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- University of Pittsburgh, Ph. D. (1993)
- International Adsorption Society, Director Board (present)
- The 3rd Pacific Basin Conference on Adsorption Science and Technology, Organizing Chairman (2003)
- General direction of Korean Institute of Chemical Engineers (present)

Research Area
- Gas Adsorption Technology
  - Adsorption Process: PSA, TSA, VSA
  - Equilibrium and Kinetics
  - New Adsorbents
- Membrane Separation: Ceramic & Metal Memb.
- SMB(Simulated Moving Bed): Fine Chemicals
- Inorganic/Organic Material Synthesis
- Supercritical Fluid Technology
- \( \text{CO}_2 \) Storage and Conversion
- Process Simulations

Gas Adsorption Technology
1. PSA and TSA Processes
   - \( \text{H}_2 \) recovery from effluent gas: \( \text{H}_2 \) Station, Reformer, FOG, COG, etc
   - \( \text{CO}_2 \) removal
   - \( \text{O}_2 \) generation
   - Air drying

2. Equilibrium & Kinetics
   - Zeolite, Activated Carbon, Alumina, Silica, CMS, Coal

3. Process Simulation
   - Dynamic Simulation
   - Cyclic Process

Simulated Moving Bed
1. New Operating Strategy
   - Partial Discard
   - FeedCol
   - Recycling Partial Discard

2. Separation Process
   - \( p-\text{Xylene Separation} \)
   - Recemic Separation

3. Chromatography
   - Equilibrium & Kinetics

4. Process Simulation
   - Dynamic Simulation
   - Cyclic Process
Membrane Separation

1. Membrane Separation
   - Organic Templating Membrane
   - Zeolite Membrane
   - Pd Membrane
   - Adsorbent/Membrane Hybrid System
   - Membrane Reactor

2. Gas Separation
   - H₂ Recovery from reforming gas
   - H₂ Recovery from WGSR gas
   - CO₂/CH₄ Separation

InOrg./Org. Material Synthesis

1. New Adsorbents for Energy
   - N- and S-compounds removal from fuels
   - S-compounds removal from natural gas
   - Mesoporous silica, Magnetite composite, MgO composite, Hybrid Silica

2. New Materials for Biotechnology
   - Functionalized materials
   - Core/Shell nanoparticles

Supercritical Fluid Technology

1. Nanoparticle Synthesis
   - YAG:Eu³⁺ Phosphor
   - Ce³⁺,Eu³⁺-Codoped YAG Phosphor
   - LiNi₁/₃Co₁/₃Mn₁/₃O₂ cathode

2. SCWO Process
   - NaFeEDTA decomposition
   - Halogenated compound decomposition
   - Anti-corrosive Reactor

3. Corrosion
   - Stainless Steel, Inconel, Titanium,
   - Metal Surface Analysis

4. Hydrocracking of VR

CO₂ Storage and Conversion

1. CO₂ Storage in Coal Seam
   - CO₂ Adsorption Capacity on Korean Coal
   - CH₄ Recovery from Coal Seam
   - Water effect & SCF

2. CO₂ Aquifer Storage
   - Saline Water Capacity for CO₂
   - Sand Stone Adsorption

3. CO₂ Conversion
   - Biological Conversion
   - Biomass Production
   - Chemical Production

Properties of supercritical water
Concept: Dual bed

- Adsorption/desorption process is exothermic/endothermic reaction.
- Pressure and temperature affect hydrogen separation process.
- Heat transfer between inner bed and outer bed in Dual bed raises efficiency of H₂ PSA process.
- Dual bed makes PSA compact and efficient

Cycle sequence of PSA process

<table>
<thead>
<tr>
<th></th>
<th>AD</th>
<th>DPE</th>
<th>DP</th>
<th>PG</th>
<th>PPE</th>
<th>FP</th>
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</thead>
<tbody>
<tr>
<td>BED 1</td>
<td>Feed</td>
<td>Vent</td>
<td>Vent</td>
<td>Product</td>
<td>Feed</td>
<td></td>
</tr>
<tr>
<td>BED 2</td>
<td>Vent</td>
<td>Feed</td>
<td>Feed</td>
<td>Product</td>
<td>Vent</td>
<td></td>
</tr>
</tbody>
</table>

Heat Exchange Pressure Swing Adsorption
Heat Exchange Pressure Swing Adsorption

Breakthrough Curve

\[ \text{H}_2/\text{CO}_2/\text{CH}_4/\text{CO} = 69/26/3/2 \text{ vol \%} \]

