

# Adsorption Techniques for CO<sub>2</sub> Capture: Modeling and Simulation Insights

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## Overview

Since the industrial revolution, carbon dioxide (CO<sub>2</sub>) has been a significant contributor to greenhouse gas emissions due to several human activities. The CO<sub>2</sub> limit in the atmosphere is considered safer if it is less than 350 ppm. However, in December 2018, it crossed safety limits and reached 409 ppm. Energy demand has been increasing enormously due to a rise in the human population and a comfortable lifestyle. India has more than 1.4 billion people, consuming energy from coal and natural gas-based power plants and emitting CO<sub>2</sub> into the atmosphere. To contribute to these needs, easily accessible fossil fuel resources are rapidly consuming. CO<sub>2</sub> is the major emitter in the transportation industry (i.e., automobiles), power generation, and deforestation in agricultural fields. There is an urgent requirement for novel technologies to reduce this carbon emissions effect on the environment. Carbon capture and sequestration (CCS) technology is getting much attention due to the rise in temperature levels. The CCS technique can be divided into three stages. In the first stage, the CO<sub>2</sub> gas is extracted from the emission gas stream, and then the CO<sub>2</sub> is concentrated and captured at high pressures. The supercritical fluid is transported to the CO<sub>2</sub> storage site, where fluid is injected into the underground rocks for permanent storage. This technology has the advantage of strategy-wise collecting CO<sub>2</sub>, storing CO<sub>2</sub> and utilising the stored gas.


Carbon capture is a significant step in the CCS technology. The adsorption based carbon capture process has advantages over the existing technologies, such as fast kinetics, excellent energy efficiency, clean environment applications, high gas storage capacities, etc. However, the thorough understanding of the conventional adsorption swing processes such as Pressure swing adsorption (PSA), Vacuum Swing Adsorption (VSA) and Temperature swing adsorption (TSA) and novel hybrid swing adsorption processes such as Vacuum Pressure Swing Adsorption (VPSA) and Temperature Vacuum Swing Adsorption process (TVSA) is missing. This course covers the fundamentals of adsorption, the advancement of adsorption in the field of carbon capture, ongoing challenges and sustainable solutions.



Significant improvements in computational power over the last two decades have encouraged researchers to develop mathematical models for accurate forecasting of experiments. Transport modelling of the carbon capture units packed with porous adsorbents mitigates the experimental effort, which is energy-consuming and expensive. In this course, we demonstrate the development of mathematical models and the application of commercial software tools to solve carbon capture units in the real world.

The course will be taught by distinguished international and national academicians and researchers who are well recognized in this field for their experience in research, teaching and consultancy. Industrially relevant case studies will be discussed as part of the tutorial session which provides Hands on experience to participants on advanced software tools. This course contributes to the nation's net zero emission goal by training manpower to pursue their career in CCUS.

<b>Course Information</b>	<b>Dates – 24<sup>th</sup> March to 28<sup>th</sup> March 2025</b>  <b>Adsorption Techniques for CO<sub>2</sub> Capture: Modeling and Simulation Insights</b>
<b>Modules</b>	<p><b>Number of participants for the course will be limited to Sixty.</b></p> <p><b><u>Day I</u></b></p> <ul style="list-style-type: none"> <li>• Introduction to CO<sub>2</sub> capture, Current Status and Future Prospects of CO<sub>2</sub> Capture, Need for Adsorption, Categorizations of Adsorptive Separation Processes.</li> <li>• Fundamentals of Adsorption Process: Adsorbents and Adsorption Isotherms, Industrial Adsorbents and various classes of materials available, Surface and pore characteristics of Adsorbent</li> <li>• Selection of Adsorbent, Equilibrium Adsorption of Pure Gases, Adsorption Equilibrium Isotherm Models, Measurements of Adsorption equilibrium (Gravimetric vs Volumetric)</li> <li>• Introduction to process modelling, Mathematical modelling basics: Differential equations, algebraic equations.</li> </ul> <p><b><u>Day II</u></b></p> <ul style="list-style-type: none"> <li>• Kinetics of sorption in batch media</li> <li>• Thermodynamics of Adsorption and Diffusion in porous media, Dynamic column breakthrough measurements for gas mixtures</li> <li>• MATLAB and Aspen software basics, unit operations, unit processes, etc.</li> </ul> <p><b><u>Day III</u></b></p> <ul style="list-style-type: none"> <li>• Introduction to differential algebraic equation systems and partial differential-algebraic equations.</li> <li>• Flow through packed beds and Dynamics of sorption column.</li> <li>• Estimation of Adsorption isotherm parameters in MATLAB and Breakthrough curve development in Aspen Adsorption</li> </ul> <p><b><u>Day IV</u></b></p> <ul style="list-style-type: none"> <li>• Adsorption separation processes by continuous systems: Introduction and Pressure Swing Adsorption (PSA)</li> <li>• Adsorption separation processes by continuous systems: Temperature Swing Adsorption (TSA) and Vacuum Swing Adsorption (VSA) Processes</li> <li>• Simulation of the CO<sub>2</sub> capture system in Aspen Adsorption and estimation of the process performance metrics</li> </ul> <p><b><u>Day V</u></b></p> <ul style="list-style-type: none"> <li>• Introduction to dynamic systems, cyclic systems, solution approaches, convergence</li> <li>• Modelling of the adsorption process to understand the CO<sub>2</sub> capture</li> </ul>

