Chinese Journal of Catalysis 39 (2018) 16–26

available at www.sciencedirect.com

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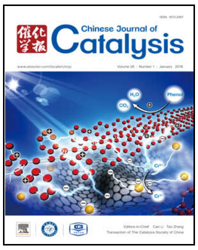
journal homepage: www.elsevier.com/locate/chnjc



Article

Availability of elements for heterogeneous catalysis: Predicting the industrial viability of novel catalysts

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ARTICLE INFO

Article history:
Received 29 July 2017
Accepted 10 November 2017
Published 5 January 2018

Keywords:
Heterogeneous catalysis
Industrial catalysis
Sustainability
Element availability
Catalyst
Catalyst design
Element abundance
Scalability

ABSTRACT

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.

1. Introduction

In the past century, huge advances have been made in industrial catalysis. Today, products of catalytic reactions contribute ca. 25% of the gross national product (GNP) in developed countries [1]. As the portfolio of catalysts grows, so does the number of industrially important catalytic reactions that use milder conditions and afford higher yields. A comprehensive list of current existing and emerging catalytic processes would be far too extensive to list here. Catalysis both improves economic returns and reduces the environmental impact of the chemical industry. Although many new catalysts have been described in the chemical literature, there is no general framework for predicting whether a new catalyst will be available in sufficient quantities to replace an existing catalyst. Currently, when proposing a new catalyst, researchers often have only the rudimentary average crustal abundance of a given element as a simple metric of technical availability. However, the crustal abundance can be an insufficient criterion for judging practical availability. Furthermore, the profitability and demand of a new catalytic product are difficult to predict. As catalyst application is ultimately a matter of economic consideration based on cost and efficiency, we now propose an improved analytic approach to determining catalyst viability based on the physi-

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DOI: 10.1016/S1872-2067(17)62979-6 | http://www.sciencedirect.com/science/journal/18722067 | Chin. J. Catal., Vol. 39, No. 1, January 2018

cal availability of sources (mineable ore streams) of a given element [2].

In the present study, we aim to equip researchers with a simple methodology to benchmark catalyst viability for a reaction and identify which catalytic elements could be substituted to create a more viable catalyst. Several factors determine catalyst compositions, including the supplier, chemical feedstock, cost of catalyst components, cost of feedstock, demand for the product and possible by-products, and local environmental legislation. Typically, catalysts are optimized for longevity with high selectivity. In some cases, particularly when the by-products are valuable, lower selectivity can be tolerated if purification is cost-effective. Based on these many factors, there is no clear way to define optimal general catalyst parameters. Therefore, catalysis offers plentiful opportunities for innovative research, as reflected in the ever-growing scientific literature in this field.

In this work, general conclusions are drawn based on an evaluation of currently employed catalysts for bulk chemical synthesis, current element availability, and estimated scalability.

The evaluation of the availability and scalability of elements is based on work published by Vesborg et al. [2], to which readers are referred for further detail. For consistency, element pricing and catalytic element consumption data are reported in US dollars (US$) from 2006, where possible.

Herein, we discuss the parameters important for predicting elements that are viable for catalysts at a given scale of industrial production. This discussion is based on selected catalytic reactions for which sufficient information on catalyst consumption was available. Although important, fine chemical synthesis is performed on a smaller scale at which catalyst availability is less likely to be the main limitation, and so is not included in this study. The selected case studies include various production scales, fuels, polymers, environmental catalysis, and a case in which the catalyst price proved limiting. Through our analysis, we have attempted to categorize catalysts as “unviable”, “viable”, or “highly viable”. We also discuss the treated elements in order of availability (primary production of element per year) using the term log(p), as introduced by Vesborg et al. [2], which is the base 10 logarithm of the annual production in kg/y. In this work, we also introduce the metric “catalyst consumption to availability ratio per annum” (CCA), which is the quantity of an element consumed by a catalytic reaction per year (in kg/y) as a ratio of the total production of that element (in kg/y). This ratio, which describes physical availability limitations, must be lower than 1.0 for any real processes, but may well be larger for hypothetical processes. Consumption refers to net consumption, which accounts for recycling of catalyst elements. The second metric introduced is the “consumed catalyst cost to product value ratio per annum” (CCP), which must be much lower than 1.0 for the process to be economically profitable.

The CCA and CCP ratios allowed the estimation of the viability a catalyst system for industrial scale production via simple calculations based on catalyst loading, catalyst lifetime, and element availability and cost. We then showed, by example, how the CCA and CCP metrics can be used to determine viability limits for the scale of production, and the product price for a catalytic process. Furthermore, we extended the previous analysis to all elements in the periodic table for which sufficient data exists to determine alternative elements that could make the process viable if substituted into the catalyst, assuming activity is maintained.

As describing each catalytic reaction individually is not feasible here, detailed descriptions are provided in the Supporting Information (SI). Selected illustrative examples are discussed from each group of availability, namely, “very low”, “low”, and “high”, grouped according to log(p).

2. Experimental

2.1. Methods

For each reaction evaluated, we estimated the net amount of catalyst consumed per year before normalizing to either kg of product produced or the market value of that product. The net catalyst consumption was calculated from the amount of catalyst needed for annual production subtracted by the amount of catalyst annually recycle and then divided by the catalyst lifetime.

2.2. Assessment of recycling lifetime

Catalyst recycling can occur either on-site, through catalyst regeneration, or off-site, such as for noble-metal catalysts used in automobiles and nitric acid production. To address the effect of regeneration and recycling to the fullest extent possible in a simple estimate of lifetime, we divided the amount of catalyst loaded into a reactor by the number of years it can be extended to run with regeneration. For example, for SiO_2-supported VO_x catalysts used for H_2SO_4 production, 10% of the catalyst is exchanged every 1–3 y [3]. Therefore, assuming the lower bound, the total catalyst amount is fully exchanged every 10 y. As another example, the Fischer-Tropsch (FT) reaction needs regeneration every 7,000 h, which extends the total lifetime to 5 y [4]. Finally, we present Pt consumption in automotive catalysts as a case study in which recycling of the active element plays a dominant role in catalyst consumption. Based on reports by Johnson Matthey [5] and Impala [6], both from 2013, the Pt demand was 104,000 kg annually, while recovery/recycling of used catalysts amounted to 34,000 kg, making the net Pt consumption 70,000 kg. This includes demand due to losses, non-recycled catalyst converters, and new catalyst converters.

2.3. Catalyst price estimates

Estimating the precise cost of a catalyst is important. The metal cost is only a fraction of the total catalyst cost, which often includes metal impregnation, wash-coating, reduction, and co-catalysts, such as zeolites. Metal prices will likely scale, at least to within an order of magnitude, with the total catalyst cost. These differences in preparation costs should be included in an advanced life-cycle analysis, but are beyond the scope of this study. Instead, we include these factors in an implicit