# Energy Technology 2018

## Carbon Dioxide Management and Other Technologies


Edited by
Ziqi Sun
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Donna Post Guillen
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Dirk Verhulst
Xiaofei Guan
Allie Anderson
Shadia Ikhmayies
York R. Smith
Amit Pandey
Sarma Pisupati
Huimin Lu



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# The Minerals, Metals & Materials Series

Ziqi Sun · Cong Wang · Donna Post Guillen
Neale R. Neelameggham
Lei Zhang · John A. Howarter
Tao Wang · Elsa Olivetti
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# Preface

This volume contains selected papers presented at the Energy Technologies Symposium organized in conjunction with the TMS 2018 Annual Meeting & Exhibition in Phoenix, Arizona, USA, and organized by the TMS Energy Committee. The papers in this volume intend to address the issues, intricacies, and the challenges relating to energy and environmental science. This volume also contains selected papers from the following symposia: Deriving Value from Challenging Waste Streams: Recycling and Sustainability Joint Session, Materials for Energy Conversion and Storage, Solar Cell Silicon, and Stored Renewable Energy in Coal.

The Energy Technologies Symposium was open to participants from both industry and academia and focused on energy efficient technologies including innovative ore beneficiation, smelting technologies, recycling, and waste heat recovery. The volume also covers various technological aspects of sustainable energy ecosystems, processes that improve energy efficiency, reduce thermal emissions, and reduce carbon dioxide and other greenhouse emissions. Papers addressing renewable energy resources for metals and materials production, waste heat recovery and other industrial energy efficient technologies, new concepts or devices for energy generation and conversion, energy efficiency improvement in process engineering, sustainability and life cycle assessment of energy systems, as well as the thermodynamics and modeling for sustainable metallurgical processes are included. This volume also includes topics on $CO_2$ sequestration and reduction in greenhouse gas emissions from process engineering, sustainable technologies in extractive metallurgy, as well as the materials processing and manufacturing industries with reduced energy consumption and $CO_2$ emission. Contributions from all areas of nonnuclear and nontraditional energy sources, such as solar, wind, and biomass are also included in this volume.

We hope this volume will provide a reference for the materials scientists and engineers as well as metallurgists for exploring innovative energy technologies and novel energy materials processing.

We would like to acknowledge the contributions from the authors of the papers in this volume, the efforts of the reviewers dedicated to the manuscripts review

process, and the help received from the publisher. We appreciate the efforts of Energy Committee members for enhancing this proceedings volume. We also acknowledge the organizers of the four other symposia that contributed papers.

## Energy Technologies Symposium Organizers

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Donna Post Guillen, Idaho National Laboratory, USA
Lei Zhang, University of Alaska Fairbanks, USA
Neale R. Neelameggham, IND LLC, USA
Tao Wang, Nucor Steel, USA
John A. Howarter, Purdue University, USA

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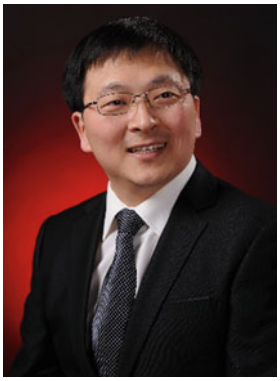
# About the Editors

**Ziqi Sun** is a senior lecturer at the School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Australia. He received his Ph.D. degree in 2009 from Institute of Metal Research, Chinese Academy of Sciences and his B.Eng. degree in 1999 from Central South University China. He was awarded with some prestigious awards and fellowships including the TMS Young Leaders Development Award from The Minerals, Metals & Materials Society (TMS, 2015), Discovery Early Career Research Award from Australian Research Council (DECRA, 2014), Alexander von Humboldt Fellowship from AvH Foundation Germany (2009), Australian Postdoctoral Fellowship from Australian Research Council (APD, 2010), the Vice-Chancellor's Research Fellowship from University of Wollongong (2013), etc. He is also serving as Vice-Chair of the Energy Committee within TMS, Associate Editor of *Surface Innovations* (ICE Science), Editorial Board Member of *Scientific Reports* (Nature Publishing Group), Editorial Board Member of *Journal of Materials Science and Technology* (Elsevier), Guest Professor at Shenzhen Institute, Peking University, and Honorary Fellow at University of Wollongong. Ziqi is the program leader for two ongoing Australian Research Council Projects. He held the roles as symposium organizer and session chair in some prestigious conferences such as TMS conferences and ACerS annual conferences. His major research interest is the rational design of bio-inspired metal oxide

nanomaterials for sustainable energy harvesting, conversion, and storage.



