Korean Journal of Chemical Engineering,
February 2025, 42(2), 195-223(29),
https://doi.org/10.1007/s11814-024-00355-3

Computation-Based Development of Carrier Materials and Catalysts for Liquid Organic Hydrogen Carrier Systems

Kiheon Sung, Yoojin Lee, Hyunwoo Yook&Jeong Woo Han
Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University

Abstract - Liquid Organic Hydrogen Carriers (LOHCs) have emerged as a promising solution for hydrogen storage, offering high hydrogen storage capacity, reversibility, thermal stability, and compatibility with existing infrastructures. Despite their potential, LOHC systems face significant challenges, including the need for specialized carriers and catalysts for efficient hydrogen storage and release. This review emphasizes the importance of computational analysis in overcoming these challenges. We summarize the computational accuracy of estimating dehydrogenation enthalpy for the carrier materials and explore molecular tuning strategies to enhance the dehydrogenation properties. In addition, we review computational studies that have investigated the impacts of catalytic adsorption/desorption and kinetic properties on the catalytic performance as well as catalyst design methods in terms of the geometry of active metal species, second metals, promoters, heterolytic hydrogen generation, and hydrogen spillover. This review further addresses the current challenges in LOHC systems, and then suggests future computational research directions to improve their efficiency and viability.

Korean Journal of Chemical Engineering,
February 2025, 42(2), 225-231(7),
https://doi.org/10.1007/s11814-024-00356-2

Donor Numbers for Ionic Liquids and Carbonate Solvents Using ^{7}Li and ^{23}Na as Probes

[1]Uddhav Kulkarni, [2]Won-Jang Cho, [3]Seunghyeon Lee, Dong Soo Hwang, [4]TaeYeong Im, You Kyeong Jeong, Kyungho Ahn & Gi-Ra Yi
[1]Department of Chemical Engineering, Sungkyunkwan University, [2]Department of Chemical Engineering, Pohang University of Science and Technology, [3]Division of Environmental Science and Engineering, Pohang University of Science and Technology, [4]LG Energy Solution, Ltd., R&D Campus

Abstract - Lithium-ion batteries (LIBs) currently dominate the commercial rechargeable battery market due to their high ionic conductivity and moderate compatibility. To enhance the development and safety of future LIBs, ionic liquids (ILs) have been introduced as additives. For the first time, we present the Lewis acid/base responses of nine ILs in terms of donor number (DN), calculated using ^{7}Li NMR spectroscopy. The anionic component of the ILs significantly influences the DN through its interaction with lithium ions. In addition, the DN of three carbonate solvents was determined using both ^{7}Li and ^{23}Na NMR spectroscopy, showing that DN of solvent is affected by the probe ion and solvent structure. These findings offer valuable insights for selecting appropriate solvents for future electrolyte development in LIBs.

Korean Journal of Chemical Engineering,
February 2025, 42(2), 233-255(23),
https://doi.org/10.1007/s11814-024-00351-7

System Design and Economic Evaluation of a Liquid Hydrogen Superstation

[1]Duho Kang, Haneul Mun, [2]Jinwoo Park [3]Inkyu Lee
[1]School of Chemical Engineering, Pusan National University, [2]Department of Chemical and Biochemical Engineering, Dongguk University, [3]Institute for Environment and Energy

Abstract - Liquid hydrogen (LH_2)-based hydrogen refueling stations (HRSs) are promising for high-capacity refueling, given the high density of LH_2, which facilitates large-scale transportation and storage. However, in LH_2 HRSs, the cryogenic cold energy of LH_2 is wasted during the vaporization process required to refuel hydrogen for fuel cell vehicles. To overcome this issue, this study proposes a novel LH_2-based hydrogen superstation (HSS) that recovers the otherwise wasted cold energy to generate electricity for the station, with any excess electricity used to charge electric vehicles. To explore the most cost-effective configuration for cold energy recovery in the HSS, two power generation cycles were designed: one incorporating a Brayton cycle followed by a Rankine cycle (BC-RC), and another using two Rankine cycles in series (RC-RC). Combining the BC-RC and RC-RC configurations, this two-stage design is adopted to efficiently recover cold energy across a broad temperature range during the vaporization process. The HSS using the BC-RC configuration achieves 53% more cold energy recovery, generates 19% more power, and experiences 8% less exergy waste compared to the HSS with the RC-RC setup. However, in smaller-scale cold energy recovery systems applied to HSS, the cost savings from using pumps instead of compressors outweigh the additional power generation benefits of the Brayton cycle. Consequently, the HSS with the RC-RC configuration demonstrates the highest economic feasibility, with a 2% higher net present value.

