

Co 2 Adsorption And Desorption Studies For Zeolite 4a

The goal of this program was to develop a low cost novel sorbent to remove carbon dioxide from flue gas and gasification streams in electric utilities. Porous materials named metal-organic frameworks (MOFs) were found to have good capacity and selectivity for the capture of carbon dioxide. Several materials from the initial set of reference MOFs showed extremely high CO₂ adsorption capacities and very desirable linear isotherm shapes. Sample preparation occurred at a high level, with a new family of materials suitable for intellectual property protection prepared and characterized. Raman spectroscopy was shown to be useful for the facile characterization of MOF materials during adsorption and especially, desorption. Further, the development of a Raman spectroscopic-based method of determining binary adsorption isotherms was initiated. It was discovered that a stronger base functionality will need to be added to MOF linkers in order to enhance CO₂ selectivity over other gases via a chemisorption mechanism. A concentrated effort was expended on being able to accurately predict CO₂ selectivities and on the calculation of predicted MOF surface area values from first principles. A method of modeling hydrolysis on MOF materials that correlates with experimental data was developed and refined. Complimentary experimental data were recorded via utilization of a combinatorial chemistry heat treatment unit and high-throughput X-ray diffractometer. The three main Deliverables for the project, namely (a) a MOF for pre-combustion (e.g., IGCC) CO₂ capture, (b) a MOF for post-combustion (flue gas) CO₂ capture, and (c) an assessment of commercial potential for a MOF in the IGCC application, were completed. The key properties for MOFs to work in this application - high CO₂ capacity, good adsorption/desorption rates, high adsorption selectivity for CO₂ over other gases such as methane and nitrogen, high stability to contaminants, namely moisture, and easy regenerability, were all addressed during this program. As predicted at the start of the program, MOFs have high potential for CO₂ capture in the IGCC and flue gas applications.

Legislation, Technology and Practice of Mine Land Reclamation contains the proceedings of the Beijing International Symposium on Land Reclamation and Ecological Restoration (LRER 2014, Beijing, China, 16-19 October 2014). The contributions cover a wide range of topics: - Monitoring, prediction and assessment of environmental damage in mining areas - Subsidence land reclamation and ecological restoration - Soil, vegetation and biological diversity - Mining methods and measures for minimization of land and environmental damage - Solid wastes and AMD treatment - Contaminated land remediation - Land reclamation and ecological restoration policies and management - Surface mined land reclamation and ecological restoration - Case study on mining reclamation and ecological restoration Legislation, Technology and Practice of Mine Land Reclamation will be of interest to engineers, scientists, consultants, government

officials and students involved in environmental engineering, soil science, ecology, forestry, mining, and land reclamation and ecological restoration in mining areas.

Characterization of gas sorption behavior on coals plays an important role on coalbed methane (CBM) and CO₂-enhanced CBM industry. In this study, the excess adsorption capacities were estimated for four coal samples with different ranks including San Juan sub-bituminous coal, Pittsburgh No. 8 bituminous coal, Hazleton anthracite and Good Spring anthracite by the volumetric adsorption experimental method. Adsorption and desorption isotherms of methane and CO₂ were directly measured for these four coal samples. Langmuir based models and Dubinin-Astakhov (D-A) based models were used to model adsorption behavior of both methane and CO₂. The experimental results showed that CH₄/CO₂ excess adsorption capacity ratio varied from 1:1.1 to 1:1.6 at maximum equilibrium pressure on these coals. Higher rank coals have higher excess adsorption capacities than lower rank coals across the experimental pressure range. Hysteresis of CO₂ is discernable and larger than methane for all coals. Higher rank coals have negligible methane hysteresis but larger CO₂ hysteresis than lower rank coals. From the modeling results, maximum CO₂ adsorption capacities are larger than methane capacities for all coals. In general, D-A based models were modeled better than Langmuir based models for these coals. Added k term reduced modeling error for both Langmuir and D-A series models. In addition, the modified Langmuir model-1 have relatively high errors for all coal samples.

An increasing interest in renewable energy resources and the search for maintainable energy policies have inspired the research contributions included in this book. Energy production and distribution need to respond to the modern world's dependence on conventional fuels. To achieve this, collaborative research is required between multiple disciplines, including materials, energy networks, new energy resources, storage solutions, waste to energy systems, smart grids and many other related subjects. Energy policies and management are of primary importance for sustainability and need to be consistent with recent advances in energy production and distribution. Challenges lie as much in the conversion from renewable energies such as wind and solar to useful forms like electricity, heat and fuel at an acceptable cost (including environmental damage) as in the integration of these resources into existing infrastructure.

In this research project, adsorption is considered in conjunction with the reverse water gas shift reaction in order to convert CO₂ to CO for synthetic fuel production. If the CO₂ for this process can be captured from high emitting industries it can be a very good alternative for reduced fossil fuel consumption and GHG emission mitigation. CO as an active gas could be used in Fischer-Tropsch process to produce conventional fuels. Literature review and process simulation were carried out in order to determine the best operating conditions for reverse water gas shift (RWGS) reaction. Increasing CO₂ conversion to CO requires CO₂/CO separation downstream of the reactor and recycling unreacted CO₂ and H₂

back into the reactor. Adsorption as a viable and cost effective process for gas separation was chosen for the CO₂/CO separation. This was started by a series of adsorbent screening experiments to select the best adsorbent for the application. Screening study was performed by comparing pure gas isotherms for CO₂ and CO at different temperatures and pressures. Then experimental isotherm data were modeled by the Temperature-Dependent Toth isotherm model which provided satisfactory fits for these isotherms. Henry law's constant, isosteric heat of adsorption and binary mixture prediction were determined as well as selectivity for each adsorbent. Finally, the expected working capacity was calculated in order to find the best candidate in terms of adsorption and desorption. Zeolite NaY was selected as the best candidate for CO₂/CO separation in adsorption process for this project. In the last step breakthrough experiments were performed to evaluate operating condition and adsorption capacity for real multi component mixture of CO₂, CO, H₂ in both cases of saturated with water and dry gas basis. In multi components experiments zeolite NaY has shown very good performance to separate CO₂/CO at low adsorption pressure and ambient temperature. Also desorption experiment was carried out in order to evaluate the working capacity of the adsorbent for using in industrial scale and eventually temperature swing adsorption (TSA) process worked very well for the regeneration step. Integrated adsorption system downstream of RWGS reactor can enhance the conversion of CO₂ to CO in this process significantly resulting to provide synthetic gas for synthetic fuel production as well as GHG emission mitigation.

Carbon-Based Material for Environmental Protection and Remediation presents an overview of carbon-based technologies and processes, and examines their usefulness and efficiency for environmental preservation and remediation. Chapters cover topics ranging from pollutants removal to new processes in materials science. Written for interested readers with strong scientific and technological backgrounds, this book will appeal to scientific advisors at private companies, academics, and graduate students.

Discover the fundamentals and tools needed to model, design, and build efficient, clean low-carbon energy systems with this unique textbook.

