3.00
	Purge	9	0.02	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.93
2	31.43	0.00
3	26.57	0.00
4	12.82	1.28
5	7.96	1.48
Total Power [kW]		12.69
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.15

A1. Candidate processes for conceptual design study

CD7.2. Hybrid PSA(CMS) & Membrane (Feed 100Lube/hr) w/ recycle

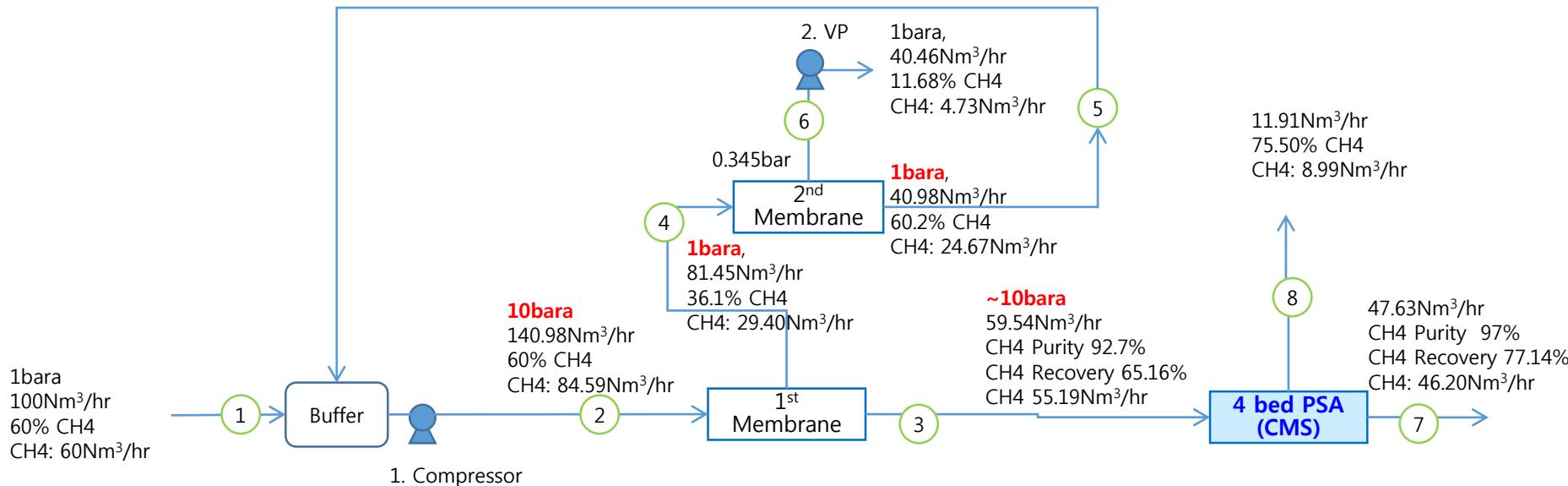


	Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO2 Conc. (mol.%)
PSA 1	Feed	1	10	25	100.00	90.00	10.00
	Product	2	1	25	68.57	97.00	3.00
	Purge	3	1	25	31.43	73.67	26.33
Mem. 1	Feed*	4	1	25	39.39	73.67	26.33
	Retentate	5	1	25	26.57	90.00	10.00
	Permeate	6	0.1	25	12.82	35.56	64.44
PSA 2	Feed	7	10	25	26.57	90.00	10.00
	Product	8	1	25	18.61	97.00	3.00
	Purge	9	1	25	7.96	73.67	26.33
	Recycled	10	1	25	7.96	73.67	26.33

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
	Nm ³ /hr	kW
1	100.00	9.93
2	31.43	0.00
3	26.57	2.64
4	12.82	1.28
5	7.96	0
Total Power [kW]		13.85
Total Power per product flow rate [kW/(Nm³/hr)]		0.16

A1. Candidate processes for conceptual design study

CD8.1: Hybrid PSA & Membrane with Recycle (Feed 100Lube/hr)
 (when low CH4 composition in feed gas)

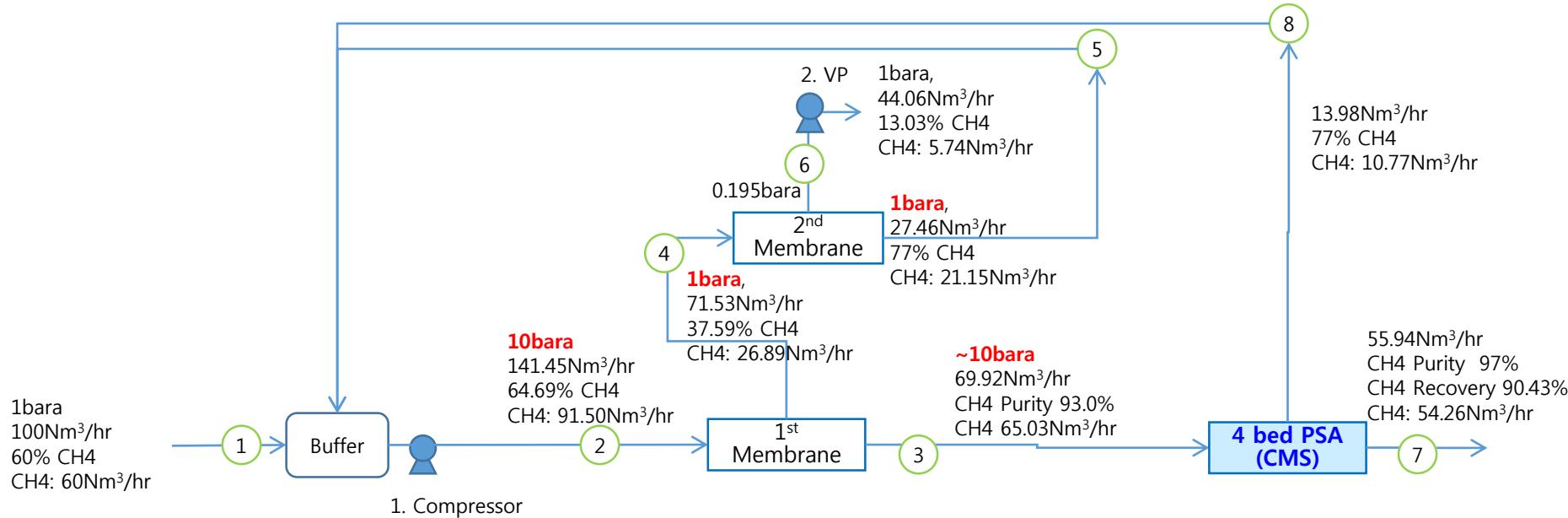


Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Feed	1	1	25	100.00	60.00	40.00
Mem. 1	Feed w/Recycle	2	10	140.92	60.00	40.00
Mem. 1	Retentate	3	10	58.38	92.70	7.30
Mem. 1	Permeate	4	1	82.54	36.10	63.90
Mem. 2	Feed	4	1	85.54	36.10	63.90
Mem. 2	Retentate	5	1	40.95	60.20	39.80
Mem. 2	Permeate	6	0.345	44.59	11.68	88.32
PSA	Feed	3	10	58.38	92.70	7.30
PSA	Product	7	1	47.63	97.00	3.00
PSA	Purge	8	1	10.75	75.50	24.50

Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
1	140.92	13.97
2	44.59	1.84
Total Power [kW]		15.81
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.33

A1. Candidate processes for conceptual design study

CD8.2: Hybrid PSA & Membrane with Recycle (Feed 100Lube/hr)
 (when low CH4 composition in feed gas)



Stream	Stream #	Pressure (bara)	Temperature (°C)	Flow rate (Nm ³ /h)	CH4 Conc. (mol.%)	CO ₂ Conc. (mol.%)
Feed	1	1	25	100.00	60.00	40.00
Mem. 1	Feed w/Recycle	2	10	137.24	64.98	35.02
Mem. 1	Retentate	3	10	68.53	93.00	7.00
Mem. 1	Permeate	4	1	68.71	37.59	62.41
Mem. 2	Feed	4	1	68.71	37.59	62.41
Mem. 2	Retentate	5	1	27.17	77.00	23.00
Mem. 2	Permeate	6	0.195	41.54	13.03	86.97
PSA	Feed	3	10	68.53	93.00	7.00
PSA	Product	7	1	58.46	97.00	3.00
PSA	Purge	8	1	10.07	77.00	23.00

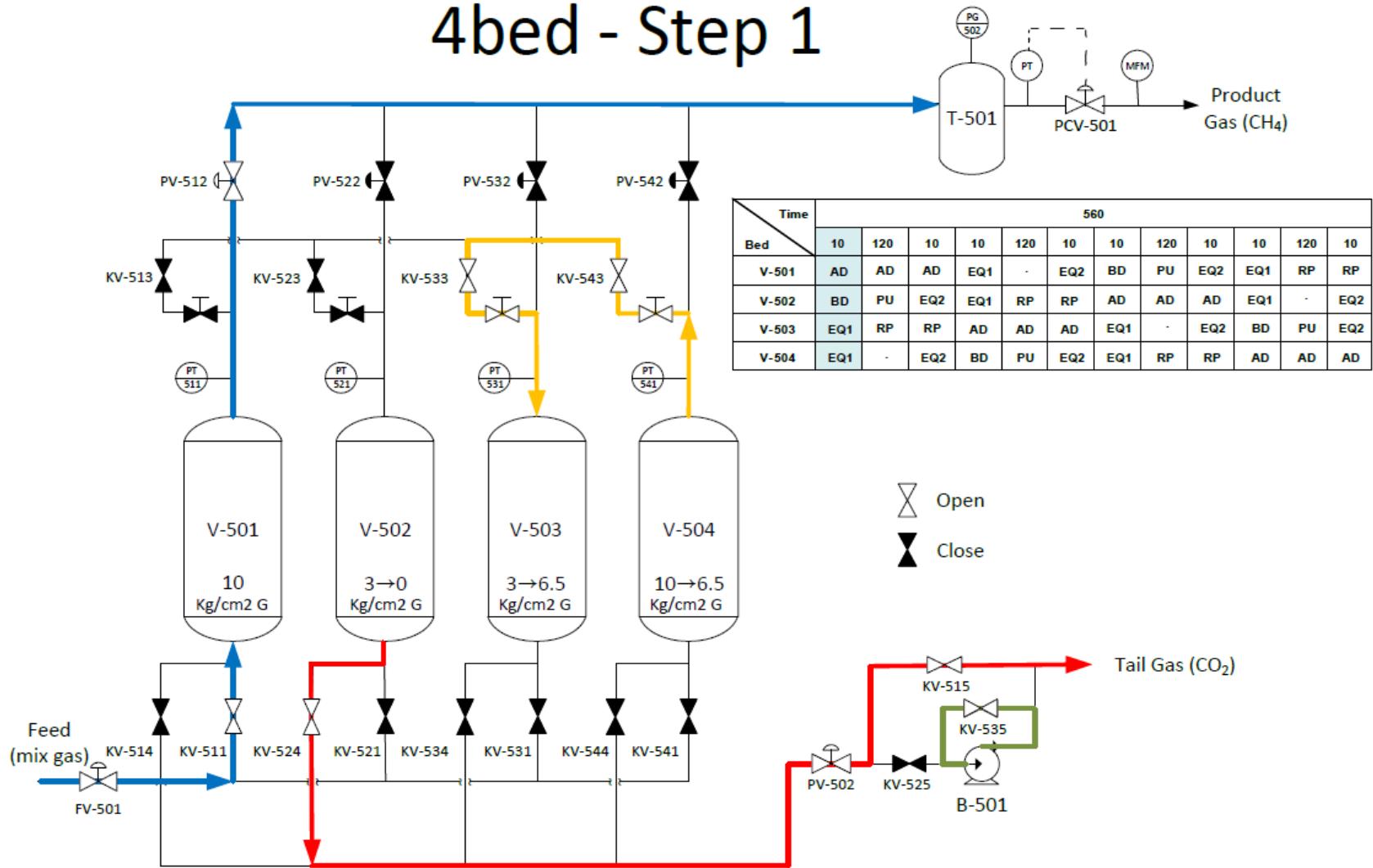
Power Unit	Flow Rate [Nm ³ /hr]	Power [kW]
1	137.24	13.99
2	41.54	3.27
Total Power [kW]		17.26
Total Power per product flow rate [kW/(Nm ³ /hr)]		0.3