Korean Journal of Chemical Engineering,
February 2025, 42(3), 529-536(8),
https://doi.org/10.1007/s11814-024-00368-y

Effect of Surface Tension on Thermocapillary Convection-Driven Droplet Transport

[1]Hyesun Hwang&Sanghyuk Wooh, [2]Syuji Fujii
[1]Department of Chemical Engineering, Chung-Ang University, [2]Department of Applied Chemistry, Faculty of Engineering, Osaka Institute of Technology

Abstract - The transport of microliter-scale droplets on solid surfaces is critical for various applications, including microfluidics and microengines. Recently, droplet manipulation strategy using thermocapillary convection has received attention due to its precise and remote controllability. The mobility of liquid droplets in this method depends on several parameters, such as laser power and the light absorption coefficient. Additionally, surface tension significantly influences droplet movement although its underlying mechanism remains unclear. In this study, we investigate the effect of surface tension on droplet movement via thermocapillary convection. Aqueous dispersions of polypyrrole (PPy) nanoparticles (NPs), which absorb near-infrared (NIR) light and convert it into heat, are employed as droplets. Upon NIR laser irradiation, the PPy droplets generate localized heat, resulting in thermocapillary convection. The lubricated surface (LuS) is used as a substrate. Due to the mobile lubricant layer, droplets are easy to move with low friction. Surface tension is modified by adding a surfactant, and the droplet movement speed increases with decreasing surface tension. Here, this phenomenon is investigating the parameters acting to Marangoni force: contact line length and surface tension gradient. We confirm that the Marangoni force, which propels the droplet, is induced more effectively by low surface tension liquids. This study provides fundamental insights into droplet behavior governed by wettability differences, advancing droplet manipulation techniques for diverse fluidic systems.

Korean journal of Chemical Engineering,
February 2025, 42(3), 537-545(9)
https://doi.org/10.1007/s11814-024-00362-4

Piecewise Response Surface Methodology for Enhanced Modeling and Optimization of Complex Systems

[1]Jiyun Kim & Kyung Hwan Ryu, [2]Jiyun Kim, [3]Do-Gun Kim
[1]Department of Chemical Engineering, Sunchon National University, [2]Department of Chemical Engineering, Kyungpook National University, [3]Department of Environmental Engineering, Sunchon National University

Abstract - This study introduces an innovative adaptation of response surface methodology (RSM) by implementing piecewise modeling to address the limitations inherent to traditional second-order polynomial models. Traditional RSM often struggles with complex, nonlinear system behaviors, particularly when variable interactions exhibit abrupt changes or asymmetrical relationships. By segmenting the response surface into distinct regions, each modeled separately, the piecewise approach enhances the methodology's adaptability and accuracy in predicting complex system dynamics. The effectiveness of the proposed piecewise RSM is demonstrated through case studies, including the optimization of tetracycline removal from water using a combined adsorption-coagulation process. This approach not only improves prediction accuracy but also integrates economic considerations into process optimization, which is crucial for industrial applications where cost-effectiveness is as important as operational efficiency. The results indicate that piecewise RSM can provide more accurate modeling of environmental and chemical engineering processes, providing a robust tool for improving experimental designs and process efficiencies while maintaining its simplicity.

Korean Journal of Chemical Engineering,
February 2025, 42(3), 659–667(9)
https://doi.org/10.1007/s11814-024-00328-6

Synthesis of Reusable IrPt/Fe2O3 Nanocatalysts Using Antisolvent Crystallization-Based Method

[1]Cun Liu, Zhe Liu, Tao Zhou, Xiaomei Xu & Taekyung Yu, [2]Cun Liu
[1]Department of Chemical Engineering, Integrated Engineering Major, College of Engineering, Kyung Hee University,
[2]College of Chemistry and Chemical Engineering, Xinjiang Agricultural University

Abstract - The antisolvent crystallization-based method, which involves forming precursor metal salt nanoparticles and converting them to metal/oxide nanoparticles by reduction/oxidation can be used to synthesize nanocomposites composed of catalyst nanoparticles and supporting materials. In this study, IrPt/Fe_2O_3 nanocomposites comprising an IrPt catalyst and magnetic Fe_2O_3 supporter with a controllable Ir/Pt ratio are synthesized using a two-step antisolvent crystallization-based method. The as-prepared nanocomposites exhibit excellent catalytic performance and reusability utilizing magnetism toward the hydrogenation of p-nitrophenol (p-NP).