Feed rate: 7 LPM, Adsorption pressure: 9 atm

\begin{align*}
\text{< Conventional bed >} & & \text{< Inner bed >} & & \text{< Outer bed >} \\
\end{align*}

\begin{align*}
\text{time [s]} & & \text{time [s]} & & \text{time [s]} \\
0 & & 0 & & 0 \\
200 & & 200 & & 200 \\
400 & & 400 & & 400 \\
600 & & 600 & & 600 \\
800 & & 800 & & 800 \\
1000 & & 1000 & & 1000 \\
1200 & & 1200 & & 1200 \\
1400 & & 1400 & & 1400 \\
1600 & & 1600 & & 1600 \\
1800 & & 1800 & & 1800 \\
\end{align*}

\begin{align*}
\text{mole fraction [-]} & & \text{mole fraction [-]} & & \text{mole fraction [-]} \\
0.0 & & 0.0 & & 0.0 \\
0.2 & & 0.2 & & 0.2 \\
0.4 & & 0.4 & & 0.4 \\
0.6 & & 0.6 & & 0.6 \\
0.8 & & 0.8 & & 0.8 \\
1.0 & & 1.0 & & 1.0 \\
\end{align*}

\begin{align*}
\text{CO} & & \text{CO} & & \text{CO} \\
\text{CH}_4 & & \text{CH}_4 & & \text{CH}_4 \\
\text{CO}_2 & & \text{CO}_2 & & \text{CO}_2 \\
\text{H}_2 & & \text{H}_2 & & \text{H}_2 \\
\end{align*}

Simulation
• The amount of adsorbent in dual bed is 81% of single bed.
• However the breakthrough time in dual bed is longer than that in single bed.
• The first H₂ concentration drop is due to the early breakthrough of CO, CH₄ and CO₂.
• The rolling-up phenomenon of CO and CH₄ breakthrough curve is due to competitive adsorption.
• Due to the heat exchange effects, the outer bed showed almost isothermal behavior.
• Roll-up phenomenon in outer bed is smaller than single bed’s tailing and roll-up.
• Heat transfer between adsorption and desorption bed raises efficiency of dual bed.
The separation performance of the Compact PSA was higher than that of a conventional PSA at the same condition.

Compared to the conventional PSA, the high purity product could be obtained from the Compact PSA with relatively small sacrifice of recovery.
H2 Pressure Swing Adsorption

COG (Coke Oven Gas): H2 56.4 %, CH4 26.6 %, CO 8.4 %, N2 5.5 %, CO2 3.1 %

Adsorption Dynamics of a Layered Bed

Effects of Carbon-to-Zeolite Ratio on Layered Bed

Effects of Feed Composition on a Layered Bed

Breakthrough curves
(a) base composition: N2=5.5%
(b) higher nitrogen composition: N2=7.5%
(c) no nitrogen composition: N2=0.0%

0.32 C/Z 0.5 C/Z 0.65 C/Z
C/Z : carbon-to-zeolite ratio.

References:
Reforming Gas: H\textsubscript{2} 38%, CH\textsubscript{4} 1%, CO 1%, N\textsubscript{2} 10%, CO\textsubscript{2} 50%

- From gasification of coal
- Low H\textsubscript{2} fraction
- Huge amount of impurities

Breakthrough curves and Temperature profile

Experimental and simulated breakthrough curves of a layered bed (AC:Z5A=7:3) under 6.5 bar pressure and 5 LPM feed flow rate

Two-bed PSA process

Effect of P/F ratio
Effect of adsorption pressure

Simulation results of four-bed PSA process

**Simulated Moving Bed (SMB) Chromatography**

**Development operating strategy to improve the separation efficiency**

**Modification of SMB configuration**

**“FeedCol” Strategy**

- The “FeedCol” operation combines a chromatographic column as a feed column with SMB system to create the “TMB effect”

- The “rectangular pulse input” is introduced to the Feed column, and partially separated feed is injected into the SMB

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**FeedCol operation (1+2-2-2-2 system)**

- Injection length and injection time are variables to operate the system

- The pre-separated feed improved the separation efficiency even extra adsorbent used in the FeedCol operation

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Initial stage of extract and last stage of raffinate in a switching period have huge amount of impurity → Purity can be enhanced by discarding these parts

However, the other performance parameter were deteriorated from the waste of product in the partial-discard operation

In the Recycling Partial-Discard operation, the discarded portions are recycled as feed to reduce the loss from discarding