**Cong Wang** is currently Professor of the School of Metallurgy, Northeastern University. Prior to joining the faculty of his alma mater, Dr. Wang had worked with Alcoa, Saint-Gobain, and Northwestern University, respectively. His expertise includes high-temperature metallurgical processing with a focus on steels. He is the incumbent TMS Energy Committee Chair. He serves on the editorial boards of several journals, including *Metallurgical and Materials Transactions A* and *B*, *International Journal of Refractory Metals and Hard Materials*, *Journal of Materials Science and Technology*, and *Journal of Iron and Steel Research International*. He is also a Corresponding Expert of Engineering, the flagship journal recently launched by Chinese Academy of Engineering. He receives Invitational Fellowship by JSPS (2017), Excellent Young Scientist Award by NSFC (2016), Outstanding Young Manufacturing Award by SME (2014) and Young Leader Professional Award by TMS (2011). He is also the finalist of the prestigious 1000 Talents Program by Chinese Government (2014). As an active member of the global metallurgy community, Dr. Wang serves as the inaugural founder of the International Metallurgical Processes Workshop for Young Scholars (IMPROWYS), and acted as organizers/advisors for various international symposia/workshop of technical significance.

**Donna Post Guillen** holds the position of distinguished research engineer in the Materials Science and Engineering Department at the Idaho National Laboratory. Dr. Guillen earned a B.S. in mechanical engineering from Rutgers University, an M.S. in aeronautics from Caltech, and a Ph.D. in engineering and applied science from Idaho State University. She has more than 30 years of research experience and has served as principal investigator for numerous multidisciplinary research projects on the topics of waste heat recovery, synthetic fuels production, nuclear reactor fuels and materials experiments, and waste

glass vitrification. The focus of her research is on multiphase computational fluid dynamics and thermal hydraulics for sustainable energy technologies. She applies numerical modeling techniques to provide understanding of a wide variety of complex systems such as, greenhouse gas generation/sequestration for dairies, working with industry (General Electric) to develop a direct evaporator for an organic Rankine cycle, and modeling the waste vitrification process for the Hanford Waste Treatment Plant and the fluidized bed for the Idaho Waste Treatment Unit. She is experienced with irradiation testing and thermal hydraulic analysis for nuclear reactor experiments and serves as Principal Investigator/Technical Lead for the Nuclear Science User Facility Program. She is the lead inventor on two patents related to the development of a new composite material to produce a fast reactor environment within a pressurized water reactor. She actively mentors students, routinely chairs and organizes technical meetings for professional societies, serves in leadership capacity for the American Nuclear Society (Thermal Hydraulics Executive and Program committees), The Minerals, Metals & Materials Society (TMS—Energy Committee Past-Chair) and the American Society of Mechanical Engineers (Thermal Hydraulics and Computational Fluid Dynamic Studies Track Co-Chair), provides subject matter reviews for proposals and technical manuscripts, has published more than 100 conference papers, reports and journal articles, and written/edited three books.

**Neale R. Neelameggham** is "The Guru" at IND LLC, involved in international consulting in the field of metals and associated chemicals (boron, magnesium, titanium, and lithium and rare earth elements), thiometallurgy, energy technologies, soil biochemical reactor design, etc. He was a visiting expert at Beihang University of Aeronautics and Astronautics, Beijing, China. He was a plenary speaker at the Light Metal Symposium in South Africa—on low carbon dioxide emission processes for magnesium. Dr. Neelameggham has more than 38 years of expertise in magnesium production and was involved in process development of

