Availability of elements for heterogeneous catalysis: Predicting the industrial viability of novel catalysts - DTU Orbit (15/03/2019)

Growing concern regarding the sustainability of the chemical industry has driven the development of more efficient catalytic reactions. First-generation estimates of catalyst viability are based on crustal abundance, which has severe limitations. Herein, we propose a second-generation approach to predicting the viability of novel catalysts prior to industrial implementation to benefit the global chemical industry. Using this prediction, we found that a correlation exists between catalyst consumption and the annual production or price of the catalyst element for 11 representative industrial catalytic processes. Based on this correlation, we have introduced two new descriptors for catalyst viability, namely, catalyst consumption to availability ratio per annum (CCA) and consumed catalyst cost to product value ratio per annum (CCP). Based on evaluations of CCA and CCP for selected industrial reactions, we have grouped catalysts from the case studies according to viability, allowing the identification of general limits of viability based on CCA and CCP. Calculating the CCA and CCP and their comparing with the general limits of viability provides researchers with a novel framework for evaluating whether the cost or physical availability of a new catalyst could be limiting. We have extended this analysis to calculate the predicted limits of economically viable production and product cost for new catalysts.

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