# Fluidized Bed Scale-Up for Sustainability Challenges. 2. New Pathway



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Review

# Fluidized Bed Scale-Up for Sustainability Challenges. 2. New Pathway

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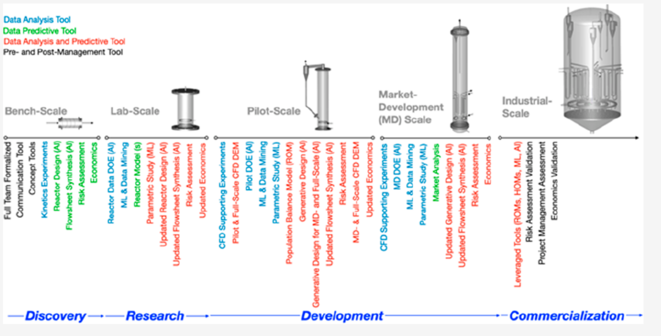
**ABSTRACT:** Despite more than 100 years of commercialization of wide-ranging fluidized bed reactors, scale-up tools and methods have remained quite similar. To exploit the benefits of fluidized beds for the time-critical sustainability challenges, scale-up has to be implemented quicker and better. Correspondingly, a companion Part 1 (*Ind. Eng. Chem. Res.* **2024**, *63*, 2519−2533) reviewed the evolution of the tools used in scaling up fluidized beds. Leveraging that, the current Part 2 aims to first overview the traditional pathway for scale-up and then propose a new pathway. Notably, instead of the traditional way of focusing on a linear sequence of progressively larger units, the emphasis is on the Phases of Discovery, Research, and Development, which apply the new tools consistently, as well as address risk mitigation and economics throughout. Based on an acrylonitrile case study, a Monte Carlo analysis indicates the new proposed pathway offers more promising economic feasibility, with net present value over 20 years ($NPV_{20}$) of \$310MM higher, along with 35% and 42% reductions in start-up and break-even times, respectively. The increase in costs for incorporating modeling efforts is insignificant compared to the overall benefits with respect to time and economics.




## INTRODUCTION

The scaling up of fluidized bed reactors from concept to commercial scale is more uncertain than with more traditional chemical reactors, resulting in a time scale that is unconscionable for the urgent sustainability challenges.[1] Fortunately, commercialization of fluidization units can be significantly expedited, as evident in catalyst cracking units (FCCUs) commercially producing abundant high-octane aviation fuel within a few years, which was driven by the then time-critical challenge posed by World War II.[2,3] This was instrumental in helping the Allied Forces win the war and is a testament to the scientific and engineering community that scale-up can be performed expeditiously with the right tools. There were other breakthrough technologies based on the fluidized bed that had similar speedy successes, with SOHIO taking four years for their acrylonitrile process[1] and Union Carbide taking eight years for their UNIPOL process.[4]

The problem is that such efforts would be unlikely in today's environment. It is clearly not from the lack of talent or technology, but the fact that scale-up today is more complicated than it was 80 years ago. Energy conservation, environmental impacts, safety, risk mitigation, waste reduction, and emissions reduction have understandably taken high priorities. Commercial units are more complex and expensive. Financial risks are higher, and markets are more transient and diverse. Feedstocks and supply chains come from multiple sources across the globe. All of these translate into novel fluidized bed scale-up typically approximating 10 years to commercialization in the private sector.

The extensive time frame for scale-up is an issue. With the pressing need for climate-neutrality, accelerating the commercial implementation of the advanced concepts and tools[1] is essential. Carbon-zero visions have been set for 2025,[5] so the engineering marvel that drove the expedited commercialization of the FCCU during World War II has to be invoked. The need for faster scale-up is real. A legally binding international climate change treaty inked in 2015 dictates the global warming limit of 1.5 °C above preindustry levels, which can only be achieved by greenhouse gas emissions peaking by 2025 and reduced by 43% by 2030. Increasing the speed in the

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scaling up of the fluidized bed reactor, which plays a pivotal role in the green transition, is critical.

Setting up and collecting data for lab-scale units are costly time- and money-wise, and pilot and process development units are even more so. To at least in part circumvent this, CFD codes of today can provide predictions within weeks and at much lower costs. Additionally, artificial intelligence (AI), which encompasses machine learning (ML), promises to be powerful tools that can play more important roles.[6] In the companion Part 1, a description and application methodology were given on advanced scale-up tools.[1] In the current Part 2, the scale-up pathway for using those tools is defined and mirrors that already implemented with product development methodologies.

## ■ BACKGROUND

Part 1 of this two-part series summarized scale-up tools that could expedite scale-up efforts,[1] starting with a focus on idealization tools to reconfirm the fluidized bed reactor configuration and operation methodology. The motivation was to move past the traditional waterfall approach,[7] which entails a defined linear sequence of execution with project stages that do not advance until a preceding stage receives final approval. As the project progresses stage by stage, it can be difficult and costly to revisit a previous one. The problem with the waterfall approach is that risk management tends not to be applied until the development stage, because risk analysis tends to be associated with the then decided process and equipment, but this is far too late to be effective. Ideally, risk management needs to be formalized and applied at conception to promote risk awareness, and the new advanced tools need to be applied to make that practice effective.

At the start, scale-up with an idealization exercise can reconfirm the original proposed design, highlight that a better design may exist, or capture gaps and constraints with a proposed design. Concept tools (e.g., Design for Six Sigma,[8] Theory of Inventive Problem-Solving (TRIZ)) are now readily accessible for the design team to speedily get onto the optimized track. This results in a documented analysis of the design that promotes team dynamics and cooperation, while providing effective communication to the stakeholders.

CFD tools have been seeing increasing use in fluidized bed scale-up efforts since 2005.[9] Common simulation tools used for fluidized beds include TFMs (two-fluid models), CFD-DEM (computational fluid dynamics−discrete element method) models, or hybrid MP-PIC (multiphase particle-in-cell) models. Today's CFD models (which include CFD-DEM and MP-PIC) are sophisticated, robust, and capable of furnishing results for the commercial-scale process within weeks using coarse graining and graphics processing units (GPUs). Reasonable predictions have been demonstrated by various industries using commercial codes.[10−12]

To account for whole particle size distributions, commercial software, regardless of whether based on the Lagrangian framework (CFD-DEM and MP-PIC) or TFM (through method of moments[9,13,14]), already have this capability, which represents a significant advantage compared to earlier ones that factor only a "representative" particle size. Nonspherical particles, particles with asperities, and particle roughness, which are known to impact fluidized bed hydrodynamics, can also be accounted for. Eppala et al.[15] showed using CFD-DEM that the fluidization regime changes from bubbling to turbulent when the particle sphericity decreases. Goldschmidt et al.[16] found that, by a hard-sphere CFD-DEM model with particle rotation, bubble behavior was better captured than with a two-fluid model.

For collisional stresses and surface roughness, which have been found to impact particle clustering behavior,[17] most CFD models do not have the capability of capturing these effects other than adjustments to the drag model.[1] Well-defined, small-scale experiments, high-resolution simulations, and AI models may change that challenge.[1,18] Experiments involving powder rheometry,[19] minimum fluidization behavior,[20,21] and the Hausner number[22,23] may provide at least a correction to the models when interparticle forces are at play. Yet, experiments are still empirical in nature, which makes the results dependent on the system and thus path-dependent. Direct Numerical Simulations (DNS) have been used to capture some particle stress behaviors in granular fluid flows. Using DNS, Tenneti and Subramaniam[24] extracted drag forces (i.e., both fluid−particle and particle−particle) for CFD models. Gu et al.[25] used CFD-DEM to derive the necessary inputs for the particle-phase stress model, but this applies only for smooth, spherical particles. Therefore, obtaining these constitutive parameters is often relegated to experience or used for tuning the model during model validation, which may stymie further use of the model at a larger scale.