its start-up company NL Magnesium through to the present US Magnesium LLC, UT until 2011. Neelameggham and Brian Davis authored the ICE-JNME award-winning (2016) paper "21st Century Global Anthropogenic Warming Convective Model," which notes that constrained air mass warming is independent of the energy conversion source—fossil or renewable energy. He is presently developing Agricoal™ and agricoalture to improve arid soils. Dr. Neelameggham holds 16 patents and patent applications, and has published several technical papers. He has served in the Magnesium Committee of the Light Metals Division (LMD) of TMS since its inception in 2000, chaired it in 2005, and in 2007 he was made a permanent co-organizer for the Magnesium Symposium. He has been a member of the Reactive Metals Committee, Recycling Committee, Titanium Committee, and Program Committee Representative of LMD and LMD council. Dr. Neelameggham was the inaugural chair, when in 2008, LMD and EPD (Extraction & Processing Division) created the Energy Committee, and has been a coeditor of the energy technology symposium proceedings through the present. He received the LMD Distinguished Service Award in 2010. While he was the chair of Hydro- and Electrometallurgy Committee he initiated the rare metal technology symposium in 2014. He is coeditor for the 2018 proceedings for the symposia on Magnesium Technology, Energy Technology, Rare Metal Technology, and Solar Cell Silicon.

**Lei Zhang** is an assistant professor in the Department of Mechanical Engineering at the University of Alaska Fairbanks (UAF). Prior to joining the UAF, Dr. Zhang worked as a postdoctoral associate in the Department of Chemical and Biomolecular Engineering at the University of Pennsylvania. Dr. Zhang obtained her Ph.D. degree in materials science and engineering from Michigan Technological University in 2011, and her M.S. and B.E. degrees in materials science and engineering from China University of Mining and Technology, Beijing, China, in 2008 and 2005, respectively. Her research interest focuses on the design and investigation of the properties of porous

materials and nanostructure-based films for energy and environmental applications. Her current research focuses mainly on the synthesis of metal-organic frameworks (MOFs) and MOF-based nanocomposites, and the manipulation of their properties and applications in gas storage, separation, and water treatment. She is also working on the development and characterization of anticorrosion coatings on metallic alloys for aerospace and biomedical applications.

Dr. Zhang has been actively involved in the activities at The Minerals, Metals & Materials Society (TMS) annual meetings. She has served on the TMS Energy Committee since 2014, and also has served on the Best Paper Award Subcommittee of the TMS Energy Committee. She has served as a frequent organizer and session chair of the symposia at TMS Annual Meetings (2015, 2016, and 2017). She was the recipient of 2015 TMS Young Leaders Professional Development Award.

**John A. Howarter** is an assistant professor in Materials Engineering at Purdue University with a joint appointment in Environmental & Ecological Engineering. His research interests are centered on synthesis, processing, and characterization of sustainable polymers and nanocomposites. His research impacts water treatment, thermal management in electronic devices, and material design for recycling and value recovery. John has been involved in the Public and Government Affairs (P&GA) Committee of The Minerals, Metals & Materials Society (TMS), where he currently serves as incoming Chair. In addition to working with P&GA, Prof. Howarter is a regular contributor to the technical programming for both TMS and Materials Science & Technology (MS&T) conferences in areas of energy, recycling, and materials sustainability. John earned a B.Sc. from The Ohio State University in 2003 and Ph.D. from Purdue University in 2008, both in materials engineering. From 2009 to 2011, he was a National Research Council postdoctoral scholar in the Polymers Division of the National Institute of Standards and Technology in Gaithersburg, Maryland.

**Tao Wang** is currently Castrip Research Lab Supervisor at Nucor Steel. He is also the lead engineer in the process and product research and development areas. Dr. Wang's current focus is to develop and modify a novel thin strip casting technology which uses up to 90% less energy to process liquid steel into hot rolled steel sheets than conventional casting methods. Dr. Wang has rich experience in metallurgical thermodynamics, thermal energy storage and transfer, steelmaking, metal solidification and casting, and metal corrosion. Dr. Wang obtained his Ph.D. and M.S. from the University of Alabama; and he received his B.S. from Xi'an Jiao Tong University in China. In his areas of research, Dr. Wang has published multiple papers and patents which led to breakthroughs in thermodynamic modeling, high-efficiency thermal energy transfer medium development, and thin strip metal casting technology.

Dr. Wang received the 2013 Light Metals Division (LMD) Best Energy Paper Award from TMS and is a 2016 TMS Young Leaders Award winner. Also, he was selected to become a member of TMS Emerging Leader Alliance (ELA) in 2015. Dr. Wang serves the technical committees, including the Energy Committee and Pyrometallurgy Committee, within TMS; and Metallurgy-Steelmaking & Casting Technology Committee, Continuous Casting Technology Committee, Southeast Chapter within Association for Iron & Steel Technology (AIST).

