Reactor Scale-up from Lab to Commercial: Bridging the "Valley of Death".

Lattner, James R*

ExxonMobil Chemical Company, Houston, Texas USA

**Corresponding author: james.r.lattner@exxonmobil.com*

Highlights

- The scale-up of a new reactor technology from lab to commercial requires design and operation of a Pilot Demonstration Unit (PDU)
- Optimum design involves answering the question: "What is the smallest thing we can build that will address the questions required to design the commercial reactor?"
- When it is important to match commercial hydrodynamics, the pilot reactor must match the height of the commercial reactor
- The job of the Reaction Engineer is to use good reaction kinetics, experience, cold flow, and hydrodynamic modeling skills to reduce the size and cost of the PDU

1. Introduction

The stage involving scaling up a new reactor technology from lab to commercial is often referred to as the "Valley of Death". New reactor technologies often have complex hydrodynamics, and it is important for the Process Demonstration Unit (PDU) used for scale-up to have commercially-relevant hydrodynamics as well. Such pilot plants are very costly, and many good technologies die at this stage, when financial support runs out before the technology is adequately demonstrated.

Every new reactor technology has unique challenges, such that there is no clear-cut recipe that will guarantee success in scale-up. The most conservative approach is to design a pilot reactor that represents the smallest vertical cross-section, which provides relevant hydrodynamics, of the proposed commercial reactor. The result is a reactor generally larger and more expensive than most companies care to undertake. It is the job of the reaction engineer to use modeling expertise, cold flow apparatuses, and other means to reduce the cost of reactor scale-up, bridging the "Valley of Death".

2. Methods

N/A

3. Results and discussion

Mass transfer-mixing and/or heat transfer are important parameters in most reactor designs. These are also parameters that do not stay constant as scale is changed, making scale-up of new reaction services particularly challenging.

An interesting case study is the hypothetical scale-up of human body metabolism. From a reaction engineering standpoint, the human respiratory system provides the mixing required to react oxygen in air with the reactant; e.g. sugar, via mechanical agitation from a pump (the heart). The reaction is exothermic (about 115W), and cooling is provided through heat transfer through the skin of the "reactor". We can look at hypothetically scaling up this reactor "technology" to sizes of commercial significance for industry, say 1,000 m^3 reactors. We find that mechanical agitation becomes impractical at this reactor size. Bubble column reactors become attractive at this scale, as the air feed to the reactor also provides the energy for mixing. Heat transfer through a jacket also fails at this scale, because the surface:volume ratio becomes insignificant. High surface area heat exchangers are required to cool the reactor. The mass transfer rate of oxygen is a function of the superficial gas velocity, such that mass transfer is improved at constant air rate and reactor volume by making the reactor taller and thinner. When designing a PDU to provide scale up data for the commercial reactor, a design that mimics the human body mixing and cooling will be completely inadequate. The PDU must be the same height as the commercial reactor in order to achieve the same gas velocity, and the diameter must be large enough to avoid slug flow from bubbles that approach the diameter of the reactor.

Packed bed reactors are typically the first choice for industrial reactors, as their simple design makes them very cost effective. The mass flux is typically high in these reactors, as this reduces the diameter, and thus additionally reduces the cost. To achieve the desired conversion and space velocity, these reactors can be quite tall, on the order of 10m or more. When designing a pilot plant reactor for scale-up, the pilot plant reactor must also be on the order of 10m high to match both the mass flux and the space velocity of the commercial reactor.

Multi-tube reactors, where each tube is packed with catalyst and the bundle placed inside a vessel with a heating or cooling medium, are frequently deployed when the reaction is very exo- or endthermic and isothermal operation is required. In addition to matching mass flux and space velocity, heat transfer becomes an important feature to be demonstrated by the PDU. In this case, the smallest reactor that matches the commercial reactor is a single tube of the same diameter and height as the commercial bundle.

Fluid bed reactors also require very large PDU reactors, if the commercial hydrodynamics and space velocities are to be matched. An example is given for scale-up of a Methanol-to-Olefins fluid bed reactor. It was desired for the PDU reactor to provide continuous catalyst regeneration in a commercially-relevant hydrodynamic regime, which resulted in a very large reactor. Large cold flow fluid beds, using air fluidization and He tracer experiments, were used to determine the effect of reactor size on the hydrodynamic parameters.

4. Conclusions

While it is the job of the Chemical Reaction Engineer to select the approach and design the Process Demonstration Unit for scale-up of new reactor technology, this is a subject that gets little or no coverage in academia. Indeed, such exercises take place only in industry and very well-funded startups, where many good ideas fail to cross “the valley of death” due to the high cost and time requirement of this stage. When the hydrodynamics of the reactor are well-characterized, the PDU can be quite small. However, when hydrodynamics are an important scale-up parameter, the size can be quite large. The Reaction Engineer should design the commercial reactor, and then ask the question: “what is the smallest thing we can build that will address all the questions required of the commercial reactor”. With a conservative approach, this means the PDU reactor will be the same height as the commercial reactor. This is typically results in prohibitive cost. Reducing the size and cost of this facility is left to the Reaction Engineer, to use kinetic and hydrodynamic modeling capabilities, cold flow mock-ups, and good engineering judgment to make compromises on hydrodynamic parameters . . . and also to the willingness of the owner to accept scale-up risk.

Keywords
Reaction Engineering; Scale-up; Fluid Beds.

ExxonMobil Document Number 2017.2025