Korean Journal of Chemical Engineering,
February 2025, 42(4), 827–841(15),
https://doi.org/10.1007/s11814-025-00414-3

Isotherm, Kinetic, and Thermodynamic Studies for Negative Pressure Cavitation Adsorption of Paclitaxel from Culture Supernatants of Taxus chinensis onto Diaion HP-20

Sangmin Yun & Jin-Hyun Kim
Center for Future Sustainable Technology, Department of Chemical Engineering, Kongju National University

Abstract - In this study, a negative pressure cavitation adsorption method was developed to efficiently recover paclitaxel from Taxus chinensis culture supernatants using Diaion HP-20 as an adsorbent. The equilibrium adsorption data were applied to Langmuir, Freundlich, Dubinin–Radushkevich, and Elovich isotherms, and the Langmuir isotherm was found to be the most feasible. The kinetic data were in good agreement with the pseudo-second-order model, and intraparticle diffusion played a dominant role in the adsorption rate of paclitaxel according to the intraparticle diffusion model. The time for the adsorption to reach equilibrium was shortened by more than eight times at all negative pressures (− 50 to − 200 mmHg) compared to the conventional adsorption. In addition, as the negative pressure increased, the maximum adsorption capacity, adsorption rate constant, intraparticle diffusion rate constant, and intraparticle diffusion coefficient increased. The values of the thermodynamic parameters indicated that the adsorption was endothermic and spontaneous. As the negative pressure intensity increased at a given adsorption capacity (qe=60–100 mg/g), the isosteric heat of adsorption decreased and the adsorbent surface became more energetically homogeneous.

Korean Journal of Chemical Engineering,
February 2025, 42(4), 877–884(8),
https://doi.org/10.1007/s11814-025-00425-0

Comparison of Radioisotope Adsorption Capability in Metal Organic Frameworks Through DFT Simulation

Hwanhui Lee, Jeongho An & Kunok Chang
Department of Nuclear Engineering, Kyung Hee University

Abstract - We compared the adsorption performance of graphene and MOF-303 for three radionuclides of significant concern in radioactive waste: Co, Sr, and Cs, using density functional theory. Additionally, we doped MOF-303 with transition metals such as Cu, Ag, and Au by replacing the hydrogen atoms in the nitrogen linker, and investigated the resulting changes in adsorption capability. The adsorption capability of MOF-303 for the Co, Sr, and Cs was superior to the adsorption capability of graphene. Furthermore, doping MOF-303 with Cu, Ag, and Au further enhanced the adsorption capability of MOF-303 for Co, Sr, and Cs. To evaluate the adsorption capabilities and characteristics of Co, Sr, and Cs on MOF-303, an initial simulation was conducted to verify the convergence of the adsorption simulations and analyze the tendencies. Subsequently, an additional simulation was performed using more refined computational parameters. Au-MOF-303 resulted in the most significant overall increase in adsorption energy for Co, Sr, and Cs among the Cu-MOF-303, Ag-MOF-303, and Au-MOF-303.

Korean Journal of Chemical Engineering,
February 2025, 42(4), 901–921(21),
https://doi.org/10.1007/s11814-024-00348-2

Optimal Design of BOG Reliquefaction Systems for LNG Carriers: A Focus on GMS Performance During Loaded Voyages

[1]Hyunjun Shin & Jong Min Lee, [2]Hyunjun Shin, Dongchan Kim & Wonjae Choi
[1]School of Chemical and Biological Engineering, Institute of Chemical Processes, Seoul National University,
[2]Hanwha Ocean. Co

Abstract - This study proposes a strategy for evaluating efficient design of the Gas Management System (GMS) on LNG carriers by decomposing its performance to subsystems: the reliquefaction system (RS) and the fuel gas supply system (FS). With increasingly stringent maritime regulations on greenhouse gas emissions, the need for efficient LNG carrier operations has become critical. A major factor in reducing fuel consumptions and carbon emissions is optimizing the design of the RS, given its significant power demand for processing NBOG. However, effective GMS design must account for variations in RS operation performance, as well as the contributions of the FS in treating NBOG with changes in ship speed. This study compares GSM configurations with reliquefaction systems based on two representative refrigeration cycles: the nitrogen reverse Brayton cycle (NRBC) and the single mixed refrigerant cycle (SMRC), both analyzing effects of cold BOG utilization. Results indicate that the RS of GMS4A-aSMRC [the aSMRC is the refrigeration cycle which utilizes cold BOG within the Single Mixed Refrigerant Cycle (SMRC)] demonstrates superior RS design performance. However, the most efficient GMS configuration varies with the Boil-off Rate (BOR): GMS2-aNRBC [the aNRBC is the refrigeration cycle which utilizes cold BOG within the Nitrogen Reverse Brayton Cycle (NRBC)] is optimal aligning with its RS performance for a 0.11%/day BOR, while GMS3-SMRC without cold BOG in RS is the most efficient for a 0.075%/day BOR, owing to increased contributions from the FS. In this study, a performance index with a consistently comparable baseline is derived to accommodate compositional deviations from flash gas recirculation at NBOG disposal streams, enabling the GMS performance to be correlated with compatible values of its decomposed subsystem.