Initial stage of extract and last stage of raffinate are collected to each storage tank and recycled to the last stage and initial stage of feed, respectively

By applying the recycle concept to PD strategy, the loss of other performance parameters are successfully reduced while the purity can be maximized

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Ceramic Membrane Separation

**Ceramic Membrane**

<table>
<thead>
<tr>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Long term stability at high temperature</td>
<td>- High capital cost for synthesis</td>
</tr>
<tr>
<td>- It has an excellent resistance to harsh</td>
<td>- Brittleness</td>
</tr>
<tr>
<td>environment, such as temperature, pressure</td>
<td>- It is difficult to achieve high</td>
</tr>
<tr>
<td>and poison</td>
<td>selectivities in large-scale</td>
</tr>
<tr>
<td>- Inertness to microbiological degradation</td>
<td>microporous membranes</td>
</tr>
<tr>
<td>- Easy regeneration after fouling</td>
<td>- Low permeability of the</td>
</tr>
<tr>
<td>- It is low capital process</td>
<td>highly selective membranes at medium temperature</td>
</tr>
<tr>
<td>- Easy catalyst modification</td>
<td>- Difficult membrane to module sealing at high</td>
</tr>
<tr>
<td></td>
<td>temperature</td>
</tr>
</tbody>
</table>

**Adsorption**

**Zeolite (Membrane)**
- micorporous, aluminosilicate minerals
- contain many cavities (over 50%)
- strong adsorption affinity to polar molecules
- possibly adsorb specific non-polar molecules

**Activate Carbon (Adsorbent)**
- the surface area: 300~2500m²/g
- the pore size: 30Å (for liquid phase use), 10~25Å (for gas phase use)

**Hybrid Membrane System**

**Purification**

**Bulk Separation**
Ceramic Membrane Separation

Characteristics

Single Gas Permeation: Transient flux

Single Gas Permeation: Steady State flux

Multi Component Transient permeation[1]

Schematic of Membrane Apparatus

Ceramic Membrane Separation

Permeation flux of Binary mixtures

What’s the Next step?

- To develop an integrated WGS reaction and Palladium alloy membrane separation process at several conditions.
- To test the separation performance by measuring permeation flux of CH$_4$/CO/CO$_2$/H$_2$ quaternary mixture.

Super Critical Water Oxidation

**Supercritical water oxidation**

<table>
<thead>
<tr>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>- High rate decomposition</td>
<td>- Corrosion on system by acid at high temperature and pressure</td>
</tr>
<tr>
<td>- Shot residence time</td>
<td>- Fouling by decreasing solubility of inorganics</td>
</tr>
<tr>
<td>- Complete decomposition</td>
<td>- Non-exist of special materials</td>
</tr>
<tr>
<td>- Low temperature</td>
<td>For corrosion at high temp. and pressure</td>
</tr>
<tr>
<td>- No effluent Nox, Sox, Dioxin</td>
<td></td>
</tr>
<tr>
<td>- Close system</td>
<td></td>
</tr>
<tr>
<td>- Minimization of Toxic gas</td>
<td></td>
</tr>
</tbody>
</table>

**Stress Corrosion Cracking in SCWO**

- Fluid discharged from the tube
- Cross section of the tube wall

In this study, the effects of metal corrosion on the SCWO of 2-chlorophenol were investigated at subcritical and supercritical conditions by using the anticorrosive SCWO system. In addition, to elucidate the corrosion characteristics of the selected metals at both conditions, a surface chemical analysis of corroded metal alloys was conducted by various methods.

C.-H. Lee et al. / J. of Supercritical Fluids 36 (2005) 59–69
Corrosion Phenomena in SCWO

Stainless 316

Before corrosion

Corrosion in the subcritical region

Corrosion in the supercritical region

AES montage displays at subcritical and supercritical conditions.

ICP-MS Results of Stainless 316 at Subcritical and Supercritical Conditions

Corrosion Phenomena in SCWO

Zirconium 702

AES montage display of the surface of each metal alloy at the subcritical and supercritical conditions (e) and (f) Zirconium 702

S.-H. Son et al. / J. of Supercritical Fluids 44 (2008) 370–378
These figure show the comparison of destruction efficiencies of 2-chlorophenol at both subcritical and supercritical conditions with the corrosion of metal alloy. It was evident that the corrosion of stainless steel 316 contributed to the improvement of destruction of 2-chlorophenol at both the subcritical and supercritical conditions, compared to the destruction efficiencies without metal corrosion.