Grid resolution and coarse graining are other challenges. The asymmetry of fluidization hydrodynamics can only be captured in 3D simulations. To adequately account for particle drag, the grid size has to be an order-of-magnitude larger than the particle size.[26,27] This translates to 1 mm even for Geldart Group A particles, which is intractable for simulating the commercial scale. To this end, subgrid models (i.e., filtered drag models) have been devised to accelerate solution times.

Regarding Lagrangian-type models, tracking all of the particles in a commercial-scale unit may appear inhibitory, but it is manageable. While CFD-DEM or MP-PIC models can model $O(10^7)$ particles, a commercial fluidized bed has approximately $O(10^{14})$ particles.[28] To address this, coarse-graining (i.e., categorizing similar particles into clouds or parcels) is employed to reduce the number of equations that needs to be solved. Analogous to grid resolution, the cloud or parcel numbers need to be judiciously determined.

Fortunately, these gaps in obtaining parameters needed in the constitutive equations, gridding, and coarse-graining may be bridged with some of today's AI tools.[6] AI models have been used to ease the challenges with the microscale physics in the constitutive equations used in CFD models. AI can be used to develop the constitutive equations or the corresponding parameters based on well-tailored experiments. Sundaresan et al.[29] suggested momentum, species, and energy transfer constitutive models can be improved via deep learning methods. Jiang et al.[30] used ML to improve a drag model for fTFM (filtered two-fluid model), and Yang et al.[31] hybridized the EMMS drag model with a neural network to extract heterogeneity indices, while Lu et al.[32] harnessed ANN to improve a filtered drag model. In addition, Lorsung and Barati Farimani[33] used AI for adaptive meshing to allow for larger meshes while maintaining the accuracy of the predictions. A similar framework can also be used for relaxing the time step constraints. As an alternative, AI models have been used to circumvent the CFD limitations altogether, specifically with respect to development of an initial process model without the complications of grid and time step restrictions. For instance, AI was used to predict syngas composition for downdraft


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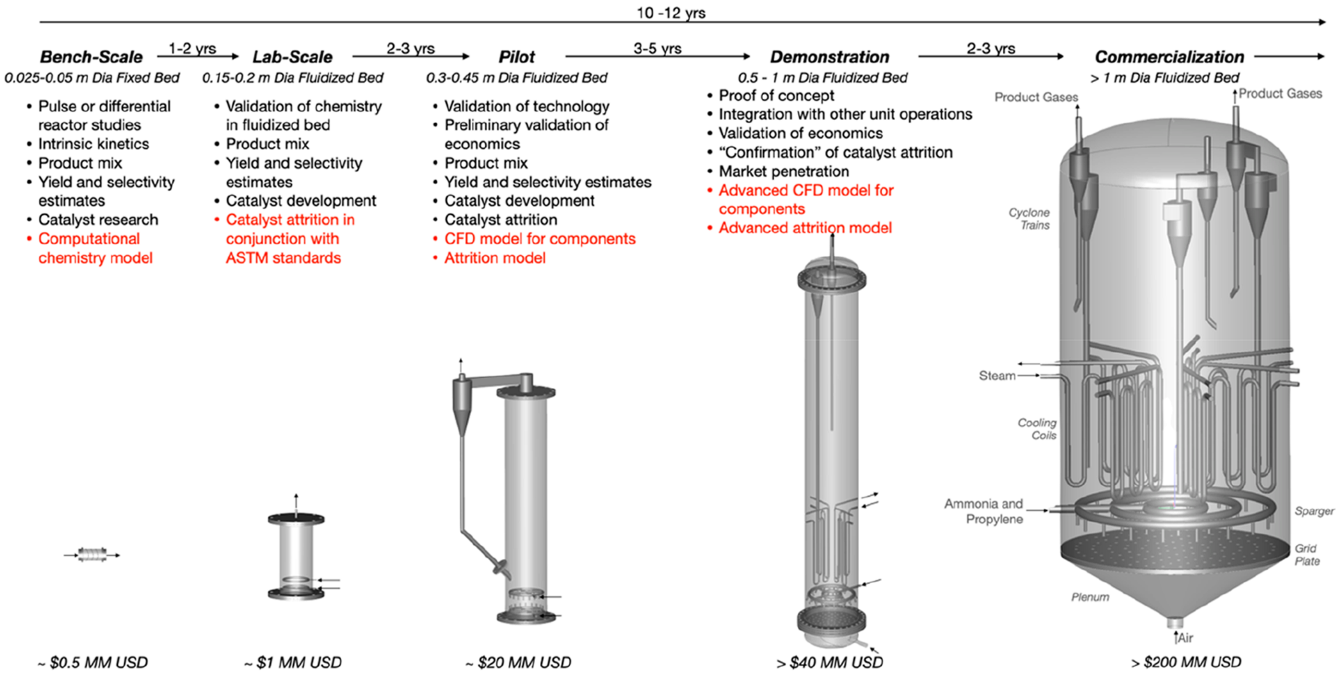


**Figure 1.** Typical fluidized bed scale-up methodology. Reproduced with permission from ref 1. Copyright 2024 American Chemical Society.

biomass gasification[34] and also hydrogen production in a bubbling fluidized bed (BFB) and a circulating fluidized bed (CFB).[35] Furthermore, AI models or augmentations are now available for many of the traditional tools used in scale-ups,[1] including Design of Experiments (DOEs),[36,37] Generative Equipment Design,[38] Flowsheet Synthesis,[39,40] and Risk Assessments Processes (RAPs).[41]

Quantum computing can also remove such restrictions with gridding and time steps, as well as the need for coarse-graining and filtering. Instead of the classical bits of today's computer architectures, quantum computing uses qubits, which is nonbinary. For some formulations, it can result in exponentially faster solution times than classical counterparts. Quantum computing has been applied to the Burgers' equation (convection−diffusion)[42] and the Navier−Stokes equations,[43] providing accuracy when compared to analytical solutions yet at significantly reduced solution times. Chen et al.[44] applied quantum computing to a finite volume method, showing that a CFD-type model is possible, augmented with a finer mesh at faster calculation speeds. Yet, quantum computing is still in its infancy and requires new and different computer architectures. CFD commercial codes are not available, and it is likely years out before they will be available given the current limits of operating systems and compilers for quantum computing platforms. Although quantum computing holds great promise for higher-order models, its application as a scale-up tool is beyond the scope of this study at this time.

While AI reactor models are in rapid development, the "black-box" nature of such approaches is somewhat incongruent with the governing physics underlying fluidization processes. AI models are only as good as the quantity and quality of the data used for training and testing. Physics-informed AI (PI-AI) may change that perception of AI. For instance, physics-informed neural networks (PINNs) hybridize a black-box neural network to white-box physical governing equations by converging the two parts to a single loss function,[45] thereby enforcing adherence to physics. Indeed, a PINN approach has already been taken for modeling flow in complex geometries such as blood vessels,[46] turbulent flow hydrodynamics sans a turbulence model,[47] two-phase flow,[48] and non-Brownian suspensions from Couette flow.[49]

Many of these AI-based tools offer a significant opportunity to reduce the scale-up time without a significant increase in investments. Still, the methodology of scale-up needs to change as well. The traditional waterfall process will not be effective for scaling up with these next-generation tools. The scale-up process needs to change to fully exploit the benefits of these tools in terms of reduced time and cost to delivery, and lower risk.