"An innovative preparation method is developed to highly improve the carbon dioxide capture capacity of the silica sorbents. In the previously used sorbent treatment method, free hydroxyl groups of silica available for further reaction are obtained by silica dehydration at high temperature. This new approach, however, grafts tetraethylenepentamine (TEPA) onto silica surface directly via incipient wetness impregnation (IWI) of TEPA/ethanol solutions at room temperature. The CO₂ adsorption/desorption performance of the catalysts is studied by Diffused Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) and Mass Spectrometer (MS) spectroscopy both qualitatively and quantitatively. The concentration of TEPA/ethanol solutions influences the deposit process of pentamine molecules onto silica particles by controlling the concentration differential of TEPA between the bulk

solution and the surface layer. Samples treated with more concentrated solutions had higher maximum carbon dioxide adsorption values, calculated from the calibrated CO₂ desorption peak area of MS spectra. The loading amount of solution also affects the mass transfer rate and equilibrium of TEPA. After the concentration is equilibrated between the bulk and the surface, the system lost the concentration gradient between bulk solution and silica surfaces, excessive pentamine solution removes the grafted pentamine molecules, and makes the carbon dioxide capture capacity curve drop from the peak point. The 0.03g silica treated by 2%, 10% and 20% TEPA/EtOH solution got the CO₂ adsorption capacity of 1545.03, 4590.28 and 7674.99 [μ]mol/g-sorbent, respectively. Two pretreatment methods of silica sorbents, ethanol pretreatment and carbon dioxide pretreatment, are used to further enhance the adsorption performance. In the former pretreatment, ethanol solvent is injected before each injection of TEPA solution, and in the latter, TEPA solution is injected in the atmosphere of a carbon dioxide gas. The principles behind these pretreatments underlie mass and momentum transfer processes. After the injection of TEPA/ethanol solution, the TEPA layer on silica surface becomes more and more concentrated with the solvent evaporation. Pores and channels are likely to be blocked by the high viscous TEPA on silica surfaces. Sufficient solvent molecules in the ethanol pretreatment help more than keep the concentration gradient between the bulk and surface and maintain a driving force to deposit the TEPA onto silica surfaces, an appropriate viscosity assists TEPA molecules diffuse deeper. 0.03g silica at the loading of 200 [μ]l, 20% TEPA/EtOH solution, the maximum CO₂ adsorption capacity is 8362.36 [μ]mol/g-sorbent with Ethanol pretreatment approach. The grafted pentamine molecules on silica surface can form inter-molecular H-bonds, which consume the functional amine groups and reduce the surface area available for CO₂ capture. Carbon dioxide was used to protect these free NH groups in the carbon dioxide pretreatment. DRIFTS and MS spectroscopy analysis shows either way gives the sorbent a higher carbon dioxide adsorption capacity than those without any pretreatment. 0.03g silica at the loading of 250 [μ]l, 20% TEPA/EtOH solution, the maximum CO₂ adsorption capacity is 9455.58 [μ]mol/g-sorbent with CO₂ pretreatment approach."--Abstract.

Adsorption/desorption isotherms were developed for methane (CH₄) and carbon dioxide (CO₂) using crushed coal saturated with coal bed methane (CBM) water. The coal samples were collected from two CBM wells in Wyoming's Powder River Basin (PRB). One located within the Canyon coal seam of the Upper Wyodak Formation and the other in Felix coal. Adsorption/desorption isotherms for a single and binary gas mix of methane and carbon dioxide gases were developed for wet and dry coal. Experiments revealed that moisture content reduces the adsorption of the various gases on the coal surface. The ratio of the gases (CH₄ and CO₂) adsorbed m dry/m wet was ~1.45 and ~1.54 for crushed sub-bituminous Canyon and Felix coals. The isotherm study results showed that carbon dioxide had a greater adsorption affinity than methane and that methane desorbed at a higher rate than carbon dioxide gas. Experiments also revealed that CO₂ gas adsorbed two to four times more than that of the CH₄ gas with the difference increasing as a function of pressure. Langmuir model was a good fit for the overall adsorption studies of the adsorbate gases on coal samples. The results of this study have important implications for microbially enhanced renewable natural gas and carbon sequestration in coal seams.

The design of space stations like the recently launched ISS is a highly complex and interdisciplinary task. This book describes component technologies, system integration, and the potential usage of space stations in general and of the ISS in particular. It so addresses students and engineers in space technology. Ernst Messerschmid holds the chair of space systems at the University of Stuttgart and was one of the first German astronauts.

The Objective of this research program is to develop a dense, non porous ceramic membrane for separation of carbon dioxide from flue gas at high temperatures (400-600 C). The research has been focused on addressing several fundamental issues of lithium zirconate (Li_2ZrO_3). In the 2nd half research, we conducted various kinds of experiments to understand the CO_2 sorption/desorption mechanism on the pure and modified Li_2ZrO_3 with the help of TGA, DSC TGA and XRD. DSC TGA results suggest that the melting of Li/K carbonates mixture may play an important role in rapid CO_2 sorption in the case of modified lithium zirconate. The CO_2 desorption experiments show that CO_2 desorption from the modified lithium zirconate follows the same mechanism as that from the pure lithium zirconate. This is different from the CO_2 adsorption on the pure and modified lithium zirconates.

7.1.1 Heavy Metals: What are They?

Adsorbent-based carbon capture is only feasible if adsorption-desorption cycles are both fully regenerating and economical. A potentially energy-saving and regenerating pH swing system is currently utilized by biocatalysts. The main objective is to develop, test and analyze a synthetic pH Swing Adsorption (pHSA) system as well as a pHSA compatible solid adsorbent to capture CO_2 from a simulated ambient air gas stream. Furthermore, comparing its performance to other CO_2 sorbent systems is necessary to determine the feasibility of pHSA implementation. The lead developed adsorbent is a carbon black co-activated with potassium carbonate and nitrogenous copolymer that is impregnated with immobilized bovine carbonic anhydrase and thereby deemed BCA/KN-CB. BCA/KN-CB has preliminarily demonstrated both a competitive CO_2 adsorption capacity and a limited regenerative ability under experimental pHSA conditions. In addition, BCA-based adsorbents achieved higher adsorption capacities than non-BCA adsorbent counterparts. BCA-based adsorbents displayed better regenerative stability when the adsorbent was chemically activated with K_2CO_3 . The point of zero charge of adsorbents BCA/KN-CB and KN-CB showed change between pHSA steps and came close to returning to the initial point of zero charge after one pHSA cycle. While the cost of the biocatalyst easily makes its use for CO_2 capture impractical, the operational and remaining material costs are competitive to MSA and TSA solid adsorbent systems. The scientific contribution of the thesis is the concept of a pH swing adsorption/biocatalytic adsorbent system that can effectively operate under ambient conditions and has competitive CO_2 adsorption capacities compared against other swing adsorption CO_2 capture systems.