**Elsa Olivetti** is the Thomas Lord Assistant Professor in the Department of Materials Science and Engineering at Massachusetts Institute of Technology (MIT). She received her B.S. in engineering science from the University of Virginia and her Ph.D. in materials science from MIT working on development of nanocomposite electrodes for lithium-ion rechargeable batteries. Olivetti joined MIT's faculty in 2014 where her current research focuses on improving the environmental and economic sustainability of materials in the context of rapid-expanding global demand. Olivetti leverages machine learning as well as data mining coupled with engineering and macroeconomic models to determine the scaled impact of novel materials and processes.

**Mingming Zhang** is currently a lead research engineer at ArcelorMittal Global R&D at East Chicago, Indiana. His main responsibilities include raw material characterization and process efficiency improvement in mineral processing and ironmaking areas. He also leads a technical relationship and research consortium with university and independent laboratory members and manages pilot pot-grate sintering test facility at ArcelorMittal Global R&D East Chicago.

Dr. Zhang has over 15 years of research experience in the field of mineral processing, metallurgical and materials engineering. He obtained his Ph.D. degree in Metallurgical Engineering from The University of Alabama and his Master degree in Mineral Processing from General Research Institute for Non-ferrous Metals in China. Prior to joining ArcelorMittal, he worked with Nucor Steel Tuscaloosa, Alabama where he was metallurgical engineer leading the development of models for simulating slab solidification and secondary cooling process.

Dr. Zhang has conducted a number of research projects involving mineral beneficiation, thermodynamics and kinetics of metallurgical reactions, electrochemical processing of light metals, energy efficient and environmental cleaner technologies. He has published over 50 peer-reviewed research papers and is the recipient of several U.S. patents. Dr. Zhang also serves as editor and reviewer for a number of prestigious journals including *Metallurgical & Materials Transactions A* and *B*, *JOM*, *Journal of Phase Equilibria and Diffusion*, and *Mineral Processing and Extractive Metallurgy Review*.

Dr. Zhang has made more than 20 research presentations at national and international conferences including more than 10 keynote presentations. He is the recipient of 2015 TMS Young Leaders Professional Development Award. He has been invited by a number of international professional associations to serve as conference organizer and technical committee member. These associations include The Minerals, Metals & Materials Society (TMS) and the Association for Iron & Steel Technology (AIST).

**Dirk Verhulst** spent the last 40 years in practical process metallurgy research on both sides of the Atlantic, bringing a number of projects from the laboratory to the pilot scale, and a few to industrial implementation. He is presently an independent consultant in process metallurgy and energy efficiency.

Until the end of 2008, he was Director of Research at Altairnano in Reno, Nevada. He participated in the development of the Altair Lithium-ion Battery, and was involved in the design and procurement of the manufacturing plant for the ceramic materials.

Over the period 2003–2008, he worked extensively on the Altair Hydrochloride $TiO_2$ Pigment Process and the operation of its pilot plant. The complex flow sheet included both hydrometallurgical and pyrometallurgical steps. Optimization of energy use was a key factor to make this new approach competitive.

From 1995 to 2000, he was Senior Development Engineer in BHP's Center for Minerals Technology at the same location in Reno. It is at BHP that the development of the hydrochloride $TiO_2$ pigment process was initiated. Other BHP projects included novel processes for nickel, cobalt, zinc, and copper.

Prior to 1995, he worked for 17 years in the research department of Umicore in Hoboken, Belgium. He was active in lead refining and in the hydrometallurgy of minor metals (indium, tellurium, selenium), but was mostly involved in the introduction of electric furnaces in lead smelting and slag cleaning. He tackled mathematical models and lab-scale experiments, ran pilot plants and participated in the start-up of industrial operations.

Dr. Verhulst has a doctor of engineering science degree in extractive metallurgy from Columbia University, and a chemical engineering degree from the Free University of Brussels. He wrote and presented publications in the areas of hydrometallurgy, pyrometallurgy, nanomaterials, and environmental science. He holds several patents and patent applications.