## ■ TRADITIONAL PATHWAY FOR SCALE-UP

Fluidized bed reactor scale-ups tend to follow a waterfall approach, whereby subsequent steps revolve around the stage gates associated with a bench-scale reactor, a lab-scale reactor, a pilot unit, an optional market development unit (MDU), and the commercial plant, as shown in Figure 1. MDU may be a necessary expense for a process involving a new technology or a new product. If the technology is not new and the product already has an established market, it is usually eliminated or circumvented with a slightly larger pilot unit.

**Stage 1: Bench Scale.** The bench-scale unit is generally a fixed bed with an inner diameter of 0.025−0.05 m, operated as a pulse or differential reactor to mimic the short gas residence times of a fluidized bed. The typical approach is trial-and-error to collect preliminary data on reaction kinetics, product mixture, yield, selectivity, and catalyst behavior. In some cases, catalyst lifetime experiments may be performed. The cost (capital, human resources, etc.) for this stage is approximately $0.5MM. At this point, a high-level economic model for a commercial plant may be attempted.

**Stage 2: Lab Scale.** The second stage starts in about 1−2 years with a lab-scale fluidized bed (diameter ∼ 0.15−0.2 m). The bed diameter is a critical parameter for the lab-scale unit and needs to be large enough that the walls do not influence the bed density and bubble hydrodynamics. A general rule of thumb is the inner diameter of the fluidized bed should be at least 0.15 m, preferably 0.2 m, for Geldart Group A particles and larger for Geldart Group B particles whereby slugging could be an issue.

A realistic bed height at this scale would be unlikely to mirror that of a commercial operation. Thus, gas residence times would be shorter than desired for the targeted product mix. Otherwise, the unit will have to be made tall, and slugging could be an issue with Geldart Group B particles. In addition, the pressure drop and shear stress to the wall in these units with tall beds can be high, resulting in the bed behaving as a piston when starting up that can persist for a surprisingly long time. Thus, tall units need to accommodate intermediate gas feeds at various axial locations along the bed. These additional feeds are only needed during start-up.

The primary objective of the lab-scale fluidized bed unit is to validate the chemical reaction, and the behavior and properties of the catalyst or bed material. Key scale-up parameters such as the entrainment rate, transport disengagement height (TDH), clustering, agglomeration, and particle attrition are unlikely to be relevant to the commercial plant operations. In some cases, a design of experiment () may be used to reduce the number of experiments with parametric studies (i.e., full factorial, half-factorial, center composite, etc.). The costs for this stage start at $1MM (including capital and human resources).

With the initial success of the lab-scale unit, additional tasks need to be completed. A reactor model may be attempted consisting of a reduced order model (ROM) such as that proposed by Levenspiel et al.,[50] Werther,[51] and Thompson et al.[52] The model should be validated with the lab-scale data in terms of reactor productivity (i.e., yields, weight hourly space velocity (WHSV), etc.) and bed density.

With a ROM in place, the commercial unit design is conceptualized. The diameter and bed height of the commercial fluidized bed reactor will still need to be estimated. CFD models may be attempted for the commercial design, but there are little data for validation. Data from the lab-scale unit tend to be limited, and wall effects could influence the bed hydrodynamics and the extrinsic kinetics. Still, having a model in place will allow other concepts to be explored and, when evaluated with the lab-unit data, may help explain some of the hydrodynamics.

Finally, the pilot unit needs to be designed, and a flow sheet with a piping and instrument diagram (P&ID) needs to be developed, assuming site logistics are a given. The validated reactor model will play an important role in the design and the flow sheet.

**Stage 3: Pilot Scale.** Lab-scale studies usually take 2−3 years, after which a pilot-scale unit (diameter ∼ 0.3−0.45 m) is typically employed to validate the technology, economics, and reactor productivity, and also to develop models for catalyst attrition and lifetime. This unit needs to be equipped to measure selectivities and conversions, bed densities, entrainment rates, transport disengagement heights (TDHs), and particle attrition. Helium residence time distribution (RTD) data can also be valuable, especially when comparing productivity numbers to the previous lab-scale reactor data. Distributor and cyclone designs are more involved with pilot units than the lab-scale units but will unlikely resemble that of the commercial unit. The cost of this stage is typically greater than $20MM because of the larger scale. This stage involves the commercial design along with the optional MDU design. CFD models (i.e., two fluid CFD, MP-PIC, CFD-DEM) of the pilot unit, MDU, and proposed commercial unit design are developed. A similar-scale model may be used to confirm the pilot unit's hydrodynamic behavior and validate the CFD model, especially if a -driven parametric study is performed. However, the best validation for the CFD model is the reactor productivity numbers from the pilot unit.

In some cases, large cold-flow experiments are performed to better understand the hydrodynamics. It should be noted that large cold-flow experiments take 6−12 months and are costly (>$500,000), and thus the benefit of this exercise should be carefully weighed. Notably, important physics, such as wall stresses, shear stresses, interparticle forces, wetting, attrition, etc., are convoluted, which may limit the viability of the data obtained from the cold-flow hydrodynamics tests. Nonetheless, this is a step in the traditional pathway, and some engineering design companies request such data as further risk-mitigation. However, such experiments rarely capture the hydrodynamics at operation conditions, certainly less so than a validated higher-order model.[1]

Coupling the pilot unit data with validated CFD (and at times with a population balance model (PBM) to track attrition, but more often not), the MDU and commercial design can be explored. The results of these models can be fed into updating the equipment, flow sheet, and P&ID designs of the MDU and commercial units. As with the previous step, the economic model, which is based on the revised equipment design and flow sheet, is further developed and used to confirm the economic viability of the proposed process.

**Stage 4: The Market Development Unit.** MDUs tend to be optional depending on if new technology or a new product is being considered. Unfortunately, the fluidized bed is still considered a new technology despite being in commercial operations for over 100 years.[3] Thus, most scale-up efforts with fluidized beds tend to involve an MDU. Whether it is needed or not hinges on the level of risk a company and/or investors is willing to absorb. MDUs are designed and flowsheeted in Stage 3, and construction may start during Stage 3 operations. Once in operation, the MDU will be used for about 2−3 years. Much of the designs and flow sheeting for the commercial unit will commence early in Stage 4.

An MDU, which typically has bed diameters of 0.5−1 m and bed heights similar to that proposed for the commercial unit, runs at the operating conditions planned for the commercial scale and is integrated with other targeted unit operations (i.e., feeders, separation columns, etc.). Cyclone trains and heat exchange coils in the MDU design need to mirror that of the proposed commercial design. Catalyst attrition and scaling models are further assessed. Bed density profile, entrainment rate, TDH, cyclone collection efficiency, cyclone pressure drop, dipleg performance, pressure drop profiles, and particle attrition are valuable scale-up data that can be collected from an MDU. However, due to the size and cost, parametric studies are rarely performed, which may not be needed if good parametric studies were performed on the pilot unit in Stage 3.