Bio-Catalysis – NSM

Surface modified NSM (Nano Size Magnetite)

Ox-NSM
Amino Acid coated-NSM
SDS-NSM
ABS-NSM

HR TEM: scale bar: 5 & 10nm

VSM

Ox-NSM
Leu-NSM
SDS-NSM
ABS-NSM

TEM: scale bar: 20 & 50nm

SDS-NSM
ABS-NSM

Bio-Catalysis – Magnetite silica

Magnetite Silica Composite

TEM & HR-TEM & SEM image

A : Ox-NSM
B : Ox-Fe3O4@SiO2
C : Fe3O4/Fe@SiO2
D : Fe2O3/Fe@SiO2
(a) MCM-41
(b) NSM
(c) and (d) : magnetic nanoparticles
(c) and (d) : magnetic/silica nanoparticles
(a) NSM (b) and (c) MCF
(d) and (e) NSM-MCF

VSM

A : Ox-NSM
B : Ox-Fe3O4@SiO2
C : Fe3O4/Fe@SiO2
D : Fe2O3/Fe@SiO2
NSM and Si-NSM-1
(a) magnetic nanoparticles
(b) magnetic core/shell
(a) NSM particles
(b) NSM-MCF

Magnesium Oxide Nano-Particles

- Toxic chemical in gas phase present a hazard to the environment.
- They are very stable molecules, they are hard to destroy and can persist in the atmosphere for long periods of time.
- Natural gas streams and crude oil streams contain \( \text{H}_2\text{S} \), which is very toxic, hazardous, and corrosive.
- MgO is an exceptionally important material, with uses in catalysis, toxic waste remediation, or as an additive in refractory, paint, and superconducting products, as well as fundamental and application studies.
- Ultrafine metal oxide particles have found use as bactericides, adsorbents, and, specifically, catalysts.
- MgO in particular has shown great promise as destructive adsorbent for toxic chemical agents.

The purpose of this work is to study the adsorptive properties of MgO. Through high surface area of these materials, we would try to improve the adsorptive capacity, affinity and selectivity toward toxic chemical in gas phase.
Magnesium Oxide Nano-Particles

TEM images

**Aerogel**
- Mg(OH)$_2$
- MgO

**Hydrothermal**
- Mg(OH)$_2$
- MgO

**Polyol thermolysis**
- MgO

XRD : MgO

![TEM images](image1)

1) Chem. Mater. 1991, 3, 175-181. / MgO Surface area : 522 m$^2$/g
2) Y. Qian, Chem. Mater, 2001, 13, 435. / MgO Size : 20~50 nm, Surface area : 143 m$^2$/g
3) T. Vasudevan, Nanotechnology, 2007, 18, 225601. / MgO Size : ~10 nm, Surface area : 112 m$^2$/g
The purpose of this work is to study the adsorption properties of Lithium (Li) modified mesoporous silica adsorbents toward nitrogen and sulfur compounds in fuels and gas.

Results: According to adsorption capacity, adsorption rate and regeneration, the Li-modified silica adsorbents (YSP-Li and MCF-Li) were better than Si-Zr cogel for diesel fuel denitrogenation. The adsorption capacity of YSP-Li was less sensitive to the applied temperature and its regeneration ability was excellent.

The effect of adsorbent concentration on nitrogen compounds uptake at 15 °C (a) and 45 °C (b) for 48 h (80 rpm) in fuel.

Kinetic of nitrogen compounds adsorption at 15°C (a) and 45°C (b) (adsorbent concentration – 10mg/ml, stirring speed – 80 rpm).

Effect of recovering sorbents by 5 ml of Toluene or MIBK at (a) 15°C and (b) 45°C (adsorbent concentration – 10mg/ml, stirring speed at 80 rpm) for 24 h and 48 h for first adsorption (with fuel).

Breakthrough curves of methylmercaptan on YSP-Li (a) and MCF-Li (b) at 25°C, and YSP-Li at 50°C (c) (activated at 150°C) and desorption curve of methylmercaptan and dimethyl disulide from YSP-Li (a) and MCF-Li (b) at 100°C. Gas mixture flow rate – 50 ml/min. The concentration of methylmercaptan in gas mixture was 291ppm.

Upgrading of Vacuum Residue (VR) in SCF

Introduction

- **Petroleum vacuum residue (VR)** consist mainly hydrocarbons with high boiling points and contains much higher portions of asphaltenes as well as much higher concentrations of sulfur, nitrogen, heavy metal (vanadium, nickel) compared with the conventional crude oils.