A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 1

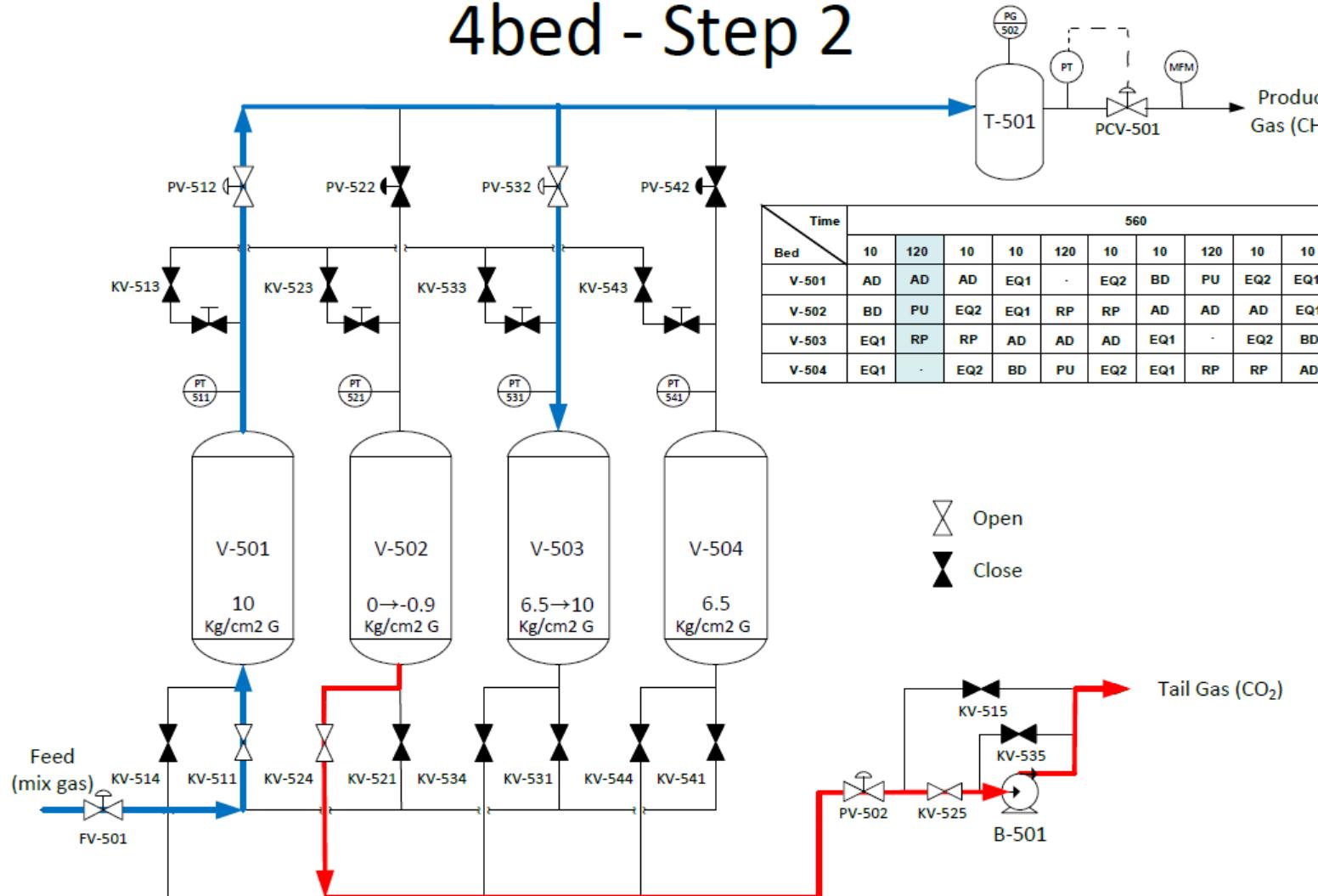


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 2

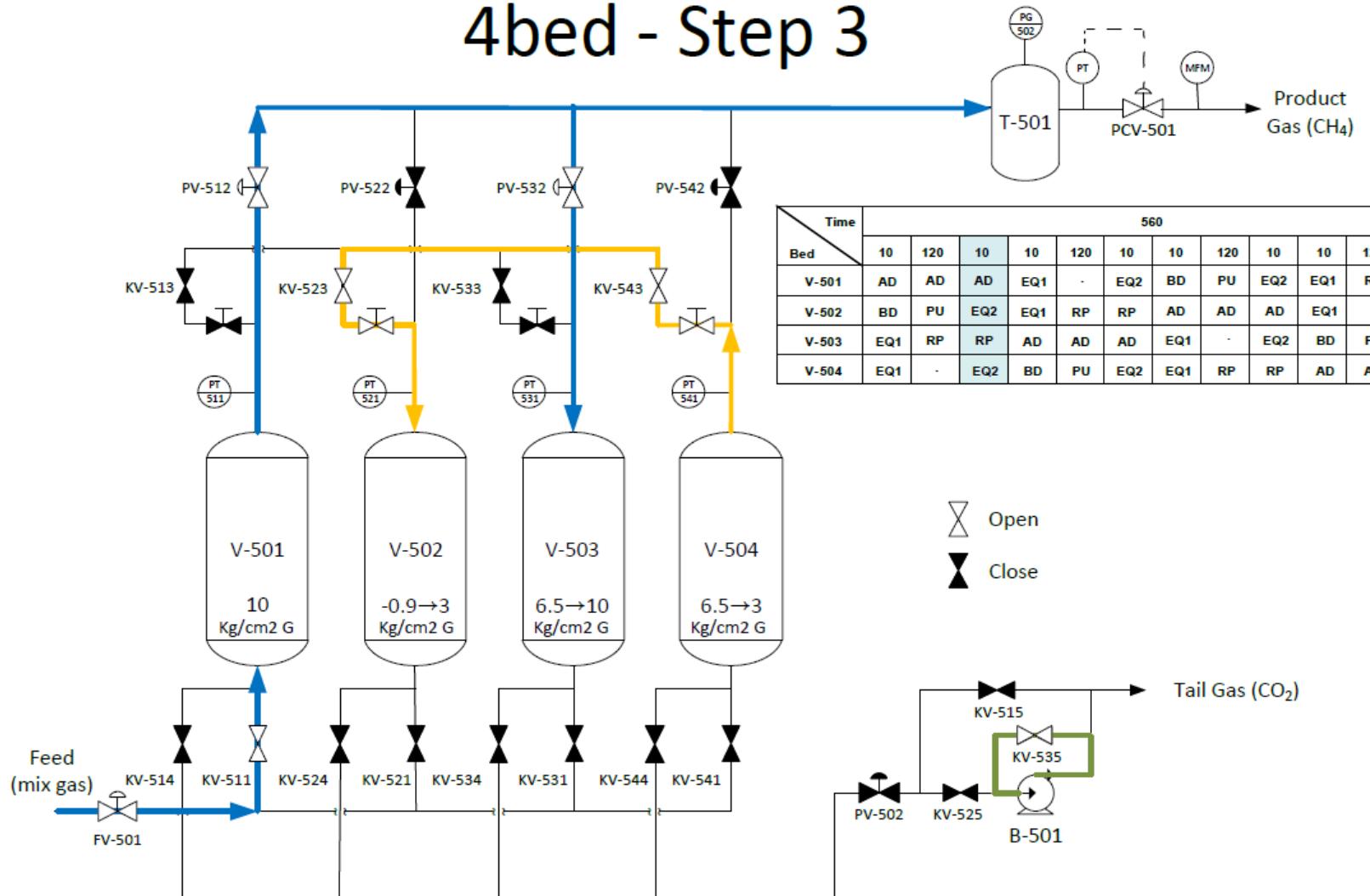


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 3

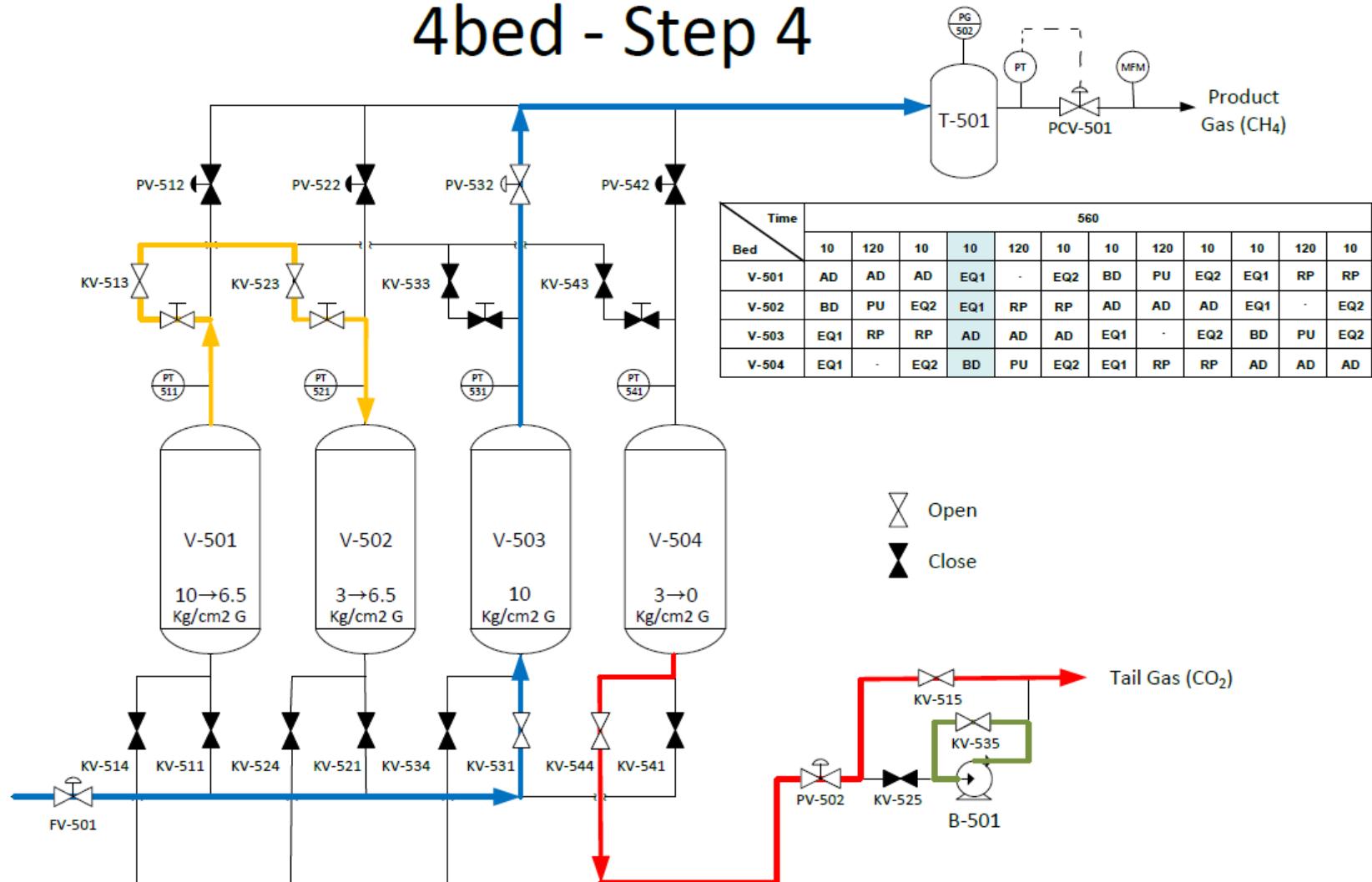


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 4