Model validation, for both the CFD and PBM, needs to be considered with the MDU data. Results from these models will help revise the equipment designs, flowsheets, and P&IDs. A process risk analysis or a risk assessment process (RAP) is often considered in Stage 4. A RAP uses the team, expertise, and a cold-eye reviewer to evaluate the probability of failure and the corresponding ramifications for each piece of equipment in the proposed design.[1] This assessment includes


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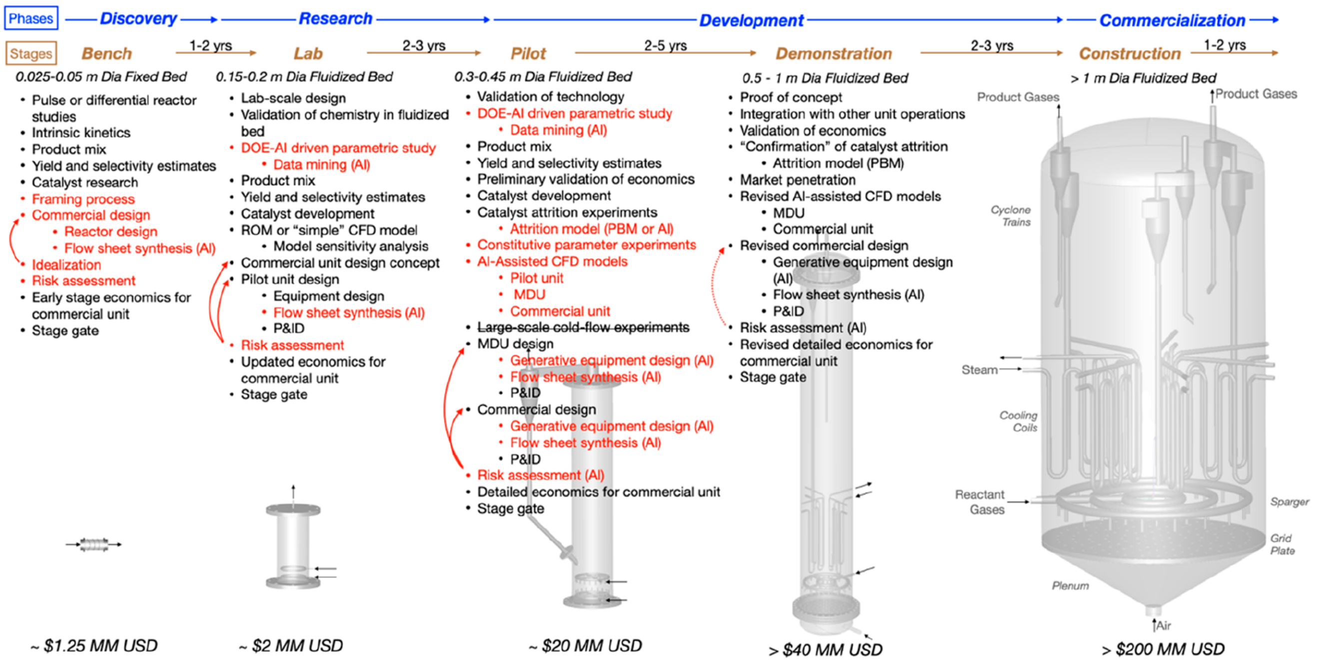


**Figure 2.** Proposed scale-up path for a fluidized bed process.

evaluation of circularity with regard to energy usage, $CO_x$ emissions, particle emissions, recyclability, and reliability. This process needs to have a systems integration approach to fully account for consequences of the failure on both up- and downstream performance. RAP, which is rooted in quantitative risk assessments (QRA) of environmental and safety risks, has been applied toward process risks involving reliability and asset management.[53]

The RAP results provide additional data for the economic model. Weak links can now be quantified, and a more realistic estimate that includes reliability can be obtained. For example, suppose the RAP highlighted that attrition could be a key challenge, and thus attrition issues were documented with a high likelihood of failure and a high consequence that goes with that failure. Consequently, catalyst replacement costs and lower reliability are added to the economic model as equipment repairs and downtime. It may suggest that the cost of failure is too high to absorb and thereby that something needs to change. The PBM can help indicate where attrition is the most problematic. Chances are it is at the gas distributor or the primary cyclone, and hence redesign is needed. In this way, RAP circumvents the possibility of having a longer start-up and/or not achieving the process objectives.

## ■ PROPOSED NEW PATHWAY FOR SCALE-UP

With additional challenges associated with today's scale-up, including safety, environmental, risk mitigation, and additional logistics, the conventional method is poorly suited for accelerating process development. Yet, it has the merit of being "tried and true", which gives a false security of risk mitigation. The commercial design and operation are often not even considered until Stage 3 with the pilot unit. However, if a different reactor configuration or operation becomes obvious, it may be too late in the process to move forward. Such is counterproductive to risk mitigation.

Based on new, available scale-up tools and leveraging product development methodology,[7,54,55] a new scale-up path is proposed with a focus on risk mitigation and economics. Figure 2 illustrates this scale-up path, which is divided into four Phases but utilizes the same Stages (i.e., bench, lab, pilot, demonstration, and commercialization) as the traditional scale-up path (Figure 1). The architecture of the new path is to circumvent the waterfall constraints that prevent the traditional scale-up path from being efficient and cost-effective.

Agile project management stems from software development efforts in the 1990s and has quickly moved into other industries such as telecommunications, banking, mining, and petrochemical.[55] Its predecessor, lean project management, was the project management methodology of choice before then, with its roots in the Toyota Production System in the 1940s.[54] The proposed phases of scale-up and the work process within each phase is based on the Scrum and Sprints methodology within the Agile project management framework.

The Scrum methodology is divided into five distinct Phases, namely, (i) Initiation, (ii) Planning and Estimates, (iii) Implementation, (iv) Review and Retrospective, and (v) Release.[7,5657] To leverage the Scrum methodology for fluidized bed scale-up, the four proposed scale-up Phases are laid out as (1) Discovery (mirrors Initiation, and Planning and Estimates), (2) Research (mirrors Implementation), (3) Development (mirrors Implementation), and (4) Commercialization (mirrors Release). However, process development takes longer and is more costly than product development. For that reason, Scrum's Review and Retrospective phase translates into Risk Assessment and Economic Evaluation at each stage of the fluidized bed scale-up pathway. Here, risk assessment is now proposed at the early beginnings of the scale-up and reassessed after each Stage. It should not be considered as a stage gate, as with the economic assessment, but as a recalculated path. It reveals what needs to be readdressed with the current Stage and what needs a higher-priority focus


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at the next Stage. It also addresses issues with circularity objectives early on in the development.

Moreover, the scale-up path needs to embrace new technology. Often, the state-of-the-art in process scale-up is very different from the state-of-practice. Many of the new tools proposed in the companion Part 1[1] for scale-up have been around for decades, but some are just starting to be considered. Other tools have gone through decades of development due to intrinsic complexity but may be now primed for process development in fluidization scale-up. These tools are key to the economic analysis required at the end of each gate and are discussed below in the context of the specific scale-up Stage. Some tools are needed to be used in every Stage. In fact, the frequency of utilizing the proposed tools is at the heart of a more efficient and cost-effective scale-up process, with the tools becoming more sophisticated with each additional Stage.

**Phase 1: Discovery.** The initiation of scale-up is now not so much a focus on bench-scale study but rather risk assessment, and the tools needed for that assessment are moved front and center. The Discovery Phase starts similarly to that of the traditional Stage 1 (i.e., bench scale) with kinetic data from a pulse or differential reactor to mimic the short gas residence times of a fluidized bed unit (Figure 2). As before, preliminary data need to be collected on the reaction kinetics, product mixture, yield, selectivity, catalyst type, and perhaps catalyst lifetime. Sometimes, a small fluidized bed reactor will be used in this phase as a "proof of concept" in conjunction with the other reactors with more defined hydrodynamics (i.e., fixed bed, pulse reactor, etc.) to demonstrate the fluidization nature of the process. These reactors tend to be too small (less than 0.15 m inner diameter for Geldart Group A particles) to provide hydrodynamics scale-up information but can provide insights into the fluidization concept. As long as the team is cognizant the hydrodynamics will be different, such experiments could be beneficial in reducing perceived risks with the chemistry and fluidization. Nevertheless, the phase involves some soft tools, with framing at the very start.