In this work, mesoporous cellular foams (MCFs) were synthesized and impregnated with different weight percentage of polyethylenimine (PEI) using wet impregnation method. The synthesized adsorbents were characterized using nitrogen adsorption/desorption, SEM, TEM, and FTIR analysis. The CO_2 adsorption capacity of PEI-impregnated MCFs was measured

using thermogravimetric analyzer (TGA). The effects of PEI loadings, adsorption temperatures, and CO₂ partial pressures on CO₂ adsorption performance using PEI-impregnated MCFs were explored. 70 wt % PEI loading was found to be the optimum for the highest CO₂ adsorption capacity of about 5 mmol/g in 95% CO₂/5% N₂ gas mixture and 4 mmol/g in 10% CO₂/90% N₂ gas mixture, at 75 °C. The effect of moisture on the CO₂ adsorption performance in simulated flue gases was studied. It was found the CO₂ adsorption performance of PEI-impregnated MCFs can be improved with the presence of moisture, especially at low adsorption temperatures. The adsorbent with optimum PEI loading was then tested for multi-cycle stability and adsorption/desorption kinetics in both humid and dry conditions. Good stability of the adsorbent in multi-cycle tests was found as no significant change in CO₂ adsorption capacity was observed. Various equilibrium adsorption isotherms, such as Langmuir and Freundlich adsorption isotherms, were applied to describe the CO₂ adsorption behavior. Different kinetic models were developed to study the CO₂ adsorption kinetics of this type of adsorbents. John-Mehl-Avrami (JMA) model was found to be well fitted with the experimental data, indicating another possible way to describe the kinetics of CO₂ adsorption process under isothermal conditions. The heat of adsorption of CO₂ adsorption process using PEI-impregnated MCFs was also calculated.

This thesis presents a combination of material synthesis and characterization with process modeling. In it, the CO₂ adsorption properties of hydrotalcites are enhanced through the production of novel supported hybrids (carbon nanotubes and graphene oxide) and the promotion with alkali metals. Hydrogen is regarded as a sustainable energy carrier, since the end users produce no carbon emissions. However, given that most of the hydrogen produced worldwide comes from fossil fuels, its potential as a carbon-free alternative depends on the ability to capture the carbon dioxide released during manufacture. Sorption-enhanced hydrogen production, in which CO₂ is removed as it is formed, can make a major contribution to achieving this. The challenge is to find solid adsorbents with sufficient CO₂ capacity that can work in the right temperature window over repeated adsorption-desorption cycles. The book presents a highly detailed characterization of the materials, together with an accurate measurement of their adsorption properties under dry conditions and in the presence of steam. It demonstrates that even small quantities of graphene oxide provide superior thermal stability to hydrotalcites due to their compatible layered structure, making them well suited as volume-efficient adsorbents for CO₂. Lastly, it identifies suitable catalysts for the overall sorption-enhanced water gas shift process.

The objective of this three-year project was to study new pressure swing adsorption (PSA) cycles for CO₂ capture and concentration at high temperature. The heavy reflux (HR) PSA concept and the use of a hydrotalcite like (HTlc) adsorbent that captures CO₂ reversibly at high temperatures simply by changing the pressure were two key features of these new PSA cycles. Through the completion or initiation of nine tasks, a bench-scale experimental and theoretical program has been carried out to complement and extend the process simulation study that was carried out during Phase I (DE-FG26-03NT41799). This final report covers the entire project from August 1, 2005 to July 31, 2008. This program

included the study of PSA cycles for CO₂ capture by both rigorous numerical simulation and equilibrium theory analysis. The insight gained from these studies was invaluable toward the applicability of PSA for CO₂ capture, whether done at ambient or high temperature. The rigorous numerical simulation studies showed that it is indeed possible to capture and concentrate CO₂ by PSA. Over a wide range of conditions it was possible to achieve greater than 90% CO₂ purity and/or greater than 90% CO₂ recovery, depending on the particular heavy reflux (HR) PSA cycle under consideration. Three HR PSA cycles were identified as viable candidates for further study experimentally. The equilibrium theory analysis, which represents the upper thermodynamic limit of the performance of PSA process, further validated the use of certain HR PSA cycles for CO₂ capture and concentration. A new graphical approach for complex PSA cycle scheduling was also developed during the course of this program. This new methodology involves a priori specifying the cycle steps, their sequence, and the number of beds, and then following a systematic procedure that requires filling in a 2-D grid based on a few simple rules, some heuristics and some experience. It has been tested successfully against several cycle schedules taken from the literature, including a 2-bed 4-step Skarstrom cycle, a 4-bed 9-step process with 2 equalization steps, a 9-bed 11-step process with 3 equalization steps, and a 6-bed 13-step process with 4 equalization steps and 4 idle steps. With respect to CO₂ capture and concentration by PSA, this new approach is now providing a very straightforward way to determine all the viable 3-bed, 4-bed, 5-bed, n-bed, etc. HR PSA cycle schedules to explore using both simulation and experimentation. This program also touted the use of K-promoted HTlc as a high temperature, reversible adsorbent for CO₂ capture by PSA. This program not only showed how to use this material in HR PSA cycles, but it also proposed a new CO₂ interaction mechanism in conjunction with a non-equilibrium kinetic model that adequately describes the uptake and release of CO₂ in this material, and some preliminary fixed bed adsorption breakthrough and desorption elution experiments were carried out to demonstrate complete reversibility on a larger scale. This information was essentially missing from the literature and deemed invaluable toward promoting the use of K-promoted HTlc as a high temperature, reversible adsorbent for CO₂ capture by PSA. Overall, the objectives of this project were met. It showed the feasibility of using K-promoted hydrotalcite (HTlc) as a high temperature, reversible adsorbent for CO₂ capture by PSA. It discovered some novel HR PSA cycles that might be useful for this purpose. Finally, it revealed a mechanistic understanding of the interaction of CO₂ with K-promoted HTlc.

Adsorption is the basis of various emerging technologies that will be essential for addressing the problems of technologies that will be essential for addressing the problems of energy conservation and environmental protection. This volume reviews recent progress and outlines the outlook for future development in adsorption theories, kinetics, pressure swing adsorption, SMB, and new nanoporous adsorbents. The contributions cover the fundamental knowledge and

methodologies for adsorption experiments and calculations regarding equilibria, heat effects, adsorbent structural modeling, diffusion measurement, and selectivity control. The volume also includes topics concerning hydrogen storage, desulfurization of fuels, and chiral separation. The contributors are internationally renowned scholars in the field of adsorption.

Addresses materials, technology, and products that could help solve the global environmental crisis once commercialized. This multidisciplinary book encompasses state-of-the-art research on the topics of Carbon Capture and Storage (CCS), and complements existing CCS technique publications with the newest research and reviews. It discusses key challenges involved in the CCS materials design, processing, and modeling and provides in-depth coverage of solvent-based carbon capture, sorbent-based carbon capture, membrane-based carbon capture, novel carbon capture methods, computational modeling, carbon capture materials including metal organic frameworks (MOF), electrochemical capture and conversion, membranes and solvents, and geological sequestration. *Materials and Processes for CO₂ Capture, Conversion and Sequestration* offers chapters on: Carbon Capture in Metal-Organic Frameworks; Metal Organic Frameworks Materials for Post-Combustion CO₂ Capture; New Progress of Microporous Metal-Organic Frameworks in CO₂ Capture and Separation; In Situ Diffraction Studies of Selected Metal-Organic Framework (MOF) Materials for Guest Capture Applications; Electrochemical CO₂ Capture and Conversion; Electrochemical Valorization of Carbon Dioxide in Molten Salts; Microstructural and Structural Characterization of Materials for CO₂ Storage using Multi-Scale X-Ray Scattering Methods; Contribution of Density Functional Theory to Microporous Materials for Carbon Capture; and Computational Modeling Study of MnO₂ Octahedral Molecular Sieves for Carbon Dioxide Capture Applications.