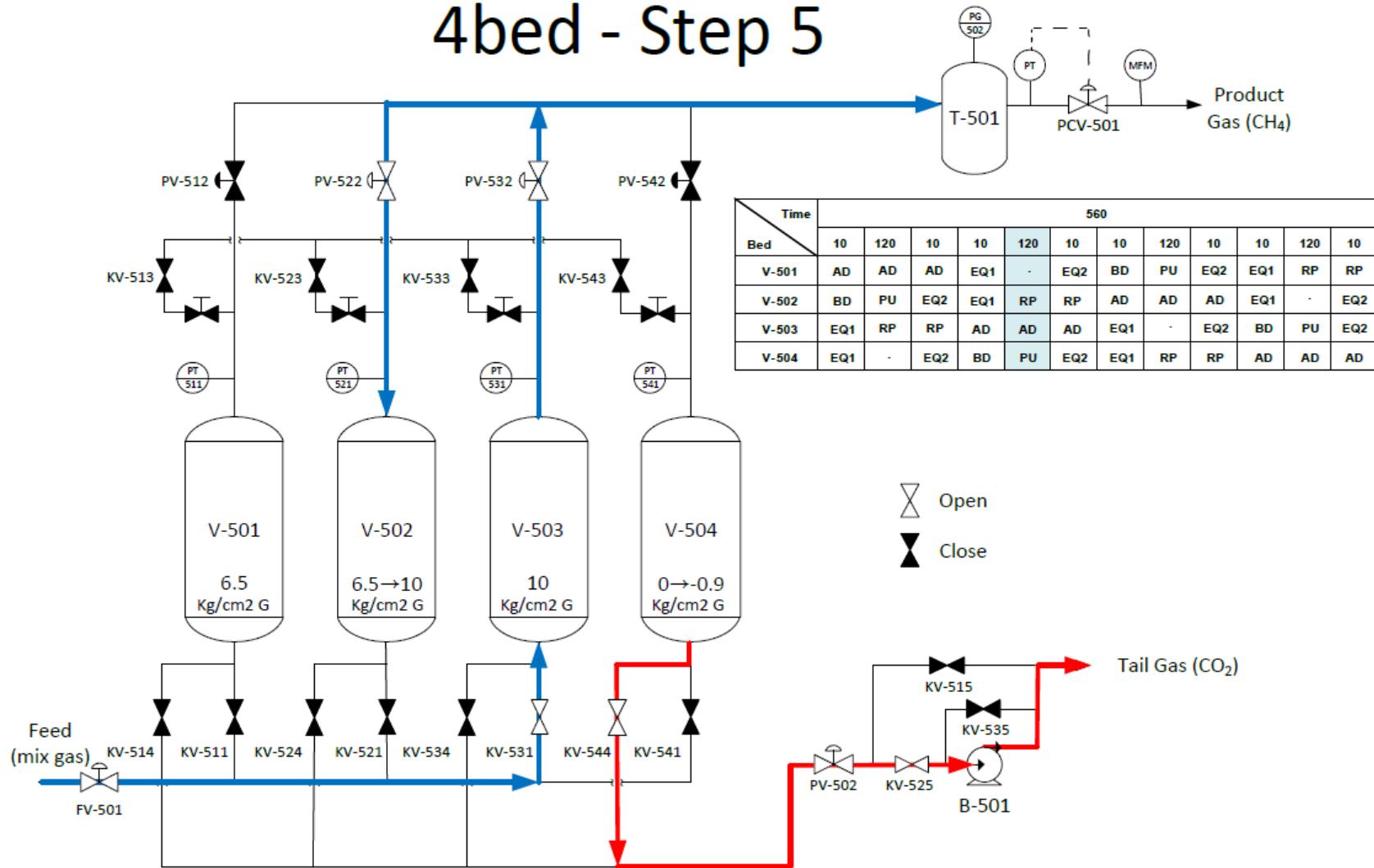


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 5

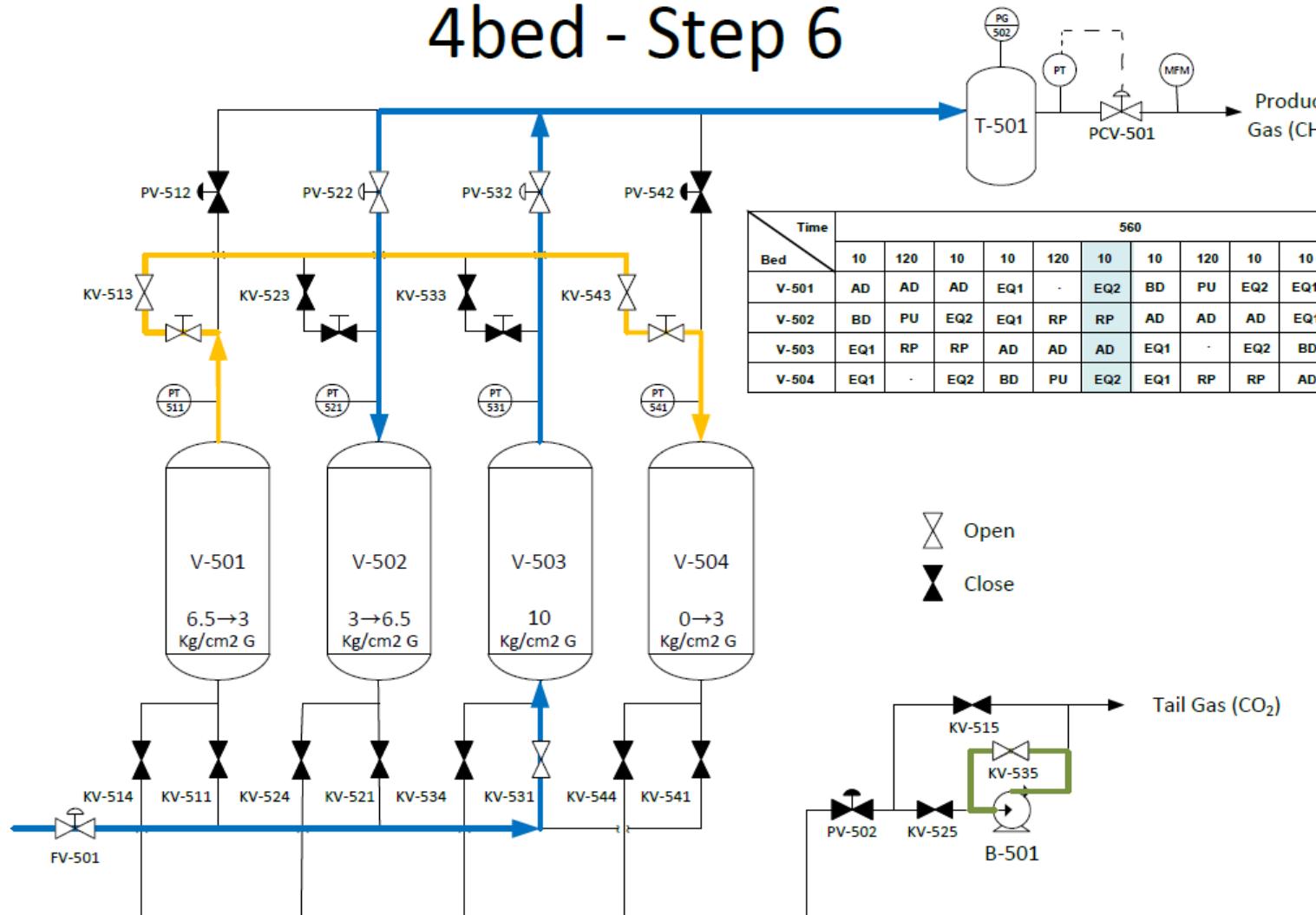


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 6

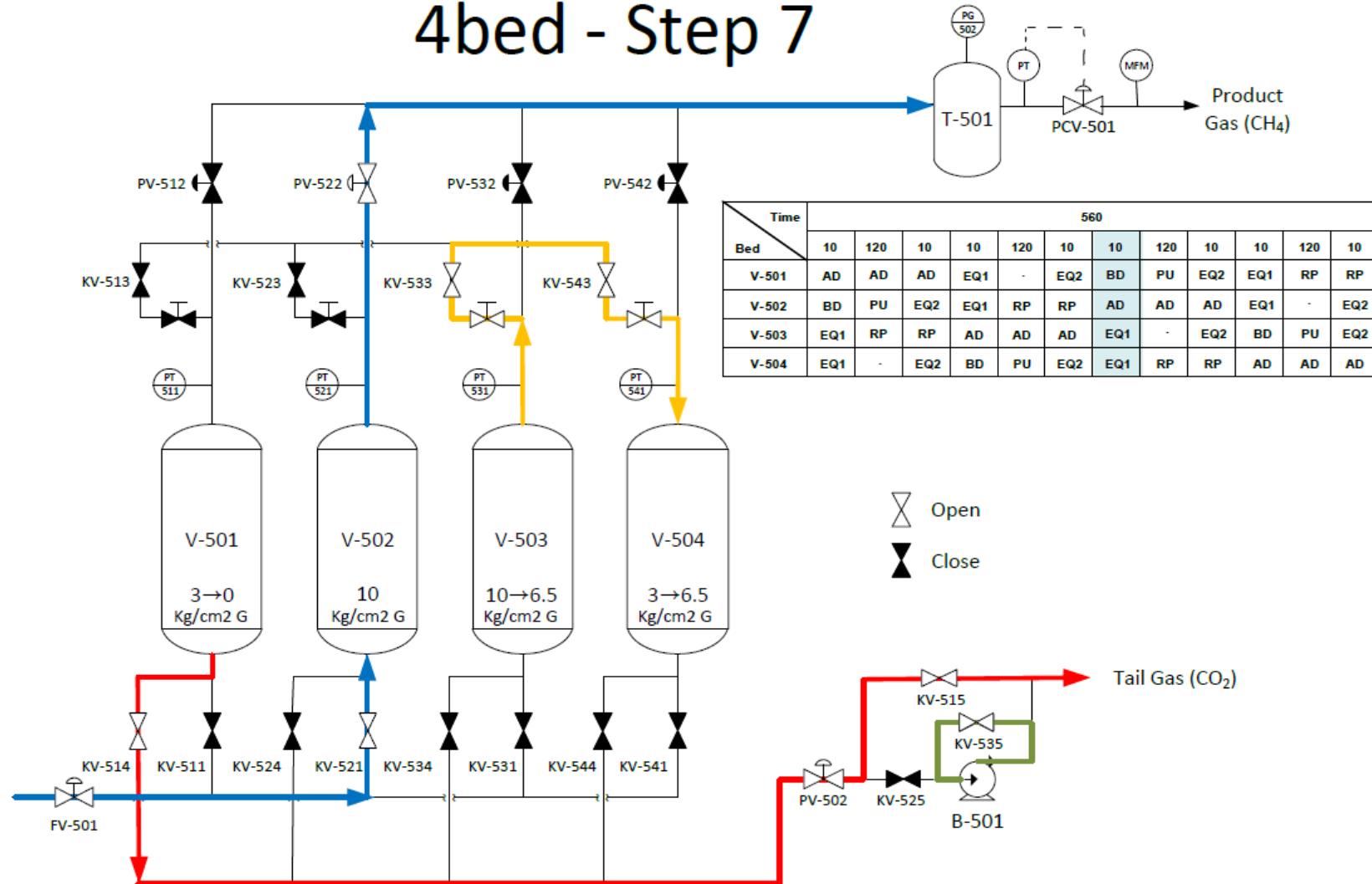


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 7

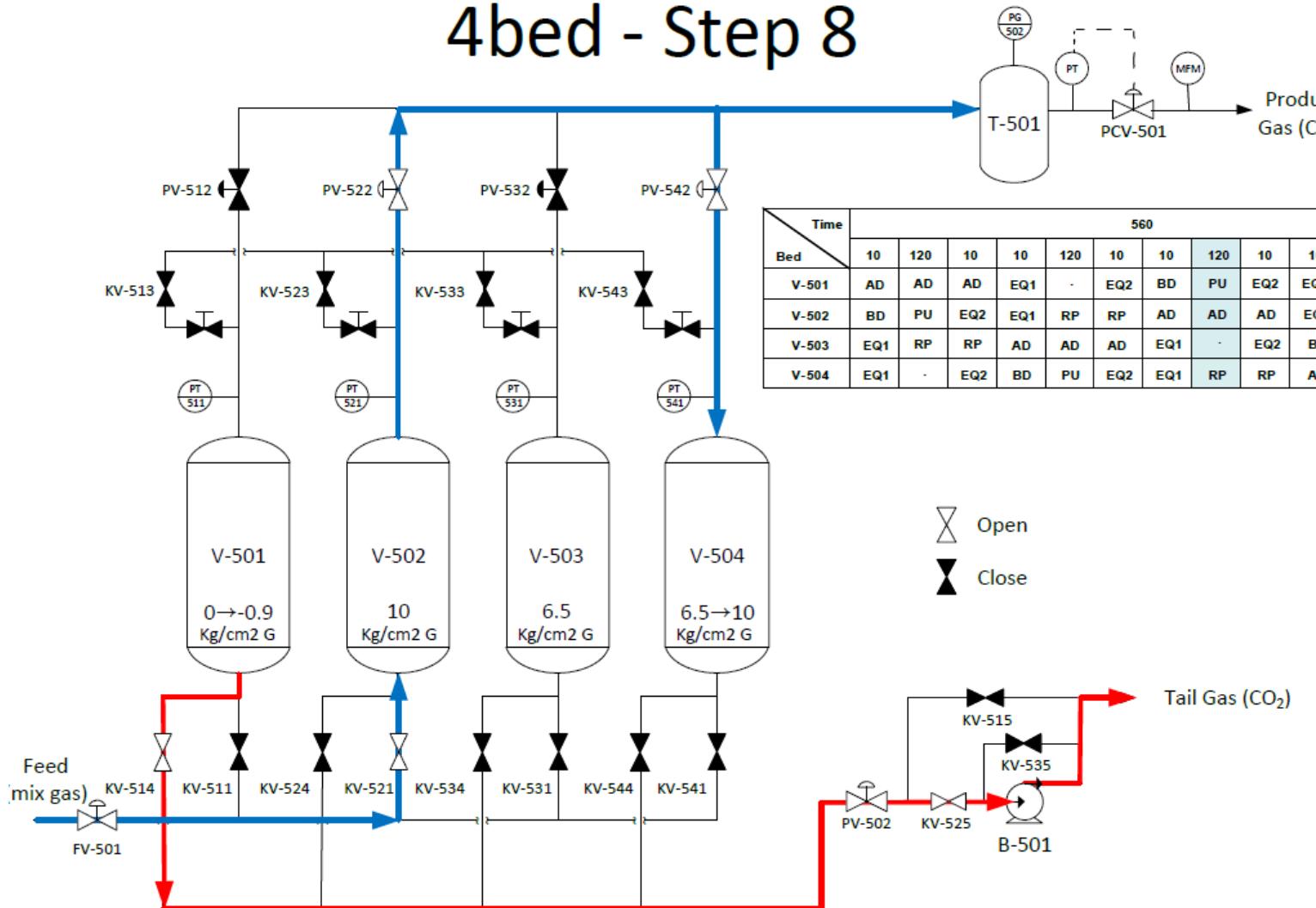