*Framing.* Framing, or the use of framing technique, is a team-building and stakeholder communication exercise. The project objective, vision, financial risk, business alignment, safety concerns, environmental concerns, stakeholders, and budget are laid out here. This is to ensure everyone on the team, including the stakeholders, is aligned concerning the purpose, concerns, and constraints. Scale-up projects can last for many years, and the team needs to understand all of this is subject to change and that such changes will be clearly communicated. At the same time, the team culture needs to be developed into one that is "in love with the problems, and not the solutions".[7] Scale-up projects should not be managed in solution space, especially at the early stages.

*Early Stage Commercial Design.* The next step being proposed is at the heart of this strategy. With only intrinsic kinetics in hand, the team needs to design the process. It will likely be wrong, but it will be enough for the subsequent risk assessment and early stage economics. Fred Brooks[58] once said, "Plan to throw one away; you will, anyhow." The design process will consist of reactor designs and flowsheets. At this point of the scale-up, the reactor design will probably be limited to the greater of the kinetics versus mass transfer time scales. The fluidized bed height is based on the required gas residence times (given the resulting time scale) with respect to the bed voidage of the predefined fluidization regime.[59] With the defined superficial gas velocity that is consistent at both scales, the diameter is based on the predefined volumetric flow rate of the commercial unit.

With a preliminary reactor design, flowsheeting is needed to define all the additional supporting equipment (i.e., feeders, cyclones, quench, heat exchangers, distillation columns, etc.). Traditionally, a flowsheet is based on institutional knowledge using Aspen Plus or Hysys. However, new tools are available that make this task faster. As noted in the companion Part 1,[1] the flowsheeting exercise can be significantly streamlined using flowsheet synthesis tools such as the Aspen Hybrid Modeler[6] or Aspen Plus piloted by HEEDs.[38] Using Simplified Flowsheet Input-Line Entry-System (SFILES), flowsheet generation, including complex topologies with splits and recycles, can be autocompleted with an AI engine based on the desired product mix, fluidized bed yields, and feedstock specifications.[40]

*Idealization Testing.* Once the process design is in place, that design needs to be tested. This is where the idealization tools come into play.[1] The incorporation of these idealization or concept tools must be done in the early months or even weeks of development. For example, some questions need to be answered in the early stages of development. Should it be a fluidized bed process? Why not a more traditional reactor? Should a circulating fluidized bed or moving bed process be considered? In actuality, a fluidized bed process may be the optimum choice but one needs to prove it. Also, what is the fluidization regime in which to operate the fluidized bed? Was it chosen based on the chemistry or other concerns?

For example, many fluidized bed projects start with the proposed operation being in the bubbling fluidized bed region to minimize solids loss rates. However, in terms of chemistry (specifically, extrinsic kinetics), most processes benefit from operations in the turbulent fluidized bed regime with its inherently higher heat and mass transfer rates that enhance extrinsic kinetics. For turbulent fluidized beds, the more chaotic nature of the bubbles or voids results in a higher bubble surface area to bed volume ratio, which impacts the extrinsic mass transfer.[60] To a lesser extent, baffles can have the same effect by breaking up large bubbles and thereby slowing the bubble rise velocity.[61,62]

Solids loss can be managed with a good distributor and cyclone design; perhaps an expanded freeboard section may be necessary. The idealization tools need to focus on these types of questions, and that focus must be done early in the scale-up process. It is much harder to convince stakeholders that the pilot plant design needs to change, than to spend upfront resources to ensure it s not have to change. Fortunately, there are a wide range of concept and idealization tools, including Design for Six Sigma,[8] TRIZ,[63] NICE or NIS,[64,65] SCAMPER,[66] CPS,[67] and SWOT,[68] that can propel the design team onto the optimized track in short order. The result will be further confirmation of the original design concept or a re-evaluation of the reactor configuration and/or operation, followed by a re-design and flowsheeting of the new concept.

*Risk Assessment.* Risk Assessment comes at the end of the Discovery Phase, followed by early stage economics. As discussed above, the Risk Assessment Process (RAP) can be used to quantify process risks entailing asset management, circularity objectives, and process reliability.[53] The probability failure mode for each component and the attendant consequences is comprehensively evaluated by the team members and possibly with external experts. RAP tools are now available based on a matrix of probabilities using an AI


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Bayesian network model to assess the reliability of the process.[41] By simulating anomalies and testing potential risks via AI, weak links in the process flow and equipment design can be identified. With RAP performed earlier, weaknesses and gaps are tackled sooner in the scale-up pathway. More importantly, communicating those weaknesses and gaps along with the strategy to address them to the stakeholders will mitigate concerns of risk with the process. Risk needs to be clear, and the path to mitigate that risk needs to be addressed, because stakeholders have much less resistance to terminating a project in the Discovery Phase.

With the risks documented and early stage economics determined comes the first stage gate. The upfront work will benefit those early stage economics analyses, and, with risks explicitly stated, give the stakeholders a higher confidence level on the path forward. It is estimated that the cost incurred at this Phase typically starts at $1.25MM, which is higher than the traditional scale-up path as additional resources are needed for the upfront work with the commercial design and idealization testing. With each subsequent stage, this commercial design will be re-evaluated. Notably, having a vetted design in the Discovery Phase will reduce the resource load with subsequent Phases.

**Phase 2: Research.** The second Phase mirrors the second Stage (i.e., lab scale) of the traditional scale-up path (Figure 2). For Geldart Group A particles, the unit should be at least 15 cm in diameter, preferably at least 20 cm in diameter. For a bed of Geldart Group B particles, the diameter needs to be large enough to prevent slugging (unless slugging is preferable). It is unlikely but not impossible that slugging will be an issue in a commercial-size unit, so analysis based on a slugging lab-scale unit would be irrelevant. Furthermore, gas residence times may be shorter than that proposed for the commercial design. Often, the lab-scale unit is limited to the facility's height. It is unlikely that a realistic bed height, mirroring that of a commercial unit, would be achievable. However, the primary objective of the lab-scale unit is to validate the chemical reaction. Even with the shorter bed heights, the extrinsic kinetics can be validated. Once validated, the kinetics can be used in a ROM to extrapolate the projected productivity of the commercial design.

Key scale-up parameters, such as the entrainment rate, transport disengagement height (TDH), bubble hydrodynamics, clustering, agglomeration, and particle attrition, are unlikely to be relevant to commercial plant operations. Validating such parameters using correlations or models may also be limited as wall effects are rarely considered or correctly considered in such correlations or models. Nonetheless, it may be worth calculating to improve confidence in relating the findings of the lab-scale unit with the larger test units.

*AI-Driven DOEs.* Test variables for the lab-scale unit should include all the important parameters (e.g., temperature, pressure, feed concentration, and superficial gas velocity), culminating in hundreds of experiments in a full-factorial matrix. Proper design of experiments (DOEs) can decrease the number of required experiments without compromising the confidence level. The traditional way is that most of the experimental matrix needs to be completed before the significance can be tested. That is changing. AI-assisted DOEs are available today. For instance, an AI-driven DOE software, called xT SAAM,[37,69] evaluates the data in real time rather than only at the end, resulting in quicker feedback.

Subsequently, AI can play a role in the data analysis of the results. As the number of experimental factors increases, so s the difficulty in recognizing the patterns and relationships with the responses. This is especially true when more than three experimental factors are being considered. Machine learning (ML) tools have certainly been used to reduce this difficulty.[70] Our earlier studies[71,72] used Self Organizing Map and Random Forest (RF) to identify the primary driver for differentiation of bubbles in the bubbling bed and clusters in risers, which was identified as the width of the particle size distribution. Fu et al.[73] used an artificial neural network model (ANN) to optimize the pressure drop and expansion ratio for fluidized bed reactors. Kim et al.[74] used RF and ANN to maximize syngas produced by a fluidized bed biomass gasifier, while Lian et al.[75] employed similar methods to maximize hydrogen. Machine learning tools thus are useful to augment the scale-up process with new insights not obtainable by more traditional methods.