Addresses one of the most pressing concerns of society—that of environmental damage caused by the greenhouse gases emitted as we use fossil fuels. Covers cutting-edge capture technology with a focus on materials and technology rather than regulation and cost. Highlights the common and novel CCS materials that are of greatest interest to industrial researchers. Provides insight into CCS materials design, processing characterization, and computer modeling. *Materials and Processes for CO₂ Capture, Conversion and Sequestration* is ideal for materials scientists and engineers, energy scientists and engineers, inorganic chemists, environmental scientists, pollution control scientists, and carbon chemists. This multi-authored book provides a comprehensive overview of the latest developments in porous CO₂ capture materials, including ionic liquid-derived carbonaceous adsorbents, porous carbons, metal-organic frameworks, porous aromatic frameworks, micro porous organic polymers. It also reviews the sorption techniques such as cyclic uptake and desorption reactions and membrane separations. In each category, the design and fabrication, the comprehensive characterization, the evaluation of CO₂ sorption/separation and the sorption/degradation mechanism are highlighted. In

addition, the advantages and remaining challenges as well as future perspectives for each porous material are covered. This book is aimed at scientists and graduate students in such fields as separation, carbon, polymer, chemistry, material science and technology, who will use and appreciate this information source in their research. Other specialists may consult specific chapters to find the latest, authoritative reviews. Dr. An-Hui Lu is a Professor at the State Key Laboratory of Fine Chemicals, School of Chemical Engineering, Faculty of Chemical, Environmental and Biological Science and Technology, Dalian University of Technology, China. Dr. Sheng Dai is a Corporate Fellow and Group Leader in the Chemical Sciences Division at Oak Ridge National Laboratory (ORNL) and a Professor of Chemistry at the University of Tennessee, USA.

Objective is to investigate the removal of CO₂ from a fuel gas produced by a coal gasifier with a K₂CO₃-modified MgO sorbent. The work consists of measuring the capacity and rates of absorption of the sorbent vs T, P, and gaseous contaminants. Effects of repeated absorption/desorption cycling on sorbent properties will be studied. During this first quarter, the Test Plan was prepared and approved. The thermobalance was prepared, and the first sorbent batch was formulated and subjected to adsorption/desorption thermobalance tests (results showed CO₂ absorption at 800 F above 400 psi).

Using inorganic solid adsorbents/sorbents is a promising approach for carbon dioxide (CO₂) capture and is attracting intense attention from both academic and industrial fields. Pre-combustion Carbon Dioxide Capture Materials presents a range of the different inorganic materials that can be used as pre-combustion CO₂ adsorbents/sorbents with specific emphasis on their design, synthesis, characterization, performance, and mechanism. Dedicated chapters cover layered double hydroxide (LDH) derived adsorbents, MgO-based adsorbents, CaO-based sorbents and alkali ceramics based sorbents. Edited and written by world-renowned scientists in each class of CO₂ capture material, this book will provide a comprehensive introduction for advanced undergraduates, postgraduates and researchers wishing to learn about the topic.

The term 'geological sequestration' stands for the capture of CO₂ directly from anthropogenic sources and disposing of it deep into the ground for geologically significant periods of time (Bachu, 2002). Coal seam sequestration as described by White et al. (2005) is "the storage of CO₂ from anthropogenic sources into deep, unminable coal seams for geologically significant limits with or without concomitant recovery of natural gas". Methane is native to coal and has its origin in coalification process. Coal is the source as well as reservoir to significant quantities of methane, a potential energy resource. Coalbed methane (CBM) a bonus non-conventional energy source is generated mainly due to geochemical transformation of the organic matter by catagenesis. CO₂ injection reduces the partial pressure of methane and

enhances desorption of methane from the matrix. CO₂ has an additional effect compared to other gases that it is preferentially adsorbed onto coal surfaces, displacing methane from adsorption sites. CO₂-ECBM sequestration is a value addition project in management of increasing atmospheric concentration of greenhouse gases (GHG) as it recovers the cost of capture, processing, transportation and storage of CO₂ by production of methane. The primary aim of this research was to develop an understanding on the coal-fluid interaction pertinent to carbon storage in coal seams with special reference to Indian coal basins. Damodar valley coalfield where production of coalbed methane is being carried out was chosen for this study. The objectives of this study included detailed knowledge of geotechnical characterization of coal measure rocks, strength characteristics of coal under saturation in different media, swelling and stress induced changes in flow behaviour of coal in multiple phases of carbon dioxide and estimation of gas storage potential of Indian coal basins. After the geological field work, petrographic and geomechanical characterization of coal measure rocks was carried out. Sandstone and shale along with varying degrees of their intercalations were identified in thin section studies under the microscope. The pertinent geomechanical characteristics of the rocks and coal were determined using laboratory tests according to the International Society of Rock Mechanics (ISRM) standards. Some data generated during these tests were used as inputs for prediction of Uniaxial Compressive Strength (UCS) and P-wave velocity using soft computing. An important aspect of coal seam sequestration is the influence of CO₂ saturation on strength parameters and failure characteristics of the host. Fluid saturation experiments were carried out to explore the effects of CO₂ adsorption on natural as well as moisture-equilibrated coal. Water saturation of coal led to high reduction in its strength implying that the seam pressure in water saturated sinks must be managed at lower levels during sequestration as compared to the dry reservoirs. Injection of CO₂ leads to sorptive weakening of coal. The scenario was worst when CO₂ was injected in wet coal. CO₂ saturation induces swelling in coal and creates or enhances the fracture lines along coal as also evident by the early crack initiation in the acoustic emission results. Coupled stress strain data during uniaxial compression were recorded and analyzed. Introduction of water and CO₂ caused early failure of coal samples at a lower value of load alongside inducing larger amount of strain at same stress values. The brittle nature of coal became less pronounced upon water saturation leading to larger time for crack initiation. To overcome the structural heterogeneity in coal, reconstituted coal specimens of uniform grain size were prepared using moulds and their strength was calculated under dry and saturated conditions. The reconstituted coal specimens were developed at different stresses and the properties of coal developed at 22 MPa and 24 MPa were found to be closest to that of natural coal. The magnitude of strength reduction in these samples was less as compared to the natural specimens. This could be due to high compaction and elimination of flow paths for fluids. Sample interiors remained largely intact and least affected by the

