Editorial

Selective Catalytic Reduction: From Basic Science to deNO_x ApplicationsFeng Gao ^{1,*} and Todd J. Toops ^{2,*}¹ Institute for Integrated Catalysis, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99354, USA² Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

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The combustion of coal, petroleum and biofuel for energy generation has resulted in unprecedented benefits to the prosperity of our modern society and will continue to do so in the future. However, rapid global climate changes, especially frequent extreme weather conditions that we have witnessed in the past two decades, remind us how fragile our planet is, and how important sustainable development is for future generations. The advancement of sciences and technologies for environmental protection, such as water purification, soil detoxification, volatile organic compounds (VOC) decomposition, plastic waste control and combustion emission control, is key for sustainability. With global awareness of the importance of environmental protection and sustainable energy development in legislation, the scientific community and the general public, we all have reasons to believe success is achievable in the 21st century.

Among the various deNO_x techniques, selective catalytic reduction (SCR) has been particularly successful. Oxide-based SCR was first commercialized in the 1970s; much more recently, zeolite-based catalysts were deployed in 2010 [1–4]. Such a success is a result of continuing research on the basic sciences of this catalytic chemistry, and the accompanying catalyst synthesis and development of auxiliary techniques (e.g., NH₃ delivery) that facilitate this catalytic chemistry. The 12 original papers and review articles of this Special Issue, contributed by ~60 authors from both academia and industry, nicely reflect this continuing effort.

Four review articles are included here, two on oxide-based catalysts and two on zeolite-based catalysts. The review article by Shan, He and coworkers [5] summarized recent progress on low-temperature activity of vanadia-based SCR catalysts, including catalyst modification with metal oxides and other elements, the use of novel supports, the application of novel synthesis approaches and the use of vanadium precursors in different forms. The authors also addressed recent advances in understanding low-temperature reaction mechanisms, and finally discussed opportunities and challenges of vanadia-based catalysts in future research. Liu and coworkers [6] reviewed the latest research on SO₂ resistance of oxide-based SCR catalysts. The authors first summarized possible catalyst deactivation mechanisms in SO₂-containing flue gas, followed by presenting strategies for alleviating such deactivation, including modification of the catalyst supports, applying complex oxide catalysts, optimizing catalyst preparation methods and catalyst acidification. The authors further summarized mechanisms for improving sulfur resistance and provided suggestions for further catalyst development.

Regarding zeolite-based SCR, Chen and collaborators [7] provided a review on recent understanding about active site dynamics in Cu-chabazite catalysts, in particular at low reaction temperatures. The authors first summarized recent advances in theoretical studies in low-temperature Cu dynamics, in particular work with ab initio molecular dynamics (AIMD) or metadynamics simulations, and then reviewed recent spectroscopic studies to follow the evolution of the coordinative environment and the local structure

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of Cu centers during low-temperature NH_3 -SCR reactions. These were then followed by presenting how understanding Cu dynamics is essential for low-temperature Cu redox, solid-state ion exchange catalyst synthesis and direct monitoring of NH_3 storage and conversion. Finally, the authors discussed new perspectives in manipulating Cu dynamics to improve low-temperature NH_3 -SCR efficiency as well as in understanding other important reactions. Finally, the review article by Gao [8] summarized recent studies on Fe-exchanged small-pore zeolite SCR catalysts. This summary included the synthesis approach of small-pore Fe/zeolites, the nature of the SCR-active Fe-species in these catalysts as determined by experimental and theoretical approaches, Fe-species transformation during hydrothermal aging, SCR reactions/structure–function correlations and a few aspects on industrial applications.

Among the eight original articles, four of them focused on new catalyst design, characterization and performance evaluation; one on in situ SO_2 poisoning; one on integrated catalyst design; one on SCR system dynamic modeling; and, finally, one on urea injection. As Guest Editors, we are pleased to see the breadth of these research topics that nicely reflect the healthy development of SCR science and technology from various approaches.

Work by Liu and coworkers [9] investigated a sulfated Fe_2O_3 SCR catalyst supported on TiO_2 . The authors discovered that the catalyst surface composition is influenced by different sequences of precursor introduction during catalyst synthesis, where catalysts with coexisting isolated Fe_2O_3 and SO_4^{2-} domains on the surface, or predominant SO_4^{2-} domain on the surface, can be readily prepared. The authors further demonstrated that such a catalyst surface composition difference affects redox capacity, NH_3 adsorption and SCR mechanisms. Wang and coworkers reported [10] the preparation and application of Sb-containing SbZrOx , SbCeOx and SbCeZrOx SCR catalysts. Via the application of a number of chemical titration and spectroscopic methods to study their catalysts, the authors demonstrated that Sb introduction influences acid distribution and redox properties, which in turn affect NH_3 adsorption and NO oxidation. The authors suggested that “dual active sites” favor NH_3 adsorption and nitrate formation, and their SbCeZrOx catalyst displayed the most balanced dual site functions and, thus, the best SCR performance.

He and coworkers [11] studied the promoting effect of Mn on a Cu-SSZ-13 catalyst. The authors discovered that impregnated MnOx species caused a decline in the crystallinity of Cu-SSZ-13 but markedly improved the redox ability. Nitrate and nitrite species were observed in the Mn-modified Cu-SSZ-13, and they suggested that the formation of these species caused the observed increase in low-temperature NH_3 -SCR activity. They further proposed that the addition of Mn is a promising method for promoting the low-temperature catalytic activity of Cu-SSZ-13. In studying the in situ SO_2 poisoning mechanism of Cu-SSZ-13, Zhang and coworkers [12] demonstrated that the formation of sulfate species, including $(\text{NH}_4)_2\text{SO}_4$, CuSO_4 and $\text{Al}_2(\text{SO}_4)_3$, are temperature dependent, where a high temperature only favors the formation of the latter two species. The authors further demonstrated that SO_2 has a negative effect on low-temperature catalytic performance due to the sulfation of active sites; however, a positive effect is found at a high temperature, owing to the inhibition of the NH_3 oxidation reaction. In joint research between industry and academia, Ogura and coworkers [13] investigated various Cu-zeolites (zeolite mining), and demonstrated the suitability of Cu-exchanged zeolite AFX as a selective and stable SCR catalyst.

It is important to realize that efforts in designing new catalysts and enhancing existing catalysts must be accompanied by many other R&D efforts in order to achieve optimal deNOx efficiency. In this regard, three more highly valuable contributions were provided. Work by Li, Yu and collaborators [14] demonstrated the fabrication of a large V-based catalyst filter to simultaneously remove NOx, SOx and dust. Yan, Sun and coworkers [15] discussed a dynamic model that was incorporated with delay estimation and variable selection to analyze outlet NOx emissions and NH_3 injection. Finally, a study by Lim and coworkers [16] on urea spray uniformity from two different urea injectors broadened the scope and increased the overall readership of this Special Issue.

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