*Reduced Order, CFD, and AI Models.* With the initial success of the lab-scale unit, additional tasks need to be completed. Reduced order models used for fluidized bed simulations are typically used to simulate axial and/or radial profiles using ordinary differential equations (ODEs). Unlike ODE models for plug flow reactors, fluidized bed ROMs need to capture the reactions in the bubbles and in the emulsion (i.e., the bubble-less part of the bed). This is achieved using compartment models. An example is the two-phase model, with the phases being the bubble phase and the emulsion phase. Levenspiel et al.[50] employed three phases, namely, bubble phase, cloud phase, and emulsion phase. The cloud phase is designated as the boundary layer surrounding the bubbles, while the bubble phase is tied to the cloud phase, and the cloud phase is tied to the emulsion phase by mass transfer coefficients. Werther[51] and Thompson et al.[52] used two phases consisting of bubble phase and emulsion phase. Most compartmental models (i.e., a type of ROM) used for modeling fluidized beds are sensitive to mass transfer or dispersion coefficients. It is recommended to do helium residence time distribution (RTD) studies to fit the ROMs' RTD curves.[50,76] As with other parameters determined from the lab-scale unit, wall effects on the bubble hydrodynamics make the mass transfer or diffusion parameters from RTD studies in the lab-scale unit only valid for the lab-scale unit. It will need to be remeasured for the subsequent larger units.

CFD models are limited in capturing wall effects and incorrectly capture radial profiles.[77] On this scale, wall effects have an influence on the bed hydrodynamics and the extrinsic kinetics. Regardless of the model, it will have to be validated with the lab-scale data in terms of productivity and bed density.

Another option is using an AI-based model to capture the lab-scale reactor's performance. Direct measurements of mass transfers can be convoluted, and empirical correlation based on bubble hydrodynamics (i.e., bubble size, bubble rise velocity, and bubble frequency) may be specific to the particle properties or properties not specified in the AI training (i.e., surface roughness, adsorbates, surface charge disparities, etc.). Fortunately, AI reactor models can relax this restriction by a more direct link to the performance indicator. Mohd et al.[78] applied such AI models for a broad range of chemical reactor systems. García-Ochoa and Castro[79] used ANN to determine the oxygen mass transfer coefficient in stirred tank reactors. Similarly, Sablani[80] used an ANN approach for determining the fluid−particle heat transfer coefficient. Guo et al.[81] used a hybrid ANN reactor model to simulate a fluidized bed biomass gasifier, which circumvented the ROM development process entirely.

AI tools are relatively new to the scale-up methodology, and some discomfort may stem from the "black-box" approach of determining key parameters or an entire reactor model with an AI tool. To this end, physics-informed AI (PI-AI) not only provides for some physical governance but also requires less data (since the abundant data needed for AI is not so feasible). Muther et al.[82] showed how PINN can filter the results from an ANN model to comply with the known physics of the process. Ji et al.[83] and Weng and Zhou[84] used PINN to solve a set of stiff ODEs related to solution kinetics. Schiassi et al.[85] used the Physics-Informed Neural Network Theory of Functional Connections (PINN-TFC) based framework or Extreme Theory of Functional Connections (X-TFC) to model a compartment model consisting of ODEs.

Once sufficiently validated, the ROM, ANN, or PINN model can be used to obtain a broad spectrum of scale-up parameters and the sensitivity of those parameters to the reactor's performance. A validated ROM, ANN, or PINN can provide a quick method of examining varying scenarios while highlighting which input factor is dominant with respect to the predefined objective function(s). As with the experimental data, machine learning can significantly improve this data analysis and is recommended. The results can have an impact on the pilot plant design and the DOE associated with the pilot plant stage.

*Commercial Unit Design Concept.* The commercial-scale fluidized bed reactor design can be estimated with an early stage model in place. Data from the lab-scale unit include the bed density, which, assuming the diameter of the lab-unit is big enough to minimize wall effects, can be extrapolated to the commercial design. With design specifications on feedstock rate, temperature, and pressure, an estimate of the bed diameter and height can be obtained. It is accurate enough for the economic analysis but not for the final design of the commercial unit.

*Pilot Unit Design.* Finally, the pilot unit needs to be designed, and a flowsheet with a piping and instrument diagram (P&ID) needs to be developed, along with site logistics. The validated reactor model plays an important role in the design and the flowsheet. The pilot reactor needs to be designed to determine key scale-up parameters, such as gas residence time versus yield, productivity, entrainment rates, TDH, bed densities, bubble hydrodynamics, and particle attrition rates. It may also need to accommodate catalyst lifetime studies, so extended operations may need to be considered.

Flowsheets follow, and, depending on the complexity of the pilot unit, an AI-assisted flowsheeting tool may be beneficial for more complex pilot unit processes. After that, P&IDs are needed along with safety procedures, environmental impacts, air permits, etc.

*Risk Assessment.* At the end of this phase, another risk assessment is warranted, which should focus on the pilot unit and the commercial design. What has changed in the understanding from Phases 1 and 2 that may affect the original design and operation of the commercial unit? The risk assessment may identify key design parameters that need further clarification or re-evaluation. It is likely that the commercial design concept and/or the pilot unit design will need to be re-designed based on the findings of the risk assessment.

It is estimated that the cost incurred at this phase typically starts at \$2MM. As with the Discovery Phase, the Research Phase cost is higher than that of the traditional scale-up path, as additional resources are needed for modeling, pilot plant design, and risk assessment. The updated risk assessment and economics documentation should be essential for the Phase 2 stage gate. Should the scale-up continue to Phase 3? Or should Phase 1 or 2 be re-done, or should the project be terminated, delayed, etc.? If the data collected in Phase 2 do not make that decision process easier, then something is amiss.

**Phase 3.1: Development with Pilot Units.** The third phase involves pilot plant experimentation and mathematical exploration of the commercial design. The key objective of the pilot plant includes obtaining (i) key scale-up data such as productivity, entrainment rates, TDH, bed density profile, and attrition rates; (ii) data for model validation such as productivity, bubble hydrodynamics,[86,87] and RTDs from gas and solid tracers;[88,89] and (iii) data for extended runtime operations. At the same time, additional development efforts need to be applied toward higher-order models (HOMs), equipment design for the commercial plant, more flowsheet synthesis, pilot experiments and analysis, population balance modeling (i.e., an ROM). Following again would be another round of risk assessment and economics evaluations.

Pilot studies in the traditional path usually take 2−3 years. However, front-loaded efforts in Phases 1 and 2 are expected to reduce this to 1−2 years. Pilot units (diameter ∼ 0.3−0.45 m) are used to validate the technology, economics, and reactor productivity, as well as develop models for catalyst attrition and lifetime. This unit needs to be equipped to measure selectivity, conversion, bed density, entrainment rates, TDH, and particle attrition. Helium RTD data can also be valuable, especially when comparing productivity numbers to the earlier lab-scale reactor data. Gas distributors (i.e., spargers, grid plates) and cyclone designs are more involved for the pilot units than the lab-scale unit but will unlikely resemble that of the commercial unit.

*AI-Driven DOE.* Measured responses from the pilot-unit experiments are going to be more difficult, more multidimensional, and more convoluted. A well-thought-out AI-driven DOE with machine learning for multivariate analysis is recommended. Machine learning tools can certainly be used to reduce this difficulty,[70] especially if this methodology was already applied in Phase 2.