fluids and hence, the strength remained closer to unsaturated reconstituted coal specimens. Permeability in coal is one of the most vital issues that determine the production or sequestration performance of coal. The permeability of CO₂ in different phases in coal samples under various possible scenarios was estimated using a newly developed, high precision P-T controlled triaxial set up. The permeability of coal decreased exponentially with increasing effective stresses for Indian coal and new empirical equations accounting for stress behaviour of coal permeability were proposed. The rate of coal matrix swelling reduced in 30-40 hours of gas injection after which coal permeability gradually increased with increasing upstream pressure. Finally, at constant pore pressure, coal permeability reduced drastically with increasing confining stresses. A similar experiment was conducted using naturally fractured coal from the same seam while maintaining a low range of confining and injection pressures to ensure a complete gas phase CO₂ flow. The permeability of coal reduced with increasing CO₂ injection pressure in four out of five cases of confinement implying that complete closure of fractures due to coal swelling took longer time of CO₂ saturation. However, permeability of coal reduced exponentially with increasing effective stresses. The next experiment investigated liquid and supercritical CO₂ permeability of coal at varying confining pressures (15 - 24 MPa), corresponding to different depths of coal. The initial liquid CO₂ permeability of coal at 10 MPa injection pressure reduced from 0.011 mD at 15 MPa confinement to 0.0004 mD at 24 MPa confinement. Further experiments revealed that the initial permeability of coal using supercritical CO₂ (0.005 mD) was nearly half of that for liquid CO₂ (0.011 mD). Nitrogen, used as a relatively inert medium, experienced a reduction in permeability in coal through which CO₂ was passed. Maximum reduction in coal permeability was observed in supercritical CO₂ flow, due to high sorption induced swelling of coal. After the role of confining stresses in different phase of CO₂ was studied, the role of CO₂ saturation period on coal permeability was studied at a fixed confining pressure of 18 MPa. Permeability of liquid as well as supercritical CO₂ reduced after each period of 20 h saturation. Maximum permeability reduction took place by nearly 27% and 43% for liquid and supercritical CO₂ saturation respectively, in the first out of three saturation periods. However, permeability of supercritical CO₂ continued to reduce after each period of saturation while minimal reduction took place at the end of second and third period of swelling with liquid CO₂. Similar trends were also observed in case of N₂ since the cleats were effectively closed due to passage of different phases of CO₂. This highlights that supercritical state of CO₂ induces maximum adsorption related swelling and the subsequent reduction in coal permeability. Based on detailed experimental understanding of the coal samples and the field information on behaviour of coal seams, reservoir simulation studies were carried out using a commercial simulator called COMET 3. Model construction was followed by history matching of the CBM wells to establish and validate those before extending the cases for CO₂ injection and enhanced recovery of the natural gas. The same established models

were used to investigate parametric influence on production characteristics of coal. In a scenario of given block size with one injection well and two production wells, the spatial distribution and relative flow of the two gases were explored with change in time. The salient findings of these studies included: coals adsorbed CO₂ quickly and surrounding matrix attained peak CO₂ matrix concentration in one month due to high adsorption potential for CO₂. The fracture gas saturation increased at first mainly near the production well due to sudden desorption of CH₄ as a consequence of dewatering. Gradually, high gas saturation resulted in the block. The statistical data generated from this study revealed that over a period of 4000 days of observation, the coal block would take in approximately 7.7 bcf of CO₂ and in lieu of which it would produce around 2.6 bcf of CH₄ and a total of 12000 bbls of water. Similar exercise was carried out for two blocks in Jharia coalfields. The study on one block showed that over a period of 4000 days, the chosen coal block adsorbed approximately 7.75 bcf of CO₂ in turn released 2.24 bcf of methane gas. The same variety of coal was simulated for a period of 20 years with an increased block size and it was found that for the chosen dimensions of Gondwana coal block in India, a total of 15.1 bcf of CO₂ may be injected for permanent storage alongside recovery of not less than 5 bcf of methane. Numerical simulation for the established Jharia model was used to predict and understand the influence of sorption time on the production behaviour of coals. It revealed that the CO₂ injection capacity into high sorption time coal was significantly higher than coal with low sorption time. Therefore, if not suitable for economical extraction of methane, these may alternatively be utilized as CO₂ sinks. It was also shown that for coal belonging to Gondwana basin setting in India, sorption time less than 10 days followed equilibrium model of desorption. Although coals with higher sorption time exhibited non-equilibrium desorption and diffusion, they were finally observed to converge with the equilibrium model at later stages of gas injection/production. Some future works based on the new findings were suggested at the end of this research work.

In chapter 1, the studies focused on the development of novel sorbents for reducing the carbon dioxide emissions at high temperatures. Our studies focused on cesium doped CaO sorbents with respect to other major flue gas compounds in a wide temperature range. The thermo-gravimetric analysis of sorbents with loadings of CaO doped on 20 wt% cesium demonstrated high CO₂ sorption uptakes (up to 66 wt% CO₂/sorbent). It is remarkable to note that zero adsorption affinity for N₂, O₂, H₂O and NO at temperatures as high as 600 C was observed. For water vapor and nitrogen oxide we observed a positive effect for CO₂ adsorption. In the presence of steam, the CO₂ adsorption increased to the highest adsorption capacity of 77 wt% CO₂/sorbent. In the presence of nitrogen oxide, the final CO₂ uptake remained same, but the rate of adsorption was higher at the initial stages (10%) than the case where no nitrogen oxide was fed. In chapter 2, Ca(NO₃)₂ · 4H₂O, CaO, Ca(OH)₂, CaCO₃, and Ca(CH₃COO)₂ · H₂O were used as precursors for synthesis of CaO

sorbents on this work. The sorbents prepared from calcium acetate (CaAc₂-CaO) resulted in the best uptake characteristics for CO₂. It possessed higher BET surface area and higher pore volume than the other sorbents. According to SEM images, this sorbent shows 'fluffy' structure, which probably contributes to its high surface area and pore volume. When temperatures were between 550 and 800 C, this sorbent could be carbonated almost completely. Moreover, the carbonation progressed dominantly at the initial short period. Under numerous adsorption-desorption cycles, the CaAc₂-CaO demonstrated the best reversibility, even under the existence of 10 vol % water vapor. In a 27 cyclic running, the sorbent sustained fairly high carbonation conversion of 62%. Pore size distributions indicate that their pore volume decreased when experimental cycles went on. Silica was doped on the CaAc₂-CaO in various weight percentages, but the resultant sorbent did not exhibit better performance under cyclic operation than those without dopant. In chapter 3, the Calcium-based carbon dioxide sorbents were made in the gas phase by flame spray pyrolysis (FSP) and compared to the ones made by standard high temperature calcination (HTC) of selected calcium precursors. The FSP-made sorbents were solid nanostructured particles having twice as large specific surface area (40-60 m²/g) as the HTC-made sorbents (i.e. from calcium acetate monohydrate). All FSP-made sorbents showed high capacity for CO₂ uptake at high temperatures (773-1073 K) while the HTC-made ones from calcium acetate monohydrate (CaAc₂ · H₂O) demonstrated the best performance for CO₂ uptake among all HTC-made sorbents. At carbonation temperatures less than 773 K, FSP-made sorbents demonstrated better performance for CO₂ uptake than all HTC-made sorbents. Above that, both FSP-made, and HTC-made sorbents from CaAc₂ · H₂O exhibited comparable carbonation rates and maximum conversion. In multiple carbonation/decarbonation cycles, FSP-made sorbents demonstrated stable, reversible and high CO₂ uptake capacity sustaining maximum molar conversion at about 50% even after 60 such cycles indicating their potential for CO₂ uptake. In chapter 4 we investigated the performance of CaO sorbents with dopant by flame spray pyrolysis at higher temperature. The results show that the sorbent with zirconia gave best performance among sorbents having different dopants. The one having Zr to Ca of 3:10 by molar gave stable performance. The calcium conversion around 64% conversion during 102-cycle operations at 973 K. When carbonation was performance at 823 K, the Zr/Ca sorbent (3:10) exhibited stable performance of 56% by calcium molar conversion, or 27% by sorbent weight, both of which are less than those at 973 K as expected. In chapter 5 we investigated the performance of CaO sorbents by flame spray pyrolysis at higher temperature with much shorter duration period. Stable high conversions were attained after 40 cycles. The results show that the sorbent could reach high CO₂ capture capacity, be completely regenerated in short time and be quite stable even at these severe conditions. Several studies were devoted to identify sorbents which could effectively capture CO₂ while survive in SO₂ atmosphere. From the group of sorbents we checked, a couple of sorbents

showed very promising behavior, namely CO₂ uptakes higher than 60% (wt/wt sorbent) while they acquired higher than 95% of their original activity/performance characteristics in a short period of time.