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 8

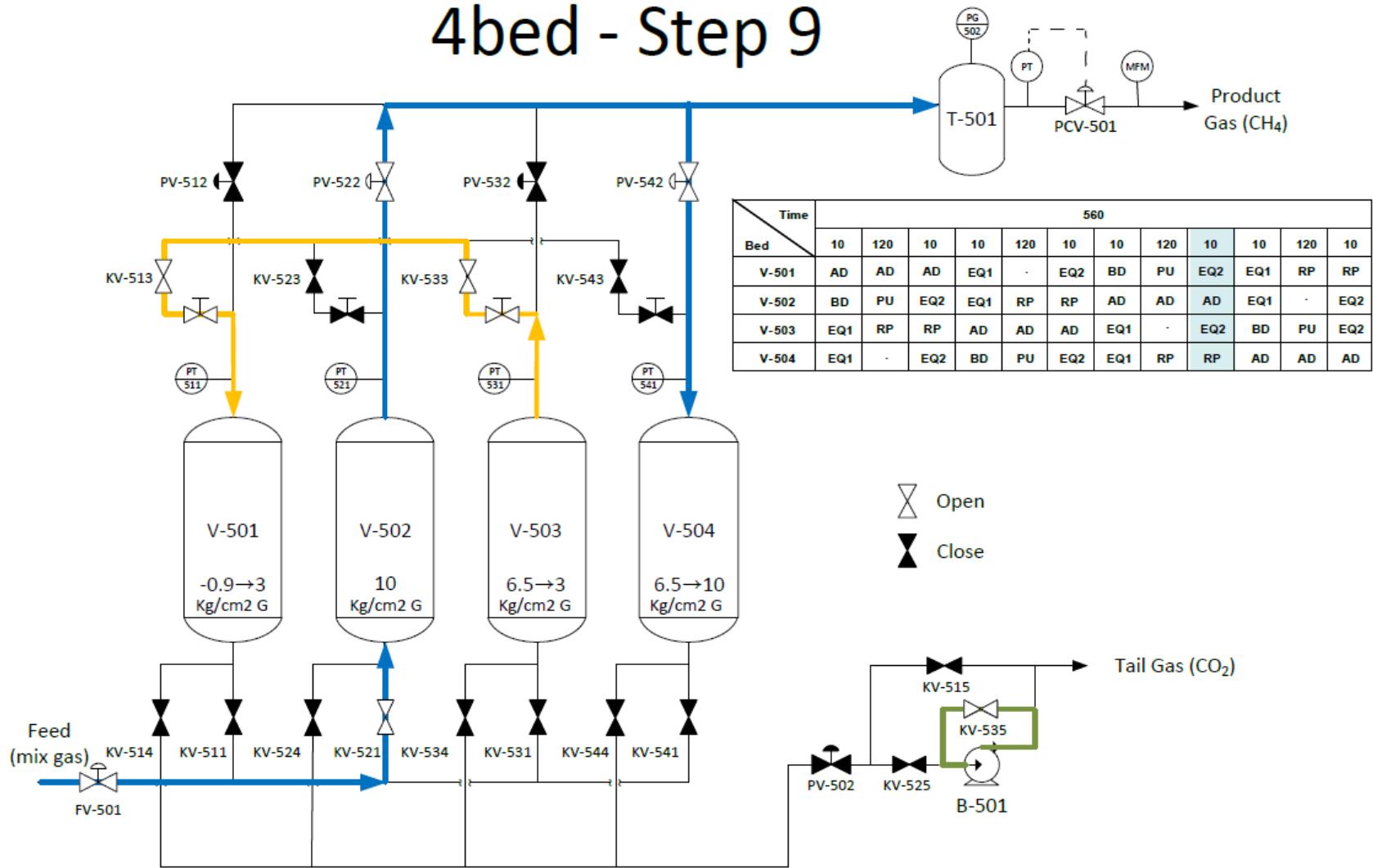


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 9

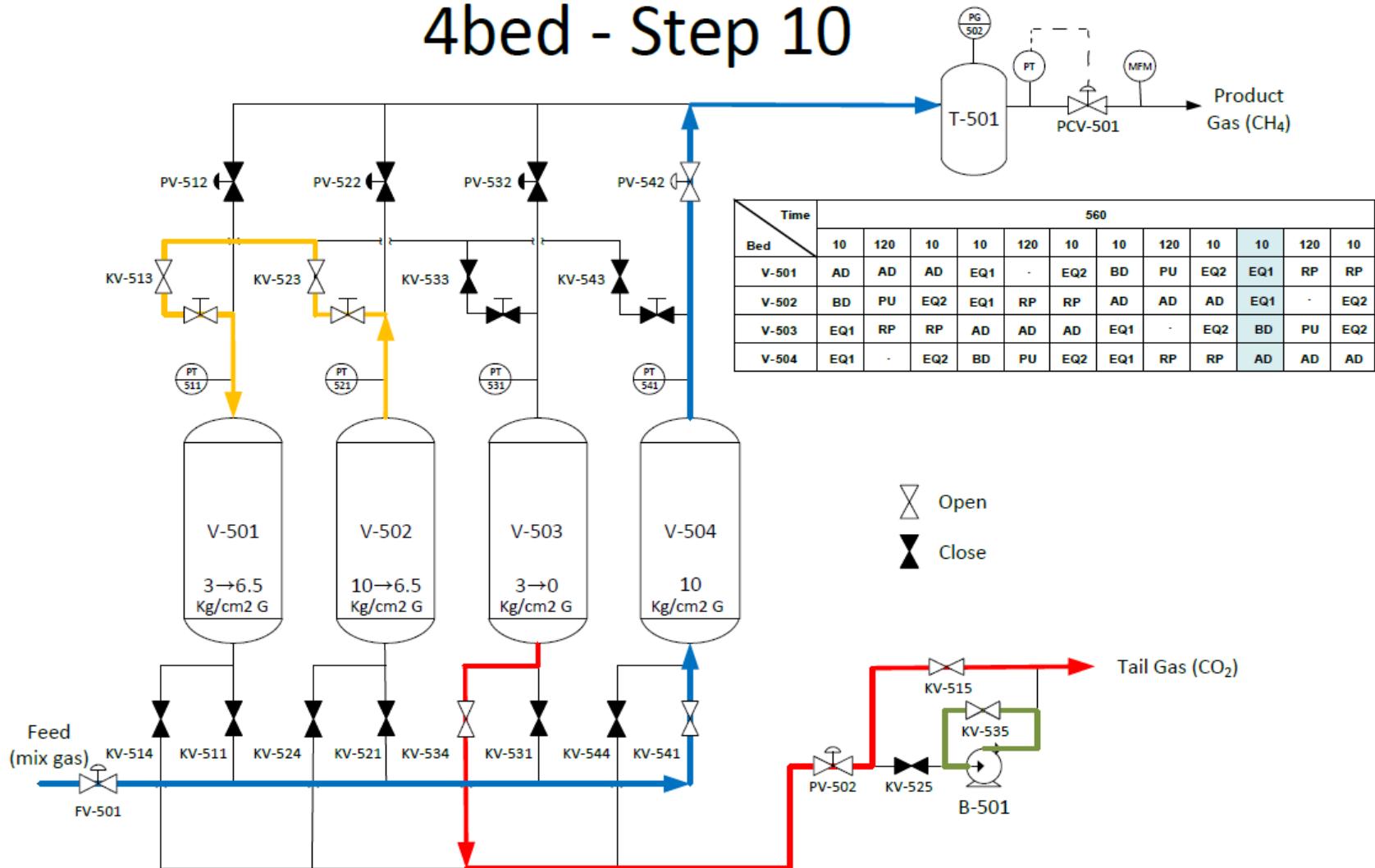


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 10

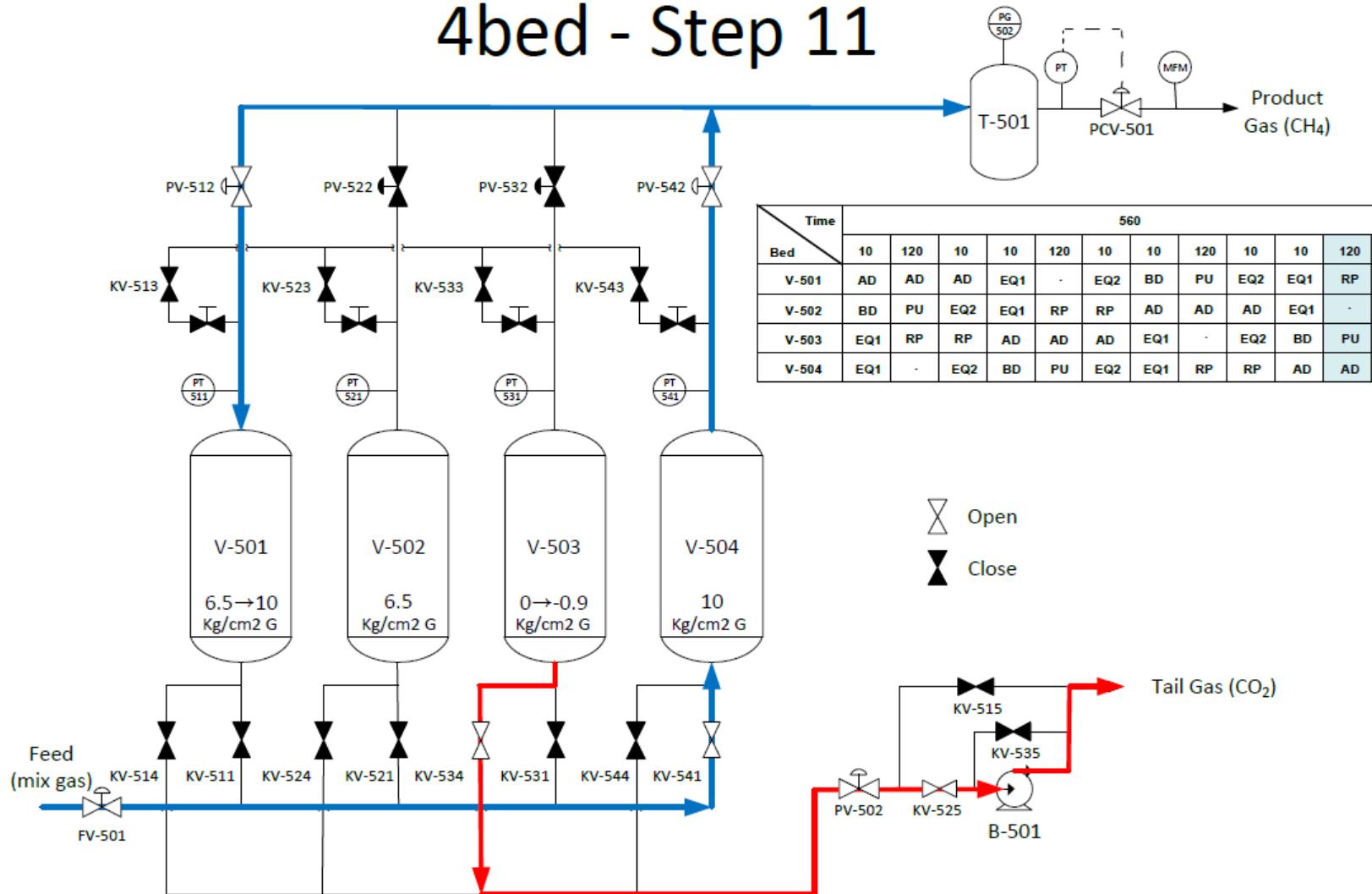


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 11