*Attrition Model.* Most pilot units are large enough that the attrition data collected are relevant to the commercial design, provided such data account for differences in particle velocities (e.g., in the presence of internals). In general, attrition in fluidized beds are mostly due to gas jets from the distributor and the primary cyclones (which process the bulk of the solids). If possible, the jet velocity penetrating the bed from a distributor and the inlet velocity for the primary cyclone need to be relevant to that proposed for the commercial unit. If so, attrition data can be developed into a population balance model (PBM).

PBMs are systems of simultaneous ODEs that describe changes in the particle size distribution. All too often, the attrition in the commercial unit is ignored during the design, resulting in a commercial plant operating at a much higher solids loss rate than initially proposed. In some cases, solids loss rates could compromise the economic viability of the


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commercial plant. A PBM is a predictive tool that can provide a more realistic attrition rate estimate well before the commercial design has been finalized. Werther and Hartge[90] incorporated attrition rate mechanisms (for jets and cyclones) and breakage patterns of attrited particles via PBM to a fluidized bed design, while Werther and Reppenhagen[91,92] provided stochastic models for the jet and cyclone as power law expressions. The breakage pattern is more complicated and usually just an estimate. These models have to be tailored to the bed material used. A more accurate breakage model could be obtained with laboratory attrition test unit (e.g., jet cup[93,94]) and particle size distribution analysis of bed samples.

With validated higher-order models (HOMs), such as a CFD and/or PBM, in place, the MDU and commercial design can be explored. The results of these models can be fed into updating the equipment design specifications, flowsheets and P&ID designs of the MDU and commercial units. As with the previous Phase, the economic model, which is based on the revised equipment design and flowsheet, is further developed and used to confirm the economic viability of the proposed process.

*Constitutive Parameter Experiments.* CFD models, and to a lesser extent, CFD-DEM models, have become an integral part of today's scale-up processes. Future efforts should emphasize and prioritize CFD efforts. Reasonable accuracy has been demonstrated and endorsed by various industries.[10−12] It should be noted though that many phenomena are still incompletely accounted for, such as interparticle force, agglomeration, clustering, attrition, and particle growth or shrinkage.[1]

Traditionally, CFD models are validated against large, cold-flow experimental data. However, such large-scale cold-flow experiments are time-consuming (~6−12 months), expensive (>$500,000), and deficient on useful physical insights (e.g., wall stress, shear stress, interparticle force, wetting, attrition, etc.). Today's CFD model would provide better predictive accuracy if the parameters used in the constitutive equations were determined from small-scale experiments specific to the physics at hand.[18] Data are needed to determine which drag model is appropriate and what the parameters for that drag model are. Also, particle collisional stress parameters such as coefficient of restitution and specularity coefficient need to be determined. Typically, collisional stress parameters are often estimated, which may be appropriate for a lower velocity fluidized bed but not for a fast fluidized bed or CFB riser where a core−annulus profile is known to develop.[95]

*Correcting Drag.* There are several ways to measure the drag or, more appropriately, correct the drag model, usually in the form of a particle cluster size. Powder rheometry tests,[19] minimum fluidization curve overshoot[21] and hysteresis tests,[20,21] and dynamic Hausner ratio tests[22,96] have all been applied to correct for drag particularly when shape effects and/or interparticle forces are involved. That correction can come as a multiplier to the drag coefficient or as a cluster size. Regarding cluster size, particles smaller than the cluster size can be assumed to be equal to the particle size for the particle size distribution.[97] The particle size distribution used in the CFD model is re-defined such that the smallest particle is the particle cluster size with a weight fraction of the sum of all the smaller particles.

Direct numerical simulation (DNS) has also been applied to correct for particle−particle drag[24] and interparticle forces.[25] Smooth, round particles are typically assumed, so the application may be limited for some systems. Nonetheless, such a model can be used to determine the microscale properties that can be extracted for a drag−filtering model.[26] Such a model reduces the grid sensitivity issue with drag models.[27]

AI models (e.g., ANN) have also been applied for drag correction.[30−32] Unlike DNS models, the underlying physics are not needed or can be generalized as a PINN model. What is needed are lots of data for the bed density and entrainment rate. Ideally, an axial profile of the solids concentration would be value-added as well, although that is a more complex experiment. At the start of Phase 3, the only data available for AI training and testing are from the lab-scale unit. It is a good start, but the AI model will have to be retrained and tested with the pilot scale data if the freeboard is significantly higher or the operating conditions (temperature, pressure, and gas velocity) are different.

Commercial CFD codes do not have AI capabilities for drag or drag correction yet, but such a model can be easily incorporated with a user-defined subroutine or a model fit to the drag−AI modeling results as a constrained subset. For lower-velocity fluidized bed simulations, the drag needs to be relevant as it is the key controlling parameter for the simulation.

*Coefficient of Restitution.* Collisional stresses, which can be quantified for either particle−particle or particle−wall, are challenging to account for in detail at the commercial scale. For most CFD models, the elasticity of the normal collisional stress is captured with the coefficient of restitution, which is an indication of the fraction of elastic momentum transfer. CFD-DEM typically uses the Hamaker constant associated with the Johnson−Kendeal−Roberts (JKR) type model. Experiments are typically performed using a particle drop experiment and a high-speed camera, whereby a change of momentum indicates the elasticity of the collision.[98−101] Oesau et al.[102] used a magnetic particle tracking procedure to quantify that elasticity.

Miao et al.[103] used particle-resolved direct numerical simulations (PR-DNSs) to quantify drag coefficients for spherical and nonspherical particles. The model was complemented with a back-propagating neural network model. Schwarz et al.[104] used a deep neural network (DNN) model for capturing erosion from the resulting particle trajectories and speeds (i.e., rebound model) for particle-laden flow through turbines. Similarly, Haghshenas et al.[105] used DNN models for particle-laden flows in sediment transport lines.

*Specularity Coefficient.* The specularity coefficient is the amount of momentum conserved when a particle impacts another particle or surface at a grazing angle.[106] Similar to measuring the restitution coefficient, the specularity coefficient or specularity reflection coefficient is usually determined from particle tracking imaging. For commercial-scale fluidized beds, the specularity coefficient may be the least important model parameter. Wall effects and shear stresses tend to have a minimal effect in a fluidized bed.

*Higher-Order Models (CFD, MP-PIC, CFD-DEM, and AI).* Perhaps the modeling component of Phase 3 is more critical than that for the traditional Stage 3 pilot-plant studies. The pilot-plant studies confirm what is expected, but it is the models that will quantify the performance of the commercial unit while serving as a data analysis tool for the pilot-plant studies. For this reason, modeling is being proposed to play a more primary role in fluidized bed scale-up, and data collected


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from the pilot unit need to go beyond productivity goals. Key hydrodynamic scale-up parameters such as bed densities, entrainment rates, transport disengagement heights, and particle attrition need to be measured and used to validate the models. Once validated, such models would be invaluable in the design and design variations of the commercial unit.

Fortunately, today's CFD codes can be accurate even for commercial-scale computational domains,[107] and industry is increasingly embracing this.[10−12] However, these codes can only capture the physics for which they have been designed. Interparticle forces,[29] drag as related to solids loadings in fluidized beds,[108] rough particles, and highly nonspherical particles are typically beyond the capabilities of commercial CFD codes (though there are some CFD-DEM codes[109−111] that can handle nonspherical particles).