The objective of this work was to evaluate the fundamentals of the currently available CO₂ separation technologies and provide a solution for the efficient capture of carbon dioxide from various point source emitting industries. In order to realize a robust approach to advancing the solution to this global issue, the versatility of the process to the range of compounds contained within the stream(s) to be processed must be maintained. It is clear that adsorption, membrane, and aqueous amine based processes are all capable. However, only aqueous amine scrubbing appears economically viable at the current stage of development. In order to challenge this, and potentially drive the separation costs lower, this work centered on hybridizing aqueous amine chemistry and dry adsorption based separations to produce a novel nanoporous material capable of efficient removal of CO₂ from flue gas (5% CO₂ balance N₂ with moisture). In order to combine aqueous amine scrubbing with dry adsorption, a few approaches were considered and evaluated. These included, amine impregnation within the vast pore volume of PE-MCM-41, surface grafting of various amino silane compounds, and finally, a novel approach of volume based amine functionalization (3D grafting). Application of pore-expanded MCM-41 (PE-MCM-41) mesoporous silica coated with 3-[2-(2-aminoethyl-amino)ethylamino]propyltrimethoxysilane (TRI) has been extensively examined for the adsorption of CO₂ from N₂. A systematic study of the amine loading as a function of the relative amounts of TRI and water used during the grafting procedure, and the temperature of the grafting reaction was carried out. Extremely high levels of active amine content were achieved using prehydrated silica surfaces at grafting temperatures below reflux in order to facilitate thermally controlled water-aided surface polymerization of the aminosilanes. Abstract iii The CO₂ adsorption capacities and rates were determined for all materials as a function of the amount of TRI and water per gram of support added to the grafting mixture. The optimal TRI grafted PE-MCM-41 adsorbent exhibited a 2.65 mmol/g adsorption capacity at 25 °C and 1.0 atm for a dry 5% CO₂ in N₂ feed mixture, which exceeded all literature reported values, for both meso- and microporous materials under the conditions used in this study. Further, the apparent adsorption and desorption rates with the amine functionalized materials were exceedingly high. When considering the grafted amine quantity, the adsorption capacity and rate were found to be mutually dependent on each other, exhibiting an apparent optimal combination. In comparison to zeolite 13X, the optimally loaded TRI-PE-MCM-41 was far superior in terms of dynamic adsorption and desorption performance. These results were further enhanced when the adsorbents were challenged with a humid stream of 5% CO₂/N₂. The TRIPE-MCM-41 exhibited a 10% increase in CO₂ adsorption capacity, whereas the 13X zeolite did not retain any significant CO₂ adsorption capacity. The novel concept of an internally variably staged permeator was

introduced. A theoretical model was developed and used as the basis for simulation studies. The advantage of the internal variably staged design was shown to permit a very high extent of separation similar to a two stage permeator for purity, while maintaining similar flux rates as per a single stage permeator. This IVSP concept has also taken existing membrane materials and mechanically translated their process performance to a higher level. As such, the unit should prove effective for front end process stream cleanup requirements prior to an adsorption process with the novel TRI-PE-MCM-41 nano-porous adsorbent.

CO₂ capture and sequestration from coal-fired power plant flue gas is an attractive technique to control CO₂ emissions. Polyamine-based sorbent is considered as a promising sorbent for CO₂ capture due to its low equipment corrosion and regeneration energy penalty. One critical aspect of development of polyamine-based CO₂ capture process is to understand the nature of the adsorbed species with amine and their evolution in adsorption / desorption process. Fourier transform infrared (FTIR) spectroscopy is a powerful and versatile tool that can provide the insights from molecular level to address these scientific issues. This dissertation is focusing on using in-situ FTIR spectroscopy to discuss several important topics in CO₂ capture and utilization processes, including (i) the structure and binding energy of adsorbed CO₂/H₂O on solid amine sorbent, (ii) the role of H₂O in CO₂ adsorption/desorption on liquid amine films, (iii) mechanism of water-enhancement on CO₂ capture by amine, and (iv) photoelectrocatalytic reduction of CO₂ on polyamine/TiO₂ thin film. H₂O vapor in flue gas has dramatic effects on polyamine-based sorbent. H₂O could affect CO₂ capture capacity, regeneration energy, and degradation kinetics of the sorbents. This in situ IR study investigated these various effects on polyamine-based sorbents. The results revealed that CO₂ adsorbed on primary amine as ammonium carbamate while H₂O adsorbed on secondary amine and promoted the formation of carbamic acid. Adsorbed H₂O increases the binding strength of CO₂ with amine and protects sorbent from SO₂ poisoning. The results of this study clarify the role of H₂O in polyamine-based sorbent for CO₂ capture and provide a molecular basis for the design and operation of polyamine-based CO₂ capture processes. The use of FTIR spectroscopy in the investigation of role of water on CO₂ capture by amine has enabled us to verify the reaction processes. The results unraveled that adsorption of CO₂ on the 20 μm tetraethylenepentamine (TEPA) film at 50 °C followed a zwitterion-intermediate pathway: zwitterion \rightleftharpoons ammonium carbamate. H₂O in the mixed TEPA/H₂O (5:1) film decreased the rate of CO₂ adsorption, but increased the amine efficiency. The presence of H₂O promotes the formation of carbamic acid and produces a broad IR band centered at 2535 cm⁻¹, which can be assigned to (O-H) of hydronium carbamate, -NCOO-...H-OH₂⁺. The broadness of this 2535 cm⁻¹ band ranging from 2100 cm⁻¹ to 2800 cm⁻¹ persists at 120 °C. These broad components of the band can be ascribed to δ (N-H) in hydrogen-bonded ammonium carbamate, a R-NH₃⁺/R₁R₂-NH₂⁺...NCOO⁻ moiety. The binding

strength of adsorbed species on the TEPA film increases in the order: adsorbed H₂O

Strong evidence exists that anthropogenic emissions of CO₂ have contributed significantly to global climate change. Therefore, it is essential to mitigate anthropogenic CO₂ emissions. Unfortunately, current technology for CO₂ capture relying on amine scrubbing is costly because of the energy requirements for amine regeneration. Accordingly, alternative CO₂ capture technologies are sought. Among these, the use of solid adsorbents appears most promising in reducing the cost of CO₂ capture. This project focused on the development of amine-based solid sorbents with a low CO₂ desorption activation energy and a high CO₂ sorption capacity. Three different porous materials including nanoporous titanium oxyhydrate (TiO(OH)₂), modified carbon nanotubes (MCNTs), and poly(divinylbenzene/2-ethylhexyl methacrylate) (polyHIPE) have been prepared as adsorbent supports. The first two CO₂ adsorbents were prepared by immobilizing tetraethylenepentamine (TEPA) onto TiO(OH)₂ and MCNTs resulting in TiO(OH)₂/TEPA and MCNTs/TEPA adsorbents. Polyethylenimine (PEI) was used to prepare a polyHIPE/PEI adsorbent through impregnation. TiO(OH)₂/TEPA was used as an adsorbent for the removal of CO₂ at a low concentration (1 vol.% CO₂ in N₂). At optimal conditions, the CO₂ sorption capacity reached 3.1 mmol CO₂/g-sorbent at 60 °C. It was observed that the activation energies for CO₂ adsorption and desorption of TiO(OH)₂/TEPA are 19.6 kJ/mol and 51.1 kJ/mol, respectively. This low CO₂ desorption activation energy can contribute to a lower CO₂ capture cost. MCNTs/TEPA and polyHIPE/PEI adsorbents were also evaluated for CO₂ capture using 10 vol.% CO₂ in N₂. At the optimal conditions CO₂ sorption capacity reached 5 mmol CO₂/g-sorbent with MCNTs/TEPA and 4 mmol CO₂/g-sorbent with polyHIPE/PEI. Kinetic and thermodynamic adsorption/desorption studies found activation energies for CO₂ desorption are 39.9 kJ/mol for MCNTs/TEPA and 36.12 kJ/mol for polyHIPE/PEI. The low activation energies for CO₂ desorption using the prepared adsorbents can contribute to a lower CO₂ capture cost. Therefore, the prepared adsorbents have potential for application to CO₂ capture from gas mixtures.