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Shadia is a member of The Minerals, Metals & Materials Society (TMS) and the World Renewable Energy Network (WREN). She is a member of the International Organizing Committee and the International Scientific Committee in the European Conference on Renewable Energy Systems (ECRES2015-ECRES2017). She is a member of the editorial board of the *International Journal of Materials and Chemistry* for Scientific & Academic Publishing, the editor-in-chief of a book for the Research Signpost. She was a technical advisor/subject editor for *JOM*. She is a guest editor for two topical collections published in the *Journal of Electronic Materials*: European Conference on Renewable Energy Systems (2015 and 2016). Shadia is a reviewer in 24 international journals and she is Chair of the TMS Materials Characterization Committee (2016–2017).

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**Sarma Pisupati** is Professor and Chair of the Energy Engineering Program, and Director of Online Education in the John and Willie Leone Family Department of Energy and Mineral Engineering at Pennsylvania State University (Penn State). He also codirects the Coal Science and Technology Program of the EMS Energy Institute. He earned B.S. and M.S. degrees in Chemical Engineering and a Ph.D. degree in Fuel Science. He has been studying and teaching the issues related to the energy and environment for the past 36 years. He has worked in industry for 5 years before joining the faculty at Penn State.

**Huimin Lu** is currently a professor in School of Materials Science & Engineering at Beihang University. He earned his Ph.D. degree in metallurgical engineering from Northeastern University in 1997. His research mainly focuses on liquid metal storage and light metal fuel cells, light metal metallurgy, and light metal materials processing and characterization. His research results were mainly on material purification technology and complete sets of equipment development and industrialization, and short process low-cost materials preparation science and technology.

Dr. Lu developed the large-capacity solid aluminum electrode three-layer electrolysis refining-oriented crystallization-ionic liquid electro-deposition combined technology, 4N, 5N, and 6N or higher than 6N high-purity aluminum could be produced and applied in integrated circuits, semiconductor, and aerospace fields. Extraction of aluminum–silicon alloy and production of solar high-purity silicon from high-alumina minerals had been applied in the industry. His new process of extracting magnesium by the aluminum–silicon alloy heat-reducing from serpentine is also applied in industry. He developed a high-strength and high-toughness graphene lithium aluminum alloy with high-pressure torsion deformation technology. High-specific energy aluminum–air batteries, magnesium–air batteries, and lithium–air batteries have made a breakthrough; especially aluminum–air batteries will soon be applied. He is studying the new wind energy utilization technology on using non-grid-connected wind power for molten aluminum energy storage, and using aluminum–air batteries for distributed power generation. In addition to teaching several courses on characterization and processing of materials, he has edited three books, published nearly 200 technical papers, and holds 24 patents.

Dr. Lu is a lifelong TMS member, participating in several TMS annual meetings. He is an editor of the TMS2018 symposium on Stored Renewable Energy in Coal.

# Part I
# Energy Technologies and $CO_2$ Management Symposium

# Gas Hydrate-Based $CO_2$ Separation Process: Quantitative Assessment of the Effectiveness of Various Chemical Additives Involved in the Process

**Hossein Dashti and Xia Lou**

**Abstract** Gas hydrates technology has been considered as an alternative method for carbon dioxide ($CO_2$) separation. A wide range of studies have been reported in the past decade on the improvement of the separation efficiency by using chemical additives. While most of these studies have shown improved kinetics, thermodynamics and/or separation efficiency at the laboratory scale, there has been no quantitative analysis of the energy consumption for viable industrial applications. Comparison of the effectiveness of the chemical additives from separate studies or groups also is impossible. The present work is focused on the modelling of the hydrate-based $CO_2$ separation process and provides a quantitative approach that is new in its analysis of the effectiveness of chemical additives in relation to the energy required and the kinetic parameters involved in the process.

**Keywords** $CO_2$ capture · $CO_2$ hydrates · Chemical additives

## Introduction

Carbon dioxide ($CO_2$) separation and capture is one of the most challenging issues to investigate in order to alleviate the problem of $CO_2$ emissions worldwide. Gas hydrate-based $CO_2$ capture/separation (HBCC) is a relatively new separation method for $CO_2$ and has attracted increasing attention in the past decade. The technology employs a unique separation mechanism that is easy to regenerate and is capable of separating various gas mixtures, which might not be achievable via conventional methods. The feasibility study of the process was first reported by Spencer [1], and later supported by Tam et al. [2] According to the authors, the cost of HBCC technology in an integrated gasification combined cycle plant was US$ 8.75 per ton of $CO_2$ captured. It was reportedly comparable to that of US$ 57 per

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ton of $CO_2$ captured through the pressure swing adsorption (PSA) method, and that of US$ 49 per ton of $CO_2$ captured using the monoethanolamine (MEA) chemical absorption method [3].