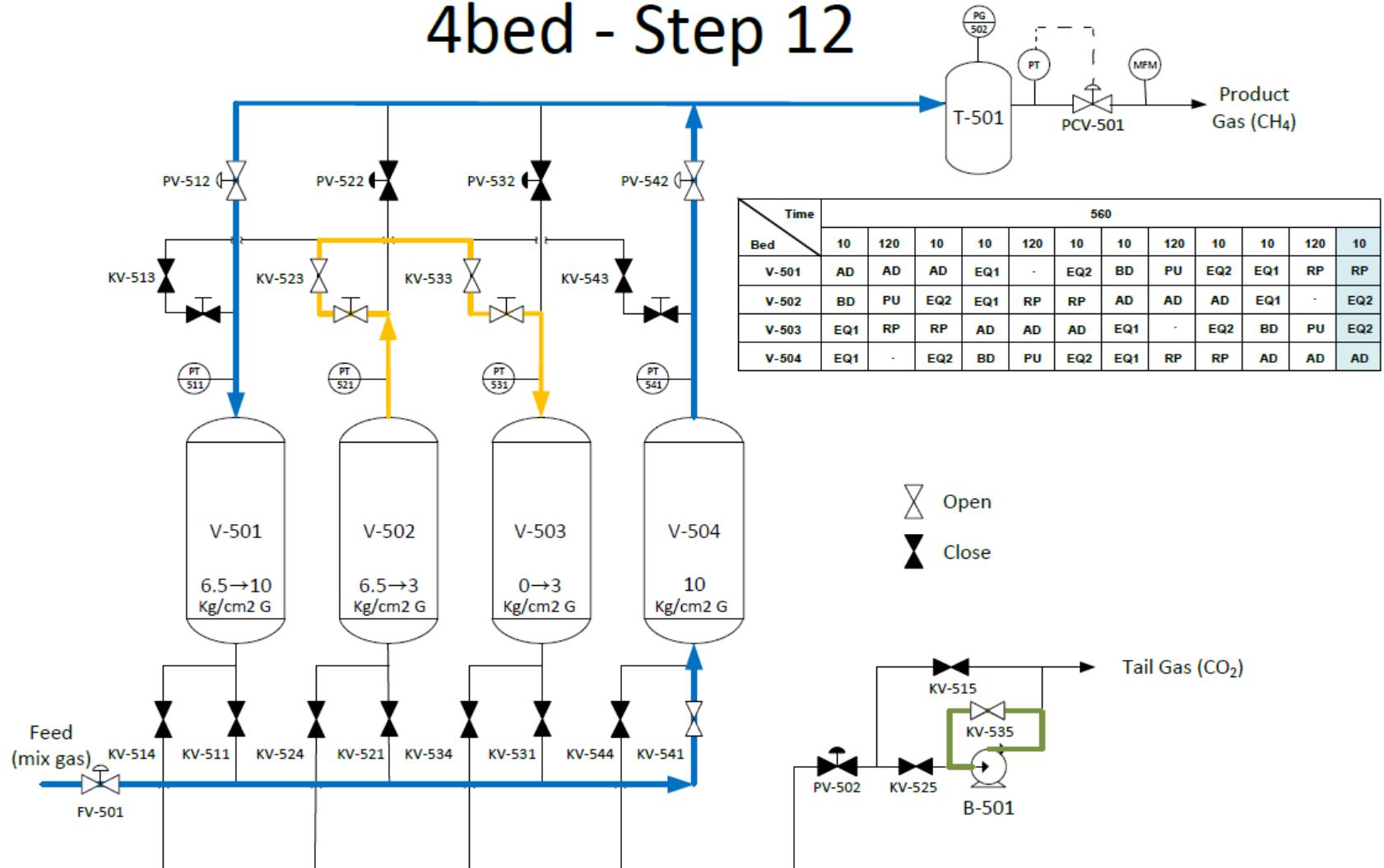


A2. Operation step of four bed PSA process

Four Bed Twelve Operating Step PSA Process



4bed - Step 12

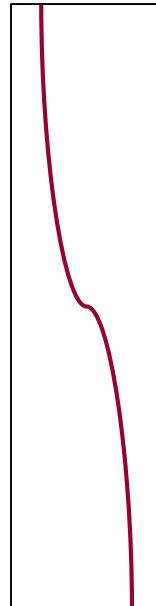


A3. Definition of cyclic steady state (CSS)

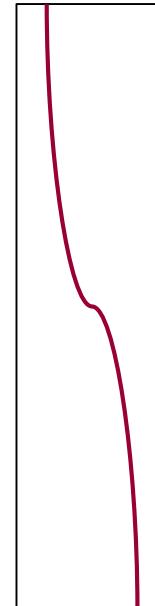


What does cyclic steady state mean?

