Scale up of hydrogenation reactions from small scale parallel reactors

High throughput research in the chemical and pharmaceutical industry is normally the term used to describe experiments in small reactions vessels, several of which are used in parallel. The question invariably raised is how reproducible the data will be, when repeated at a larger scale. This is especially true of high pressure processes where gas-liquid reactions are performed using a solid (dispersed) catalyst. Many commercially important hydrogenations are performed using such multi-phase (heterogeneous) catalytic media. There are many variables that influence the reaction rate and chemists often struggle to appreciate the key ones. This is not helped by fact that much of the equipment used in studies is so simple and poorly instrumented that elucidation of the controlling variables is virtually impossible.

This article will review data from three sizes of experimental equipment that is used for development of heterogeneous hydrogenation processes, covering a volume range of two orders of magnitude (10ml to 1000ml).

In evaluating this data,"mixing rate" will be quantified in a manner amenable to chemists - involving only the reaction rate and time to reaction, rather than more complex parameters often used by engineers.

This will be used to show that in well controlled and instrumented reactors that reliably record the progress of the reaction, much useful and scalable information can be obtained even at the very small scale. This can be achieved without knowledge of reaction kinetics and using only information directly reported by the reactor instruments.

This will then be used to identify the relative importance of mixing and reaction kinetics - and hence to highlight what is truly controlling the reaction.

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