	<ul style="list-style-type: none"> <li>Advanced CO<sub>2</sub> capture adsorption separation processes: Hybrid swing processes such as Vacuum Pressure Swing Adsorption (VPSA) and Temperature Vacuum Swing Adsorption (TVSA)</li> </ul>
<p><b>You Should Attend If You Are...</b></p>	<ul style="list-style-type: none"> <li>Executives, Engineers, and Researchers from industries, service, and government organizations, including R&amp;D laboratories.</li> <li>Students at all levels (BTech, MSc, MTech, PhD) from reputed academic and technical institutions.</li> <li>Faculty Members from reputed academic and technical institutions</li> <li>Students who would like to pursue their career in Carbon Capture Utilization and Sequestration (CCUS)</li> </ul>
<p><b>Fees</b></p>	<p>The participation fees for taking the course is as follows:</p> <p><b>Participants from abroad: US \$250</b></p> <p><b>Industrial Organizations: INR 6000+18% GST</b></p> <p><b>Research Organizations: INR 3000+18% GST</b></p> <p><b>Faculty/Scientists: INR 3000+18% GST</b></p> <p><b>Post Doc: INR 2000+18% GST</b></p> <p><b>Students: INR 1000+18% GST</b></p> <p>The above fee includes all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hr. free internet facility. The participants will be provided with accommodation on payment basis.</p> <p><b>Note:</b> <u>There is no central registration on the GIAN portal (<a href="http://gian.iith.ac.in">gian.iith.ac.in</a>); registration will be managed directly by the hosting institute.</u></p>

	<p>Dr. Debangsu Bhattacharyya is the professor at West Virginia University. His research interests are in the area of advanced modeling and simulation, condition monitoring, fault diagnosis, state estimation, optimization, uncertainty quantification, sensor placement, scheduling, biomimetic control, artificial intelligence and machine learning including reinforcement learning, and advanced manufacturing. His group is applying these process systems engineering approaches to energy-generating and energy storage processes including green and blue hydrogen generation and utilization processes, carbon capture and utilization systems, and natural gas and biomass utilization processes. Till now, he has authored/co-authored more</p>
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	<p>than 125 research papers, 5 book chapters, 300 oral presentations and 60 poster presentations</p>
	<p>Dr. Ravi Chandra Dutta is an Assistant Professor in the Department of Chemical Engineering at the Indian Institute of Technology Dharwad since April 2023. He completed his PhD at The University of Queensland (2019) and post doc at Max Planck Institute for Polymer Research Germany (2021). He worked as postdoctoral research fellow at the University of Queensland during 2021 to 2023. His research interests lie in the development of gas separation membranes, AI material discovery and the design of energy storage materials.</p>
	<p>Dr. Sridhar Palla is an assistant professor at the Indian Institute of Petroleum and Energy, Visakhapatnam, and a researcher specializing in multiscale modeling, molecular simulations, and the integration of artificial intelligence (AI) and machine learning (ML) to address energy and environmental challenges.</p>

Course Co-Coordinator

Dr. Sridhar Palla, Phone: 91-9492462493, E-mail: [sridhapalla.che@iipe.ac.in](mailto:sridhapalla.che@iipe.ac.in)

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Registration link:

<https://iipe.ac.in/GIAN2/registration/giancourse2.php>