Variable profiles (temperature, concentration, adsorbed amounts) within the bed at the start of a cycle are same as those at the end of the cycle



=



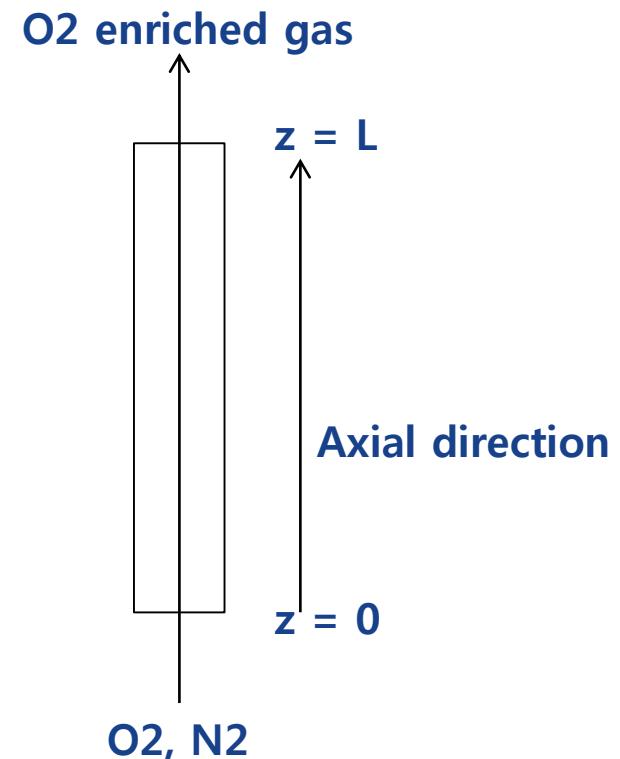
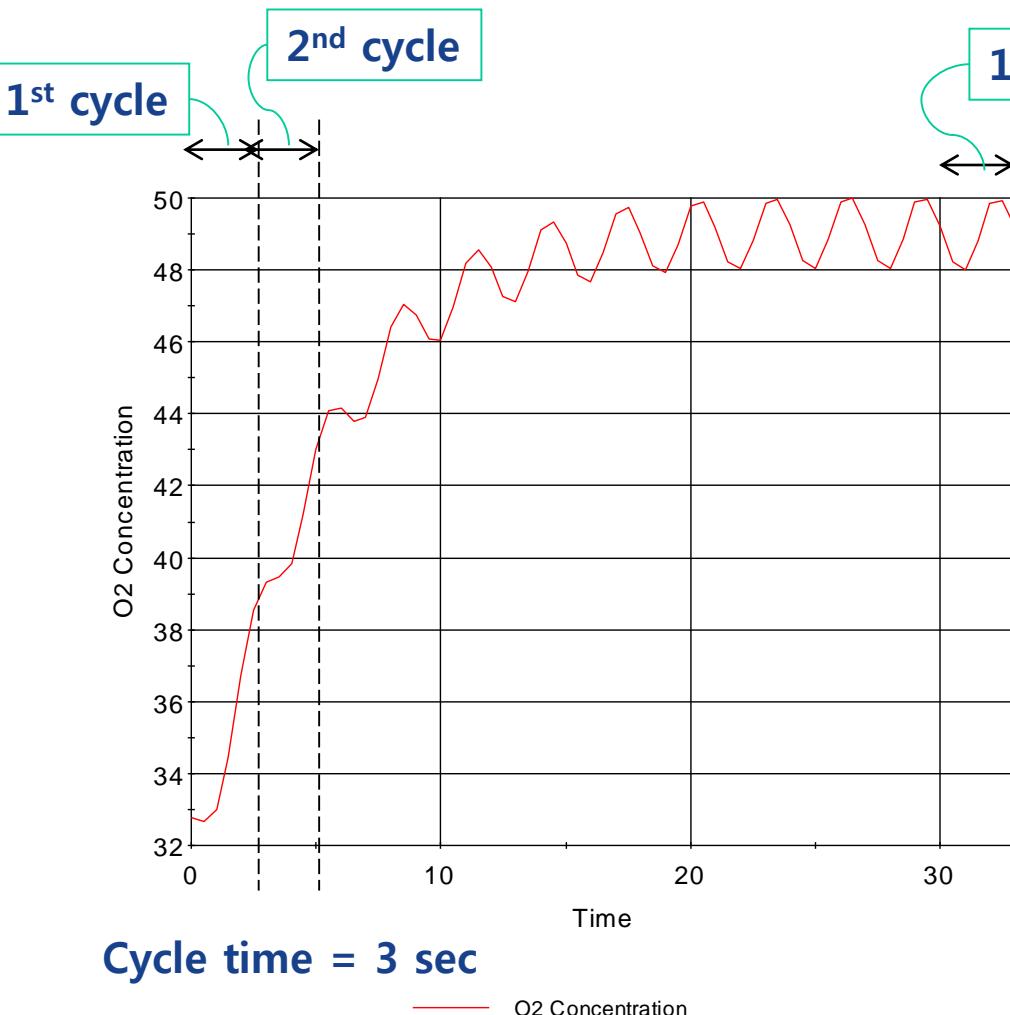
Time = 0

Time = t_{cycle}

A3. Definition of cyclic steady state (CSS)



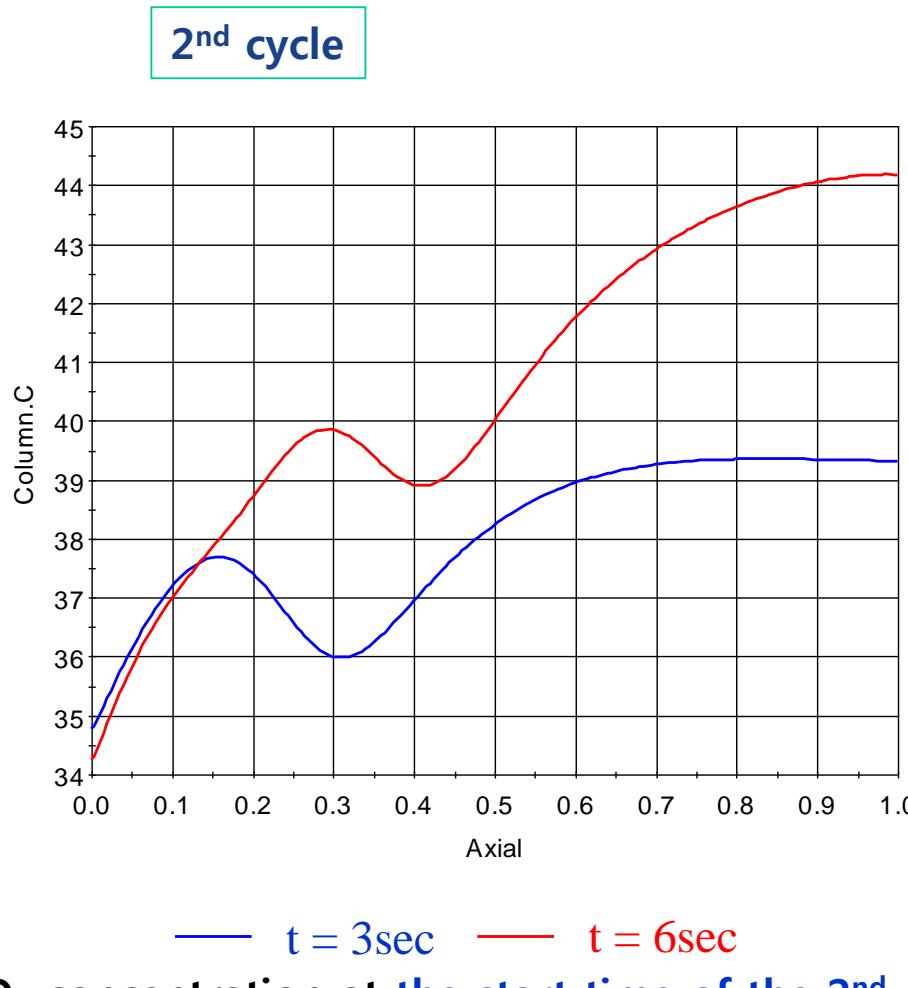
What does cyclic steady state mean?



