Effective rate constants for nanostructured heterogeneous catalysts
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There is currently a high level of interest in the use of nanostructured materials for catalysis [1,2]. With precious metal catalysts such as platinum, palladium and gold in high demand, the use of these materials in nanoparticle form can also substantially reduce the cost of the catalyst through the exposure of more surface area for the same volume of material [3]. When reactants are plentiful, the activity by mass of a nanoparticulate catalyst will increase as its surface area increases. Under diffusion-limited conditions, however, 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 [4,5] to derive simple expressions for the effective reactivity of a nanostructured catalyst under diffusion limited conditions that relate the intrinsic rate constants of the surface sites presented by the catalyst to an effective rate constant. We show that distinct limiting cases emerge depending on the degree of overlap of the reactant depletion zone about each site. 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 of the gas molecules, so the effective reactivity will depend on the structure of the catalyst on that scale.

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