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Effective rate constants for nanostructured heterogeneous catalysts SHAUN HENDY, NICOLA GASTON, PHILIP ZHANG, Industrial Research Ltd, NAT LUND, Victoria University of Wellington — There is currently a high level of interest in the use of nanostructured materials for catalysis. For instance, gold, which is largely inert in the bulk, can exhibit strong catalytic activity when in nanoparticle form. With precious metal catalysts such as Pt and Pd in high demand, the use of these materials in nanoparticle form can also substantially reduce costs by exposure of more surface area for the same volume of material. When reactants are plentiful, the effective activity of a nanoparticulate catalyst will increase roughly with its surface area. However, under diffusion-limited conditions, the reactant must diffuse to active sites on the catalyst, so a high surface area and a high density of active sites may bring diminishing returns if reactant is consumed faster than it arrives. Here we apply a mathematical homogenisation approach to derive simple expressions for the effective reactivity of a nanostructured catalyst under diffusion limited conditions that relate the intrinsic rate constants of the surfaces presented by the catalyst to an effective rate constant. When highly active catalytic sites, such as step edges or other defects are present, we show that distinct limiting cases emerge depending on the degree of overlap of the reactant depletion zone about each site. In gases, the size of this depletion zone is approximately the mean free path, so the effective reactivity will depend on the structure of the catalyst on that scale. We discuss implications for the optimal design of nanoparticle catalysts.

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