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Guest Editorial

Applications of Modelling at Johnson Matthey

The theme for this issue of the journal is modelling and its usefulness to Johnson Matthey in a wide range of research and development (R&D) areas. Modelling is one of three core competencies within Johnson Matthey, together with the ability to control materials at the atomic scale, and to characterise materials using state of the art techniques. It forms a crucial component of the company's strategy to design and develop high performance, more resource efficient products.

Modelling can encompass many techniques from models based on robust physical principles to those based on empirical and statistical parameter fitting. While this latter approach is widely used in the analysis of experimental data, it is the former approach that comprises the articles in this issue and the subject of this editorial. The use of physical parameter models is much more versatile than empirical fitting models as it allows the prediction of properties over a much greater parameter space than a model based on fitted parameters derived from a specific data set.

Techniques from computational chemistry (electronic structure and force field), thermodynamics and process simulation to kinetic reaction engineering form the basis of modelling based on physical principles, and all are used within Johnson Matthey in both R&D and applied contexts.

Modelling approaches have long been used in chemical engineering activities, including areas such as reactor modelling, alloy development and emissions control systems, as evidenced by the three articles by Stitt *et al*. (1), Heiss *et al*. (2, 3) and Watling *et al*. (4). In particular, the advent of computer based techniques such as computational fluid dynamics (CFD) and discrete element method (DEM) have revolutionised the ability to simulate complex shapes and processes with high precision and sensitivity. These methods have also benefited from the availability of inexpensive large computer resources (5).

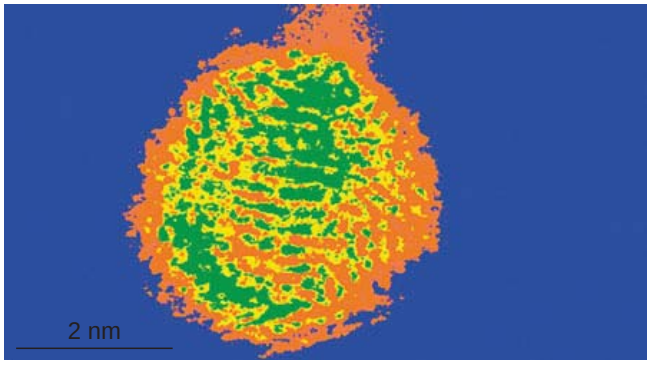
Materials and Catalyst Design

The application of modelling to materials and catalyst design is a more recent innovation and has been in part dependent on the continued falling cost of computing power, including the appearance of relatively inexpensive local clusters of hundreds to thousands of processors, together with access by companies to a growing network of national supercomputer facilities. Johnson Matthey established an atomistic modelling group in 2004 with a single modeller and in the last eleven years this has grown to a group of nine split between Johnson Matthey Technology Centre (JMTC) facilities at Sonning Common, UK, and Pretoria, South Africa. The work from this group is tightly focused on areas where there is strong interest and collaboration with experimental R&D across the company. This allows good definition of the problem that the modelling aims to inform and continued exchange of data between modelling and experiment to better understand and apply simulation results.

Given that atomistic modelling originates within the physics community, one of the challenges has been to establish a common language to allow modelling concepts to be understood by the predominately chemistry-based experimental community within Johnson Matthey. A simple example of this is that energies calculated by atomistic modelling are usually expressed as electronvolts (eV), while chemists are used to energies in (kilo)joules (1 eV = 96 kJ mol^{-1}). One consequence of this is that although physicists may be comfortable with energies of a few eV, to a chemist this would represent energies of many hundreds of kJ which can have a significant effect on whether a material would be stable or whether a chemical reaction is favourable or not. To help overcome these possible barriers, the Johnson Matthey modelling group includes modellers with both physics and chemistry backgrounds and a strong emphasis is put on communication skills to

help experimentalists fully understand the implications of modelling results.

With the emphasis of catalysis and catalysts amongst Johnson Matthey's products, the atomistic modelling group has focused on modelling surfaces as well as bulk structures. The ability to understand how a surface structure is different from the bulk is key in explaining and predicting reactivity. A good example is work carried out by the group on the calculation of surface compositions of metal alloy surfaces and how adsorbates change these compositions. Taking a range of Pt alloy surfaces with a range of transition metals in the absence of adsorbates, Pt tends to segregate to the surface, therefore maximising the number of possible reaction sites (for Pt specific reactions). However, in the presence of OH and O adsorbates (as would be present in an O_2 containing reaction feed such as in a cathode of a fuel cell), many other transition metals are segregated to the surface due to the greater strength of the M-O(H) bond. This has the effect of limiting reaction sites and makes these less noble metals (than Pt) susceptible to chemical leaching. Therefore, the effect of reaction conditions on the surface of catalyst materials can be predicted, further refining the prediction of modelling in terms of reactivity and stability. A forthcoming article in this journal is expected to present the work in more detail, as well as providing a more general overview of the group's activities.



'Core-shell' catalyst where a core of one metal or alloy is encased with a layer of different atoms

Catalysis and Collaboration

As part of developing modelling methods to be more applicable to Johnson Matthey products and processes, the company has extensive collaboration with academic groups. In general, we work with these groups in areas such as code development to overcome limitations in current commercial atomistic software. One example of this is a collaboration with the group of Dr Chris Skylaris of Southampton University, UK. Dr Skylaris is working with a linear scaling atomistic code called Order-N Electronic Total Energy Package (ONETEP) which has been designed to model large molecular structures such as proteins and macromolecules. In our current collaboration we have been applying ONETEP to the modelling of large metal nanoparticles (such as Pt particles of >1000 atoms). These systems are currently beyond standard density functional theory (DFT) codes using reasonable computation resources and if the efforts continue to be successful have the potential of bridging the current modelling gap between small nanoparticle clusters and the bulk surface.

In summary, it is hoped that this issue of the *Johnson Matthey Technology Review* highlights some of the scope of recent developments in modelling across the chemical and chemical engineering length scales and the reasons why Johnson Matthey has invested in modelling research as a key tool in continuing to develop advanced products for demanding markets.

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