$CO_2$ form hydrates between 1.1–4.3 MPa and 273–283 K respectively. Separating $CO_2$ from the other gases such as oxygen and nitrogen can be achieved by first forming a solid hydrate phase that is enriched with $CO_2$, followed by separation of the hydrate phase from the gaseous phase and dissociation of the hydrates, leading to the recovery of $CO_2$ that is much higher in concentration than in the original gas mixture. Upon dissociation, one volume of $CO_2$ hydrates can release 175 volumes of $CO_2$ gas at standard conditions [4]. However, the high operation pressures required in the HBCC process lead to the high compression costs and energy consumption. This has limited the viable industrial application of the HBCC [5]. The relatively low separation efficiency also is a challenge [6, 7]. Many chemical additives have been investigated in an attempt to lower the operation pressure, and to increase the formation rate, of $CO_2$ gas hydrates. Among the most commonly studied chemical additives, tetrahydrofuran (THF) and cyclopentane (CP) have been found to be useful in reducing the operating pressure and increasing the $CO_2$ recovery rate. Other additives, like tetra-n-butyl ammonium bromide (TBAB), dodecyl-trimethyl-ammonium chloride (DTAC) and $TBANO_3$, have been found to be useful in increasing the gas storage capacity and reducing the operating pressure. Surfactants, such as sodium dodecyl sulphate (SDS), only enhance the hydration rate of the process. Mixed chemical additives also have been studied to enhance their effects in HBCC.

Studies on chemical additives have been mostly focused on the effect of the chemical additives upon the kinetics, the operational conditions and the separation efficacy. Details of the progress in chemical additives improved HBCC can be found in a few recent review papers [6–8]. Other work on chemical additives associated HBCC includes thermodynamic modelling of the $CO_2$ fluid and hydrate phase behaviour. For instance, Herslund et al. [5, 9, 10] modelled the fluid phase and hydrate phase in the presence of THF, CP and the mixture of both. Verrett et al. [11] developed a thermodynamic model to simulate the HBCC process in the presence of TBAB. Another study by Shi and Liang [12] proposed a thermodynamic model to investigate the effects of TBAB, tetrabutyl ammonium fluoride (TBAF) and tetrabutyl ammonium chloride (TBAC) in HBCC process. Kinetic studies on gas hydrate formation are mostly based on the model established by Englezos et al. [13] that considers both mass transfer and crystallisation processes at the gas-liquid interface. The driving force in this model is the difference between the fugacity of the dissolved gas and the fugacity at equilibrium. However, the report on kinetic models for chemical additives enhanced HBCC process is limited. A recent study by ZareNezhad et al. [14] reported a single component gas ($CO_2$) hydrates kinetics in the absence and presence of SDS. In this model, the crystallization theory was coupled with the mass transfer phenomena but the gas composition difference between the liquid phase and the solid-liquid interface was considered as the driving force. Sun and Kang [15] also proposed a two-parameter kinetic model to predict the $CO_2$ hydrate formation rate in presence of THF. In this

work, the Gibbs free energy difference was considered as the driving force. In terms of quantitative analysis of the energy consumption associated with the HBCC, Tajima et al. [16] reported the energy consumption by a designed HBCC process for separating $CO_2$ from the emitted flue gases, using the thermodynamic approach. There was no chemical additive used in the design. A later report by Duc et al. [17] used the process simulator PRO II, to estimate the energy consumption involved in a multi-staged HBCC process in the presence of TBAB.

The present work is focused on the development and validation of a quantitative approach for the energy estimation of the HBCC process using the production scale reported by Tajima et al. [16]. The proposed approach will then be applied to the reported HBCC processes in the presence of THF [18, 19], TBAB [20, 21], and a mixture of TBAB with DATC [22]. The impact of the chemical additive on the energy consumption in relation to the formation pressure and temperature, and the kinetics of the $CO_2$ hydrates will be discussed.