The aim of the book is to provide an understanding of the current science underpinning Carbon Capture and Sequestration (CCS) and to provide students and interested researchers with sufficient background on the basics of Chemical Engineering, Material Science, and Geology that they can understand the current state of the art of the research in the field of CCS. In addition, the book provides a comprehensive discussion of the impact of CCS on the energy landscape, society, and climate as these topics govern the success of the science being done in this field. The book is aimed at undergraduate students, graduate students, scientists, and professionals who would like to gain a broad multidisciplinary view of the research that is being carried out to solve one of greatest challenges of our generation.

Contents:Energy and ElectricityThe Atmosphere and Climate ModelingThe Carbon CycleIntroduction to Carbon

Capture Absorption Adsorption Membranes Introduction to Geological Sequestration Fluids and Rocks Large-Scale Geological Carbon Sequestration Land Use and Geo-Engineering List of Symbols Credits Readership: Students taking courses on environmental sciences and research level individuals who are interested in environmental issues related to CCS. Key Features: The first comprehensive textbook on Carbon Capture and Sequestration (CCS) A comprehensive discussion on the science of CCS and its impact on society and climate A multidisciplinary approach to CCS by the leading US research centers on CCS Keywords: Carbon Capture; Carbon Storage; Carbon Sequestration; Gas Separations "The following describes a novel passive approach to control the indoor CO₂ levels in enclosed spaces, primarily focusing on commercial buildings. Amine impregnated silica sorbents were identified as suitable candidates and synthesized; the amine loading ratio was varied to create a range of materials. These samples along with other commercial zeolite candidates have been tested over a range of CO₂ concentrations to determine the CO₂ adsorption capacity in laboratory systems and under simulated room conditions. The research work also focuses on the CO₂ desorption capacity of the candidate adsorbents. The desorption is allowed to occur gradually over time with the concentration gradient as its sole driving force; usually a pressure or temperature swing is applied to desorb CO₂ from the adsorbents. Results have shown TEPA impregnated silica to have a good adsorption capacity (1.5 mmol/g); and by decreasing the amine content, the silica-TEPA samples showed good initial desorption of almost 31% of the adsorbed CO₂. They exhibited lower capacity but a greater desorption percentage with repeated cycles. At room temperature and pressure conditions, cyclic tests were conducted in a small chamber simulating real indoor environment. The adsorbent reduced the CO₂ concentration by almost 8% reduction. Further studies conducted to investigate the effect of adsorbent weight showed that adsorption increased from 3% to 8% on increasing the quantity of adsorbent used. Similarly, the effect of relative humidity of chamber air was studied. Results showed a 4% decrease in CO₂ uptake when the RH was dropped to 15% from 50%; and an increase of 10% uptake was observed at 90% RH"--Abstract, page iii.

Strong evidence exists that anthropogenic emissions of CO₂ have contributed significantly to global climate change. Therefore, it is essential to mitigate anthropogenic CO₂ emissions. Unfortunately, current technology for CO₂ capture relying on amine scrubbing is costly because of the energy requirements for amine regeneration. Accordingly, alternative CO₂ capture technologies are sought. Among these, the use of solid adsorbents appears most promising in reducing the cost of CO₂ capture. This project focused on the development of amine-based solid sorbents. Specifically, an inorganic-organic CO₂ sorbent was prepared by immobilizing tetraethylenepentamine (TEPA) onto nanoporous titanium oxyhydrate (TiO(OH)₂). At the optimal conditions, the CO₂ sorption capacity reached 3.1 mmol CO₂/g-sorbent for 1 vol.% CO₂ in N₂. It is observed that the activation energies for CO₂ adsorption and desorption of TiO(OH)₂/TEPA are 19.6 kJ/mol and 51.1 kJ/mol, respectively. This low CO₂ desorption activation

energy means a high CO₂ desorption rate, thus a low CO₂ capture cost.

An innovative, low-cost, and low-energy-consuming carbon dioxide (CO₂) capture technology was developed, based on CO₂ adsorption on a high-capacity and durable carbon sorbent. This report describes the (1) performance of the concept on a bench-scale system; (2) results of parametric tests to determine the optimum operating conditions; (3) results of the testing with a flue gas from coal-fired boilers; and (4) evaluation of the technical and economic viability of the technology. The process uses a falling bed of carbon sorbent microbeads to separate the flue gas into two streams: a CO₂-lean flue gas stream from which > 90% of the CP₂ is removed and a pure stream of CO₂ that is ready for compression and sequestration. The carbon sorbent microbeads have several unique properties such as high CO₂ capacity, low heat of adsorption and desorption (25 to 28 kJ/mole), mechanically robust, and rapid adsorption and desorption rates. The capture of CO₂ from the flue gas is performed at near ambient temperatures in which the sorbent microbeads flow down by gravity counter-current with the up-flow of the flue gas. The adsorbed CO₂ is stripped by heating the CO₂-loaded sorbent to ~ 100°C, in contact with low-pressure (~ 5 psig) steam in a section at the bottom of the adsorber. The regenerated sorbent is dehydrated of adsorbed moisture, cooled, and lifted back to the adsorber. The CO₂ from the desorber is essentially pure and can be dehydrated, compressed, and transported to a sequestration site. Bench-scale tests using a simulated flue gas showed that the integrated system can be operated to provide > 90% CO₂ capture from a 15% CO₂ stream in the adsorber and produce > 98% CO₂ at the outlet of the stripper. Long-term tests (1,000 cycles) showed that the system can be operated reliably without sorbent agglomeration or attrition. The bench-scale reactor was also operated using a flue gas stream from a coal-fired boiler at the University of Toledo campus for about 135 h, comprising 7,000 cycles of adsorption and desorption using the desulfurized flue gas that contained only 4.5% v/v CO₂. A capture efficiency of 85 to 95% CO₂ was achieved under steady-state conditions. The CO₂ adsorption capacity did not change significantly during the field test, as determined from the CO₂ adsorption isotherms of fresh and used sorbents. The process is also being tested using the flue gas from a PC-fired power plant at the National Carbon Capture Center (NCCC), Wilsonville, AL. The cost of electricity was calculated for CO₂ capture using the carbon sorbent and compared with the no-CO₂ capture and CO₂ capture with an amine-based system. The increase in the levelized cost of electricity (L-COE) is about 37% for CO₂ capture using the carbon sorbent in comparison to 80% for an amine-based system, demonstrating the economic advantage of CO₂ capture using the carbon sorbent. The 37% increase in the L-COE corresponds to a cost of capture of \$30/ton of CO₂, including compression costs, capital cost for the capture system, and increased plant operating and capital costs to make up for reduced plant efficiency. Preliminary sensitivity analyses showed capital costs, pressure drops in the adsorber, and steam requirement for the regenerator are the major variables in determining the cost of CO₂ capture. The results indicate that further long-term testing with a flue gas from a pulverized coal fired boiler should be performed to obtain additional data relating to the effects of flue gas contaminants, the ability to reduce pressure drop by using alternate structural packing, and the use of low-cost construction materials.

