Oxidation Reactor Scale-up:
Translating Pilot Plants to Commercial Scale through Modeling

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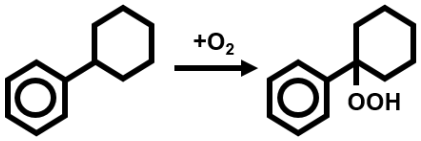
Highlights

- Multiphase reactors often present significant scale-up challenges.
- Measuring and modeling intrinsic kinetics are essential
- Scale-up models ranging from phenomenological reactor models to computational fluid dynamics are critical to projecting commercial reactor performance from pilot data and de-risking scale-up.

1. Introduction

Conventional routes for producing chemical products such as phenol and cyclohexanone involve liquid phase oxidation reactions as a key reaction step. This class of reactions is well-studied in literature with extensive experimental data and modeling work for the conversion of hydrocarbons such as cumene, p-xylene, and cyclohexane [1]. A novel route to produce both phenol and cyclohexanone from benzene requires the liquid phase oxidation of phenylcyclohexane—optimizing this step is critical to minimize process yield losses and byproduct make [2]. To design a full-scale commercial reactor to conduct this reaction efficiently requires a range of tools: pilot reactor experiments to probe the chemistry at a range of conditions, a comprehensive kinetic modeling of the oxidation reaction built on that pilot data, an understanding of the transport phenomena at scale that may impact performance, and a commercial reactor model to predict performance at scale. The complete analysis presented here allows for a confident and efficient commercial-scale industrial reactor design while managing risk.



Reaction 1. Primary oxidation reaction of phenylcyclohexane to its hydroperoxide. Secondary reactions will be discussed in the full paper.

2. Methods

In order to progress the reaction scale-up, we use a range of models and experiments: small-scale kinetic experiments in batch and continuous pilot plants, free radical kinetic models, 1-D and 3-D phenomenological models at laboratory and commercial scale, and hydrodynamic and mass transport experiments [3-6]. These models are tools to scope reactor performance *a priori* to identify preferred operating conditions and aid in selecting reactor configurations that will achieve target performance. These tools illustrate a framework for approaching gas-liquid reaction chemistry and bubble column reactor scale-up that is translatable to other chemistries.

3. Results and discussion

The kinetic experiments and model show that the thermal phenylcyclohexane oxidation demonstrates low yield to desired products, but the use of free radical chain transfer agents such as *N*-hydroxyphthalimide (NHPI) can dramatically improve hydroperoxide production rate and selectivity (see Figure 1). Mass transfer limitations must also be managed at both the laboratory and commercial scale to maximize hydroperoxide selectivities. We will discuss the impacts of reactor geometry and configuration to minimize byproduct formation and achieve desired performance at scale. Cold flow

hydrodynamic experiments with real process fluids and computational fluid dynamic modeling were used to evaluate commercial reactor geometries and de-risk potential scale-up issues.

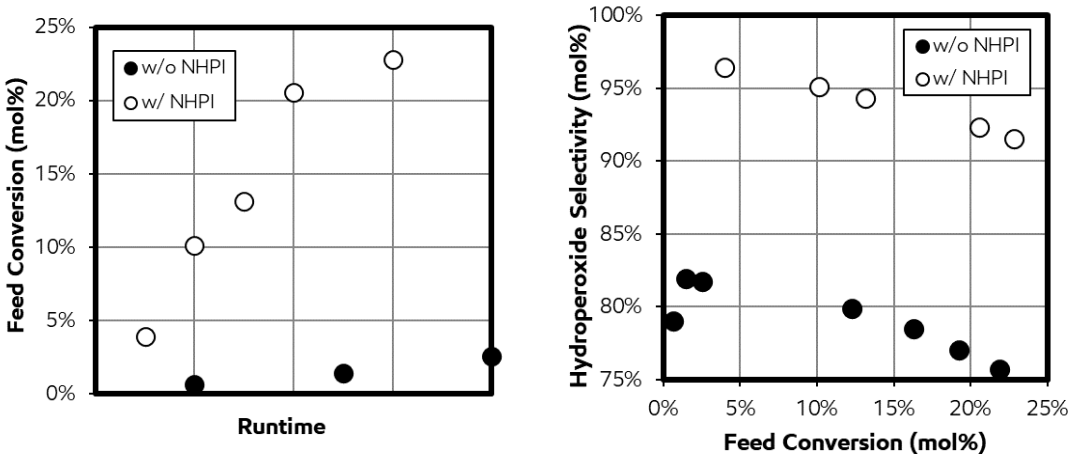


Figure 1. Batch reactor evaluation of the impact of *N*-hydroxyphthalimide (NHPI) on the phenylcyclohexane oxidation rate (left) and product hydroperoxide selectivity (right) [7].

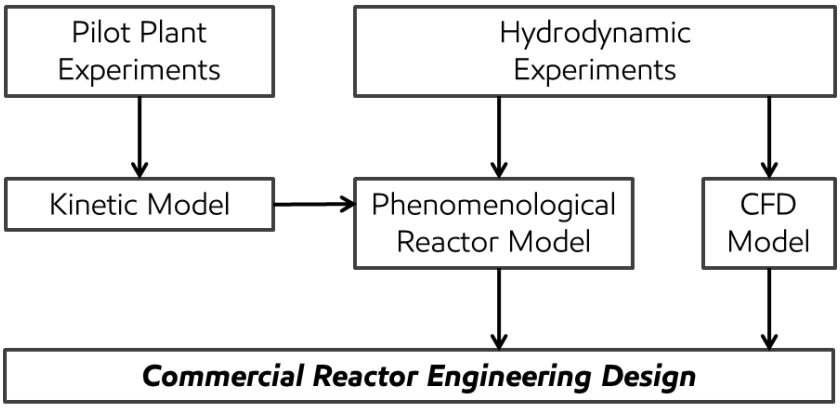


Figure 2. Reactor scale-up methodology and tools employed.

4. Conclusions

Oxidation reaction scale-up is discussed from the evaluation of the fundamental chemistry through its translation to commercial scale. This work presents a comprehensive experimental and modeling framework applicable to gas-liquid reactions that enables such efforts. This approach is a valuable methodology for conceptualizing commercial reactors based on novel reaction chemistries.

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Keywords
Multiphase reactors; Bubble column reactors; Reactor modeling; Reactor scale-up