A3. Definition of cyclic steady state (CSS)



What does cyclic steady state mean?



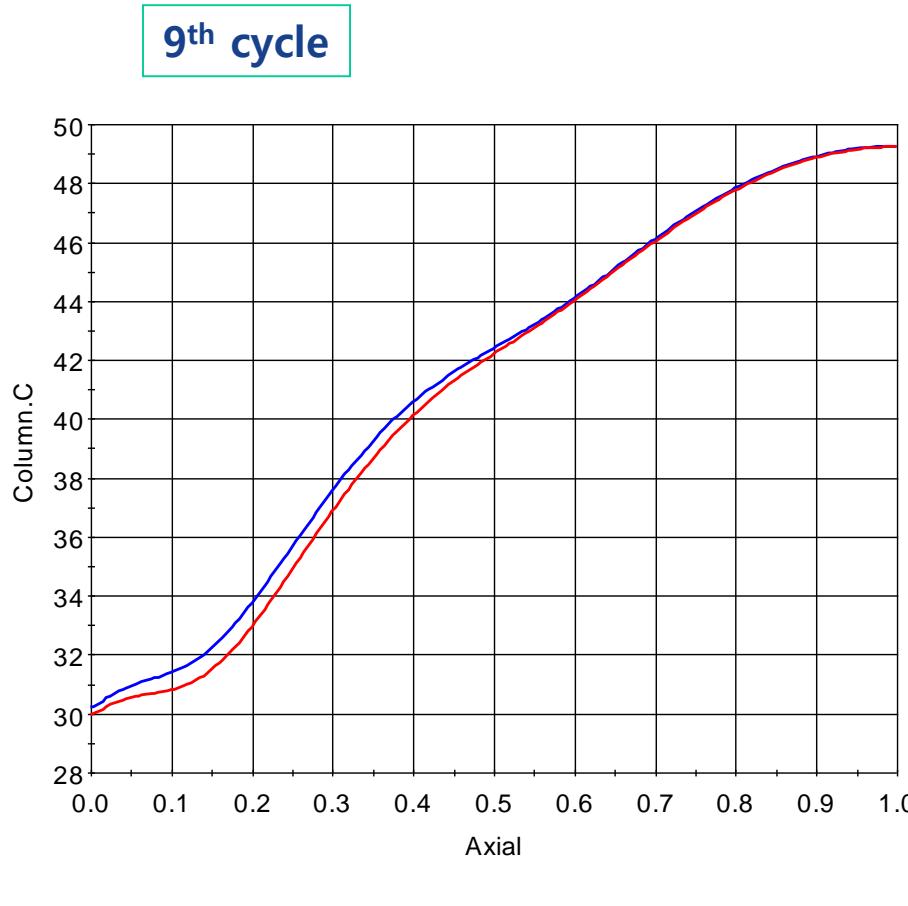
$\phi|_{t=0} \neq \phi|_{t=t\text{cycle}}$
Not Yet
Cyclic Steady State

Fig. O₂ concentration at the start time of the 2nd cycle & the end time of the 2nd cycle

A3. Definition of cyclic steady state (CSS)



What does cyclic steady state mean?



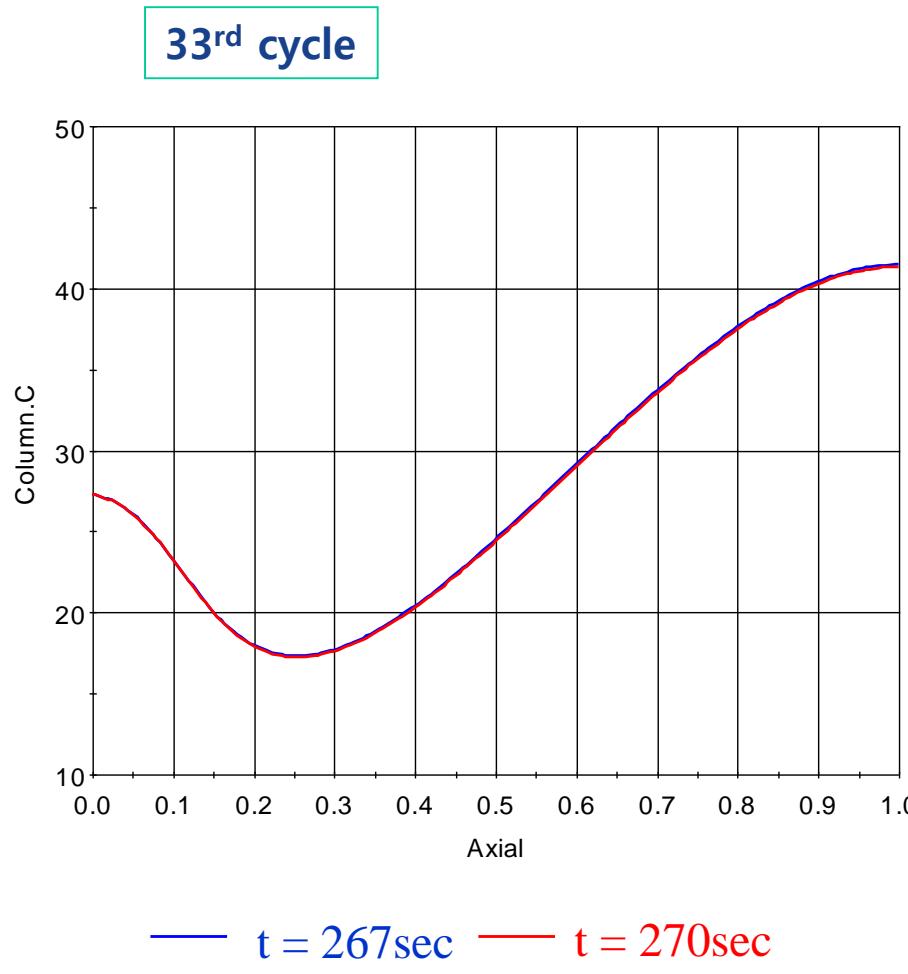
$\phi|_{t=0} \neq \phi|_{t=t\text{cycle}}$
*Not Yet
Cyclic Steady State*

Fig. O₂ concentration at the start time of the 9th cycle &
the end time of the 9th cycle

A3. Definition of cyclic steady state (CSS)



What does cyclic steady state mean?



$\phi|_{t=0} = \phi|_{t=t\text{cycle}}$

*Almost
Cyclic Steady State
(CSS)*

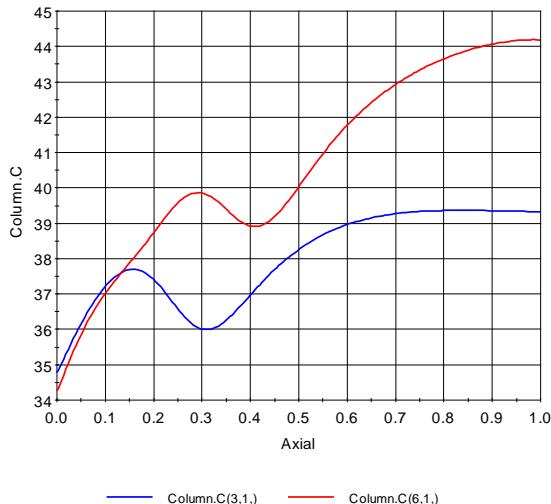
Fig. O₂ concentration at the start time of the 33rd cycle & the end time of the 33rd cycle

A3. Definition of cyclic steady state (CSS)



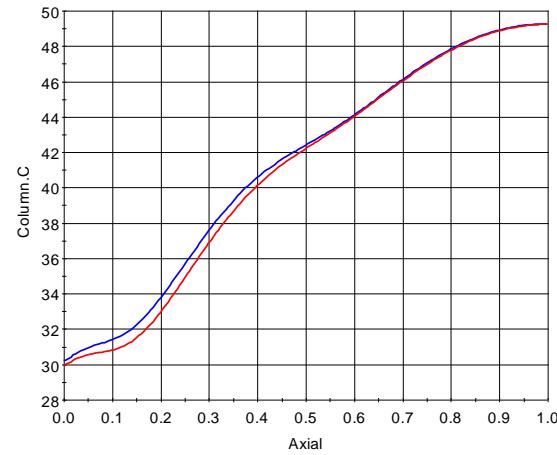
What does cyclic steady state mean?

2nd cycle



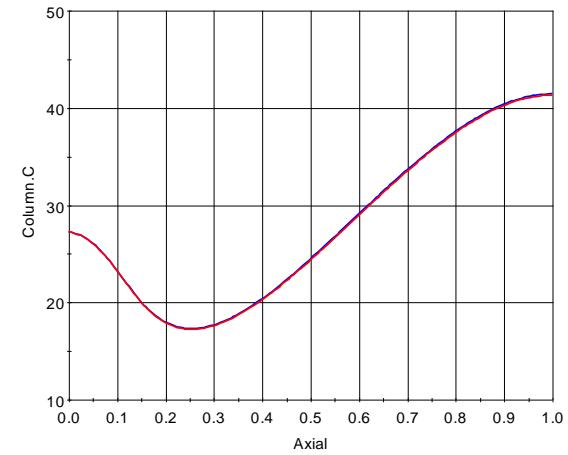
$$\phi|_{t=0} \neq \phi|_{t=t\text{cycle}}$$

9th cycle



$$\phi|_{t=0} \neq \phi|_{t=t\text{cycle}}$$

33rd cycle



$$\phi|_{t=0} = \phi|_{t=t\text{cycle}}$$

Cyclic Steady State
= CSS

A4. PSA optimisation approach at CSS

How to optimize cyclic adsorption processes (CAP) in a mathematical way?