- The processes that convert these residues into low boiling, value-added products, less concentrations of heterocyclic species and metals are called **residue upgrading processes**.

- **Advantage of upgrading VR in supercritical hydrocarbon solvent process:**
  + Mild operating temperature (about 390-420°C)
  + Improve the diffusion rate, enhance coke extraction, retard coke deposition at the supercritical hydrocarbon solvent state.
  + The combination between activated carbon and hydrocarbon solvent make the “hydrogen – shuttling” mechanism would enhance solvent effect significantly.

Goal of Work

In this work, we investigate the effectiveness of various kinds of catalysts and hydrocarbon solvents in the upgrading of VDU-VR at supercritical condition in a batch reactor.

Upgrading of Vacuum Residue (VR) in SCF

Figure 1. Schematic diagram of the experiment apparatus.

Figure 2. SimDis analysis plot

Figure 3. Boiling point distribution plot

These peaks of kerosene, naphtha which were appears in DimDis analysis plot were proved that the carbon–carbon bonding of VR were cleaved under supercritical fluid condition.

The fractions of naphtha, kerosene and distillates, which is shown in the boiling distribution plot, were generated by the VR upgrading reaction.
The Geological Storage of CO₂

Increasing CO₂ atmospheric concentration & global surface temperature

Experimental Apparatus

- Themogravimetry analyzer
- Automatic High Pressure Gas Adsorption Analyzer
- High pressure gravimetric analyzer

- Establishment of Database for CO₂ Sequestration
- Measurement/Evaluation of CO₂ storage capacity in Coal Bed & Deep Saline Formations
- Optimization of CO₂ storage process design
The Geological Storage of CO₂

Texture of sample Coal

Pure CO₂ & CH₄ Adsorption on Coal

Dry coal plate’s diameter change of CO₂ adsorption at 318.15 K[1]

Adsorption and desorption of CH₄ and CO₂ on dry coal and wetted coal at 338.15K[2]

Mixture gas Adsorption on Coal

High pressure CO₂/CH₄ mixture gas preferential sorption measurement on dry coal at 318.15K[2]

Model Fitting

M-DR and M-DR+k fitting of CO₂ adsorption at 338.15K[2]

Properties of Sandstone

<table>
<thead>
<tr>
<th>Properties</th>
<th>Sample</th>
<th>Borcung sandstone</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk specific gravity (g/cc)</td>
<td></td>
<td>2.71</td>
</tr>
<tr>
<td>Absorption ratio (%)</td>
<td></td>
<td>0.13</td>
</tr>
<tr>
<td>Effective porosity (%)</td>
<td></td>
<td>0.32</td>
</tr>
<tr>
<td>P-wave velocity (m/sec)</td>
<td></td>
<td>5150</td>
</tr>
<tr>
<td>S-wave velocity (m/sec)</td>
<td></td>
<td>2870</td>
</tr>
<tr>
<td>Uniaxial compressive strength (MPa)</td>
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<td>301</td>
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<tr>
<td>Brazilian tensile strength (MPa)</td>
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<td>23</td>
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<tr>
<td>Young’s Modulus (GPa)</td>
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<td>64</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
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<td>0.25</td>
</tr>
</tbody>
</table>

Biomass: Renewable and available essentially for all countries. Contains negligible sulphur, nitrogen and metal contents. Does not result in a net increase in the CO$_2$ concentration in the atmosphere.

Wood is the preferred raw material for biomass conversion based on resource and process evaluations.

Problem of conversion: Lignocellulose

Lignocellulose consists mainly of:
- Cellulose (35–50%)
- Hemicellulose (20–35%)
- Lignin (5–25%)

Structure of cellulose (chain conformation) (left) and Lignin (right)
**Supercritical fluids** provide unique transport properties:
- Gas-like diffusivity
- Liquid-like properties
- Have the ability to dissolve materials not normally soluble in either liquid or gaseous phase of the solvent. Therefore it promotes the gasification/ liquefaction reactions.
- Acid and sulfur containing groups on the surface have been found to be an effective catalyst for cellulose liquefaction.\[1\]

**The purpose of this work:**
- Study decomposition pathways of microcrystalline cellulose, lignin and lignocellulose in various solvents at sub- and supercritical conditions.
- Check the catalytic ability of surface modified magnetic nanoparticles. \[2,3\]
- Combine with technology of VR upgrading.