## Methodology

A schematic flow diagram (Fig. 1) is first established based on the reported HBCC process by Tajima et al. [16]. Two compressors and three heat exchangers are used before the flue gas enters the reactor where the flue gas mixes with water with or without chemical additives. Gas hydrates form in the reactor. The hydrates slurry is separated from the gas phase and sent to a hydrates dissociation reactor from which purified $CO_2$ is collected.

According to the authors: (1) the process was applied to the treatment of total emission from a 1,000 MW power plant; (2) the total flow rate of the input flue gas was $1.0 \times 10^6 \mathrm{N\,m^3.h^{-1}}$; (3) the volume of the reactor was about 7,000 $m^3$; (4) the pressurisation was performed using adiabatic compressors with 80% efficiency; (5) the inlet and outlet temperatures of coolant were 253 K and 263 K, respectively; (6) the coefficient of performance (COP) in heat exchangers is assumed to be 3 and (7) the composition of $CO_2$ in the hydrates stream is 100%. Based on these

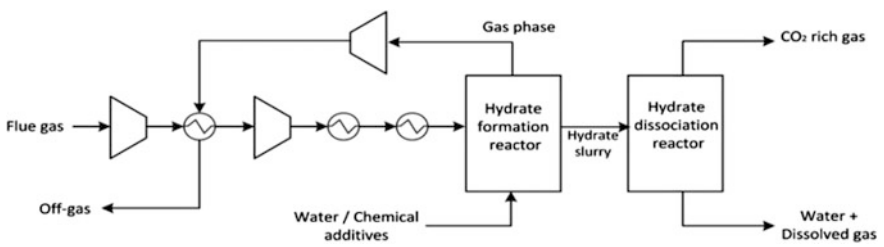


**Fig. 1** A schematic flow diagram of the gas hydrate-based $CO_2$ separation process

assumptions, the total energy consumption involved in this process was calculated using Eq. 1:

$$E_{total} = E_{compression} + E_{cooling} + E_{hydrates} \quad (1)$$

in which $E_{compression}$ and $E_{cooling}$ represent the energy consumption during the compression and cooling stages and $E_{hydrates}$ is the energy consumption associated with hydrate formation and dissociation.

## *Estimation of $E_{compression}$ and $E_{cooling}$*

The energy consumption values in the pressurising and cooling processes were simulated using Aspen HYSYS (V.8.6). The temperature and pressure of the input flue gas were, reportedly, 298 K and 0.1 MPa [16].

## *Estimation of $E_{hydrates}$*

For the estimation of $E_{hydrates}$, an energy balance around the formation and dissociation reactor (Fig. 2) was first established (Eq. 2).

$$E_{hydrates} = \sum_{i=1}^{5} F_i H_i - r_f \Delta H_f + r_d \Delta H_d \quad (2)$$

where $F_i$ is the flow rate of stream $i$, $H_i$ is the enthalpy of stream $i$, $r_f$ and $r_d$ are the rates of hydrate formation and dissociation, respectively, and $\Delta H_f$ and $\Delta H_d$ are the enthalpies of hydrate formation and dissociation, respectively. Below are the details of the modelling of each of the parameters.

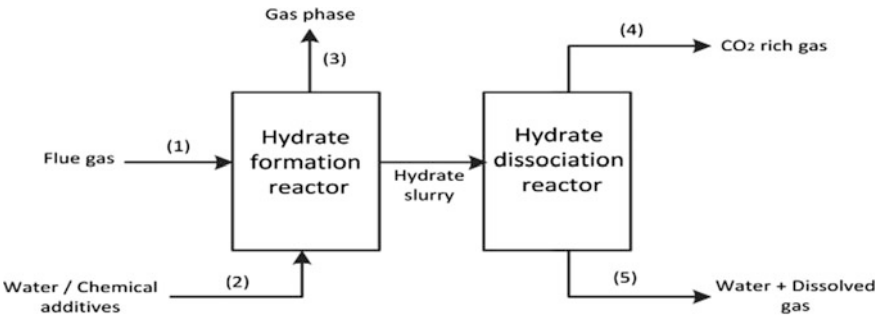


**Fig. 2** $CO_2$ hydrates formation and dissociation unit