Characteristics of CAP

- Cyclic Steady State (CSS):
Not steady state but dynamic steady state
Periodical operation
- Nonlinear PDE bed model
- **More than one operating steps**
- Difficult to express CSS for optimization

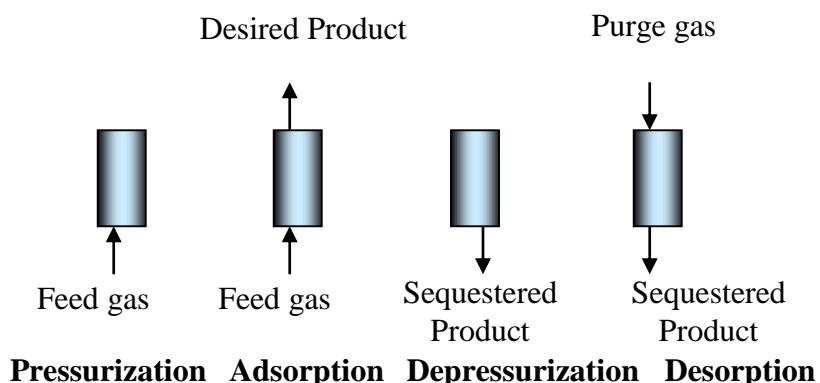
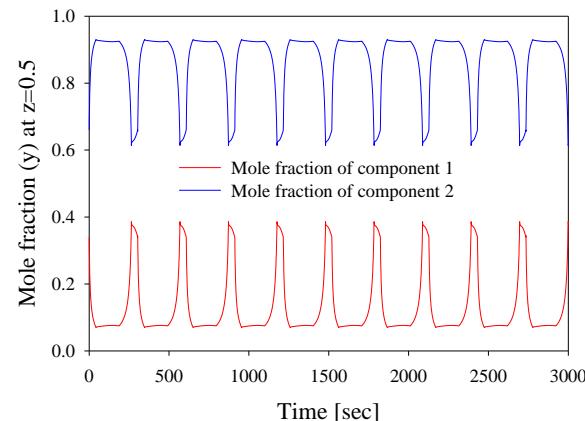


One of the **most difficult**
processes **to be optimized**



Improved Mathematical Optimization method

- Tailored Single Discretization (TSD) method
(Ko et al., 2003)
- updated Tailored Single Discretization (uTSD)
(Ko et al., 2005)

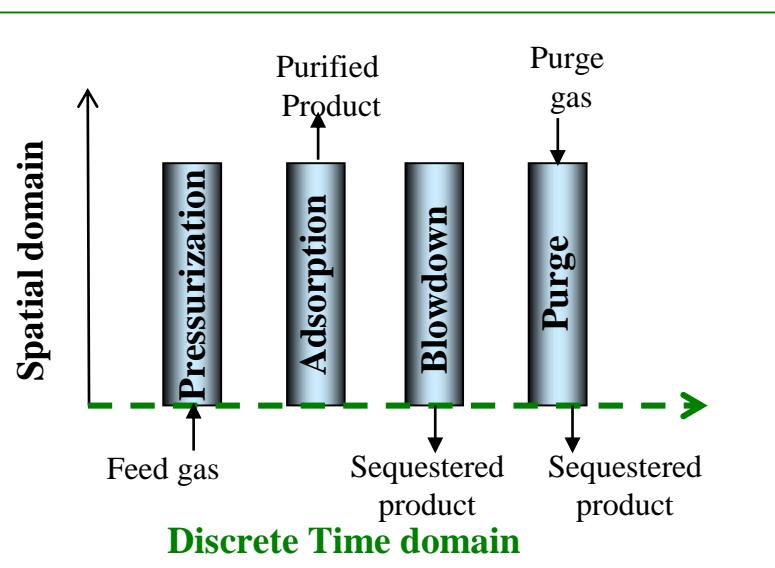


A4. PSA optimisation approach at CSS

The Concept of CD and SD

CD approach

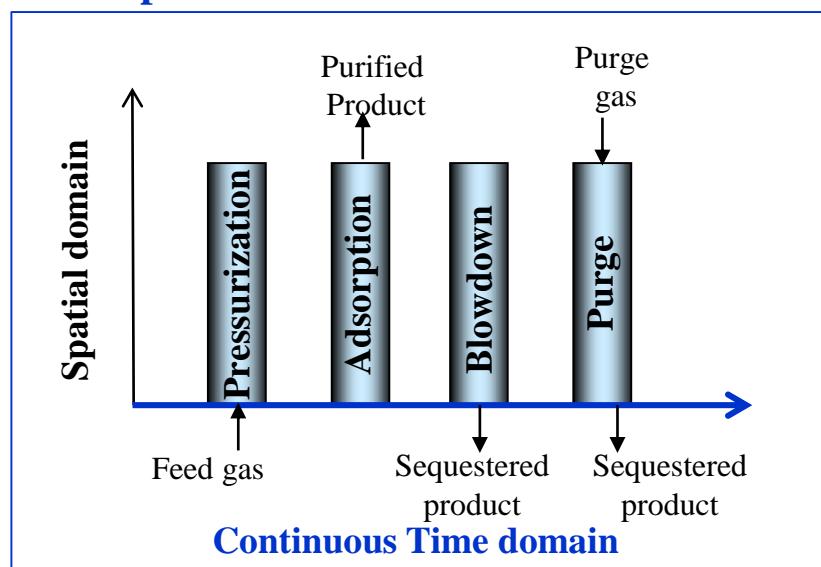
Complete discretization (CD) means the dynamic simulation adopts two discretization of the spatial domain as well as **the time domain as a new axis**.



Time domain is discretized by FDM(finite difference method) or OCFEM(orthogonal collocation finite element method). Then, **the discrete time domain** is used in the cyclic steady state(CSS) expression for the CSS optimization.

SD approach

Single discretization (SD) means the dynamic simulation adopts only one discretization of the spatial domain, not the time domain as a new axis. Instead, **variable time step (=continuous time) is adopted within the simulation solver.**

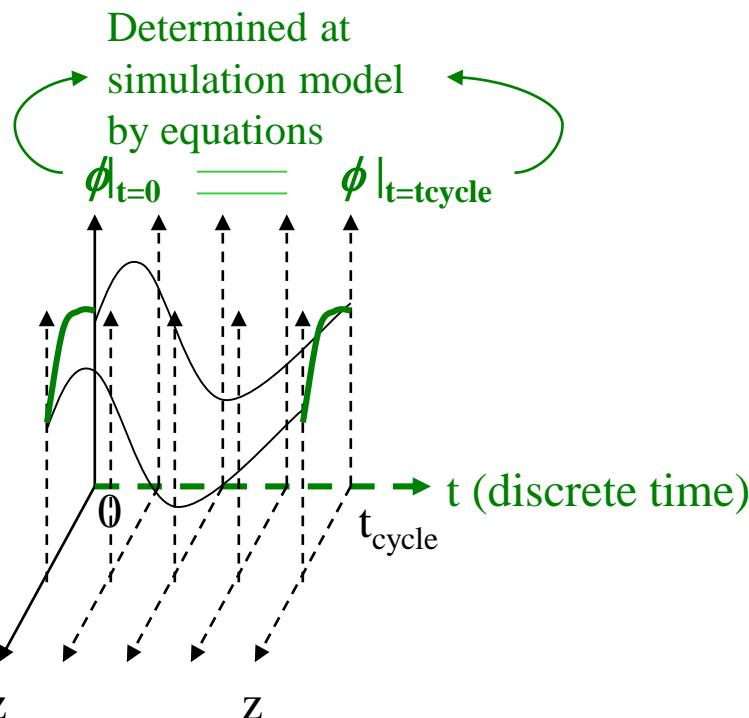


Continuous time domain model can be used in the cyclic steady state expression for the CSS optimization by **using binary variables**

A4. PSA optimisation approach at CSS

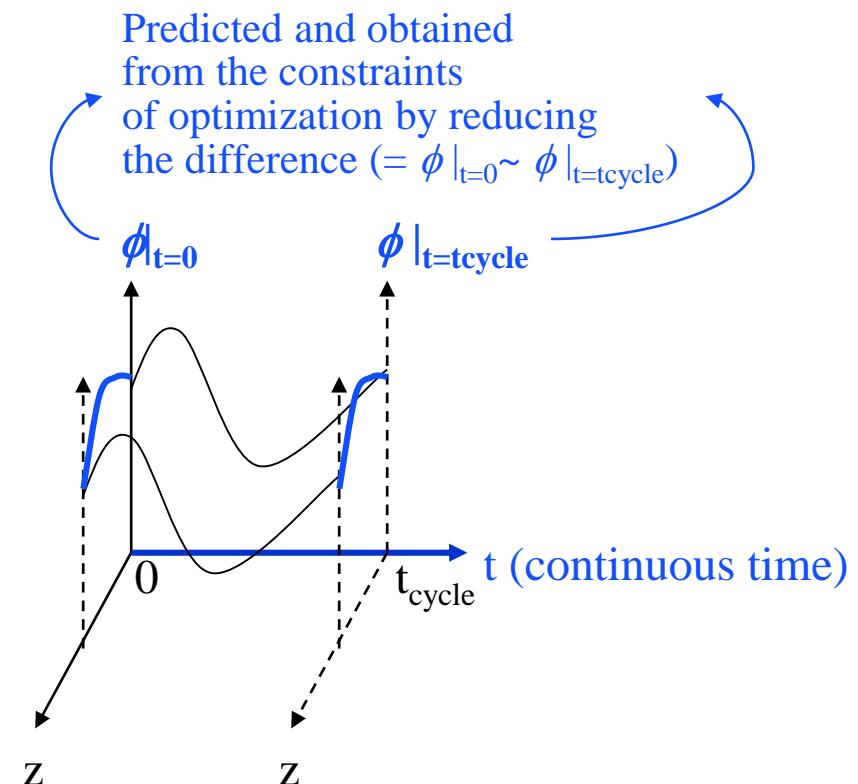
Implementation of CD and TSD (Ko et al., 2003 & 2005)

**CD (Complete Discretization) approach,
also called “Double Discretization”**



CSS Expression:
Discrete Time model
By adopting new time axis

TSD(Tailored Single Discretization) approach



CSS Expression:
Continuous Time model
by using binary variables