The sorbents for separation of CO₂ from ultra dilute gas streams are required to be able to achieve high CO₂ sorption capacities,

although CO₂ concentrations of such gases are extremely low. They are also expected to have fast adsorption kinetics at low temperature ranges (e.g., 5-30°C). In addition, their CO₂ desorption kinetics should be fast, as is expected for any other sorbents. An alternative amine-based sorbent (referred as RFAS) developed in this work was assessed under various conditions. Studies showed that the CO₂ sorption capacities of the sorbent increased considerably with N loading, slowly with increasing temperature (apparently contrary to the prediction with the isothermal equation of exothermic sorption), and gradually with the decrease of gas flow rate in the tested range. In addition, CO₂ sorption capacity increased and then decreased with increasing H₂O:CO₂ mole ratio and the stoichiometric ratio 1:1 is the turning point. The CO₂ sorption capacities achieved by the sorbent with 8.07 mmol N/g for air with 400 ppm CO₂ and the CO₂-N₂ gas mixtures containing 1 vol-% CO₂, were 1.78 mmol CO₂/g and 1.92 mmol CO₂/g, respectively, higher than those reported in the most recent literature. A kinetic model corresponding to three proposed pathways was derived and expected to quantitatively predict the CO₂ sorption characteristics given that the involved parameters can be established in the future. The half-CO₂-adsorption and desorption times of the sorbent along with temperatures were used to evaluate the dynamics of the sorbent. The adsorbed CO₂ can be completely desorbed at only 80°C within as short as 30 minutes. The CO₂ sorption capacities of the sorbent within 10 sorption-desorption cycles are repeatable. All the results confirmed that the sorbent is a highly adsorptive, reversibly dynamic, and regenerable sorbent for capture of ultradilute CO₂ from gas mixtures. Key words: carbon dioxide emissions, carbon dioxide capture and sequestration, amine-based solid adsorbents, air capture, adsorption capacity.

Carbon capture is essential for reduction of carbon dioxide (CO₂) pollution from flue gas which is emitted during fossil fuel combustion. The flue gas is mainly composed of 15% CO₂ and 85% N₂ and it requires high selectivity for gas purification. Some methods have been developed for carbon capture such as Pressure Swing Adsorption (PSA) and Temperature Swing Adsorption (TSA). Unfortunately, these techniques use a lot of energy during the desorption step that reduces power generation efficiency. An ideally effective carbon capture technique needs to promote CO₂ adsorption and desorption at the proper times during the separation cycles, without incurring a large parasitic energy load. A new gas adsorption technique is presented, Supercapacitive Swing Adsorption (SSA), in which CO₂ is either actively adsorbed or desorbed by repeated capacitive charge and discharge of supercapacitor carbon electrodes and energy used in adsorption can principally be recovered upon desorption. It is shown that reversible adsorption/desorption of CO₂ from a 15% CO₂ and 85% N₂ gas mixture can be achieved when an electrically conducting high surface area porous carbon material is brought into contact with carbon dioxide gas and an aqueous sodium chloride electrolyte. When the supercapacitor carbon electrodes are charged, the electrolyte ions are spontaneously organized into an electric double layer at the surface of each porous carbon electrode. The presence of this double layer leads to reversible, selective adsorption and desorption of the CO₂ as the supercapacitor is charged and discharged. Moreover, it is also shown that SSA has the ability to separate CO₂ from N₂, with a high selectivity for CO₂ and only a weak dependence on the CO₂ partial pressure in a CO₂/N₂ gas mixture. The amount of adsorbed CO₂ scales with applied voltage and with the mass of the porous

carbon sorbent, which is inexpensive, robust and environmentally friendly. The effect barely depends on temperature. CO₂ sorption studies were conducted for Raniganj coals of India from the point of view of CO₂ adsorption & desorption and the effect of temperature, coal particle size and media pH. Adsorption and desorption studies were conducted for 4 samples with the highest adsorption capacity reported as 11.09mL/g of coal and lowest as 5.15mL/g at 30°C. Desorption studies revealed the existence of both positive and negative hysteresis curves. The minimum desorption capacity was attained for S -2, 1.29ml/g at the pressure of 22.361Psi. Hysteresis was minimum for sample 1. While sample 3 and sample 5 showed maximum positive hysteresis. The hysteresis increases with increasing pressure initially and extended till 600Psi. Experimental data were verified using several adsorption isotherms such as Langmuir, BET, Dubinin-Astakhov (D-A) and Dubinin-Radushkevich (D-R). The Langmuir isotherm model was failed to predict the data accurately. The D-A model gave an enough satisfactory representation suggesting that the pore filling model proposed by the Polany. Sorption studies conducted at 30, 31.1, 40 and 50°C revealed that adsorption decreased with increase in temperature. These values were also compared with those obtained through the characteristic plots defined by the Dubinin-Ashtakov equation. CO₂ adsorption behavior at new temperature fit in with the experimental data reported for CO₂ adsorption below its critical temperature. The effect of particle size was studied by considering samples of 150µm, 650µm and 850µm and it was found that adsorption capacity decreased with increase in particle size. As far as the effect of pH was concerned, the adsorption capacity was highest for acidic media followed by alkaline media and neutral media. The experimental results of CO₂ adsorption and desorption in a packed column indicated that the concentration wave front at the center of the packed column differs from those which are close to the wall of column filled with adsorbent material even though the ratio of column diameter to the particle size is greater than 20. The comparison of the experimental results with one dimensional model of packed column shows that in order to simulate the average breakthrough in a packed column a two dimensional (radial and axial) model of packed column is needed. In this paper the mathematical model of a non-slip flow through a packed column with 2 inches in diameter and 18 inches in length filled with 5A zeolite pellets is presented. The comparison of experimental results of CO₂ adsorption and desorption for the mixed and central breakthrough of the packed column with numerical results is also presented.

This book summarises the advanced CO₂ capture technologies that can be used to reduce greenhouse gas emissions, especially those from large-scale sources, such as power-generation and steel-making plants. Focusing on the fundamental chemistry and chemical processes, as well as advanced technologies, including absorption and adsorption, it also discusses other aspects of the major CO₂ capture methods: membrane separation; the basic chemistry and process for CO₂ capture; the development of materials and processes; and practical applications, based on the authors' R&D experience. This book serves as a valuable reference resource for researchers, teachers and students interested in CO₂ problems, providing essential information on how to capture CO₂ from various types of gases efficiently. It is also of interest to practitioners and academics, as it discusses the performance of the latest technologies applied in large-scale emission sources.

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