CFD models need to be tuned to the data collected from the pilot unit.[112] Ideally, tuning needs to be minimized as much as possible. A higher level of tuning is a direct result of the amount of physics that the model is missing (i.e., drag, particle shape, particle roughness, interparticle forces, etc.). It could be an important piece of physics that stymie direct use at another scale. Clearly, the ability to confidently extrapolate to larger computation domains depends on a fundamental model. The higher the level of tuning, the more the model becomes a curve-fit and less a prediction tool. To address this, data from small-scale experiments can be conducted to obtain key constitutive parameters that are more in line with a fundamental model than that from tuning.[18]

Nevertheless, tuning is often needed. For the tuning, it should be based on a large amount of statistically significant data that spans the operating range and physical properties that will be relevant to the commercial system. For low-velocity fluidized beds, tuning is generally done with a multiplier to the drag coefficient.[113] It has been done through adjustments to the particle size or size distribution,[114] but that change will also change the collisional stress values. For circulating fluidized beds (CFBs), the adjustments to the coefficient of restitution can significantly impact the collisional stress model, perhaps too much.[115]

Grid resolution and coarse graining also need to be resolved. For grid resolution, a size of 1 mm may be needed for Geldart Group A powder,[24,25] which is too small for simulating commercial-scale units. That requirement can be relaxed if a filtered drag relationship is used.[26] However, the grid still needs to be resolved, which requires several simulations, each one with a better grid resolution. If two simulations of different grid resolutions have the same answer, then the more relaxed gridding may be valid. The axial pressure profile and a mid-bed radial pressure profile at a steady state could be good metrics for the effectiveness of the grid resolution.

Coarse graining (i.e., clouds or parcels) has the same issue. Coarse graining reduces the number of equations by categorizing similar particles into groups. That number of particles per cloud or parcel needs to be resolved much like the gridding by comparing multiple simulations of different levels of coarse graining. For fluidized bed simulations, the metric should be the axial bed density profile instead of the averaged bed density.

The restrictions with getting constitutive equation parameters, grid resolution, and coarse graining can be reduced or eliminated with an AI model (e.g., ANN). AI has been used for quantifying the scale dependency,[18] optimizing the filtered drag model,[30,32] measuring the heterogeneity index (i.e., level of clustering) for an EMMS drag model,[31] and optimizing adaptive gridding to relax time step constraints.[33] Others[34,35] have removed the Navier−Stokes equations altogether by replacing the CFD modeling with AI modeling.

Such distancing from fundamental physics could be disconcerting, which is why PINN models are actively being developed for fluid flow problems.[45−47] As noted above, it still uses the neural network, but an additional layer is added to filter the physics. In the case of fluidized bed models, this would be the Navier−Stokes equations and drag model. However, such models are not commercially available yet.

*MDU and Commercial Design.* With higher-order models and/or AI models (ANN or PINN) along with key scale-up data from the pilot unit (i.e., bed density, gas RTDs, entrainment rates, TDH, yields, etc.), detailed MDU and commercial designs can be obtained. Using a generative equipment design tool can better optimize this design.[38] Such a tool will not only optimize the reactor size and configuration, but also be used to optimize the gas distributor design, number of cyclones and geometry of cyclones, placement of the diplegs, design of the heat exchange tubes, etc. The design of the commercial unit should be done first, as it will predetermine some of the design parameters for the MDU.

After the design of the units, flowsheeting is needed. As with Phase 2, a flowsheet synthesis tool can reduce the resource load and perhaps deliver an optimized configuration.[40] Our earlier study[1] discussed the algorithm and commercial application of such tools. With an optimized flowsheet design in place, the P&IDs are needed to complete the design of the commercial unit and the MDU.

*Risk Assessment.* The Phase 3.1 risk assessment needs to be the most involved exercise of all the risk assessments, as it needs to identify weak links in the detailed process flow and equipment design. The risk assessment team should include the scale-up team, any external consultants, and one new consultant as a cold-eye reviewer. The first risk analysis should start with the commercial unit as it will help discern what the MDU needs to resolve. It should be noted that the risk assessment is a stage gate process. In general, if the team is not going back to redo some of the commercial and/or MDU design, the exercise is not detailed enough. Afterward, another economic analysis is needed based on the resulting designs. This needs to be a detailed economic model that encompasses all of the equipment, supporting equipment, utilities, resources, market pricing, reliability estimates, etc.

The subsequent stage gate is for the stakeholders with documentation on the design, risks, and economics in hand. Their decisions will determine if the project progresses to or skips the next stage (i.e., MDU). Reaffirming the skilling of the next phase or going directly to commercial construction, performing additional tasks in Phase 3.1 again, terminating, delaying, or slowing down the project are all important considerations.

**Phase 3.2: Development with MDUs.** The second part of Phase 3 involves the construction and operation of the MDU, additional data analysis, validation of the pilot unit data, revised design for the commercial unit, revised models, a detailed risk assessment, the final economic analysis, updated supply chain availability and pricing, and updated market penetration. MDUs are time-consuming and expensive. Thus, this stage tends to be applied toward vetting new technology or for market penetration. Tasks for this phase mirrors that of the demonstration-unit stage. Data are collected from the MDU


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and compared to pilot-plant results. In addition, all reactor models and PBMs need to be further validated. The commercial unit will go through another design exercise using AI-driven tools for equipment sizing and flow sheeting.

A risk analysis is needed and should mirror that performed for Phase 3.1. If done right, there are always changes to the design, almost to the very end. At this point, each of those changes needs to go through a cost−benefit evaluation. However, the work process needs to be set up to embrace such changes and not be exposed to negative feedback. A design change may not be used, which is fine, but it should always be disclosed.

The MDU is a good indicator of the scale-up efforts. If data from the MDU are consistent with what was learned from the pilot and lab units, and the corresponding models, then the scale-up methodology was correct. In other words, if the result of this phase is that the phase was not needed, then consider the scale-up successful. If all of this was performed in the time proposed, then acknowledgment of the scale-up team is warranted.

**Benefits of Using Tools.** What has been proposed here means that more resources are needed for data analysis, modeling, and technical management to accelerate the commercialization of a proposed fluidized bed process such as biomass gasification or pyrolysis, methane decarbonization, plastic-to-chemicals, or carbon capture chemical looping. The question then is, why should more resources be used? As Figure 3 reflects, the profitability of any chemical process

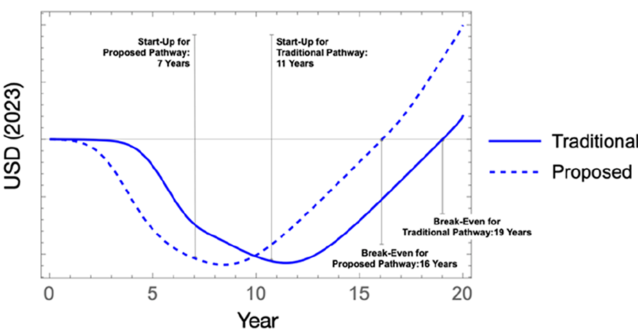


**Figure 3.** Cumulative cash flow for a hypothetical fluidized bed acrylonitrile plant with 2MM kg of acrylonitrile product per year.

depends on controlling costs during the Research and Development (R&D). Naturally, the more the spending on R&D is, the harder it is to recover when revenue does start coming in. Specifically, the net present value over 20 years ($NPV_{20}$) needs to be positive on the order of \$10MM. That is achieved by starting up the process earlier or incurring lower scale-up costs. For the traditional scale-up pathway for a hypothetical fluidized bed acrylonitrile plant, Figure 3 shows that break-even (i.e., net profit) does not occur until 19 years after the start of the project. This results in a $NPV_{20}$ of \$20MM. If this can be moved a few years earlier, perhaps by using the proposed tools and methodology, the break-even time is now 16 years, but the $NPV_{20}$ is now significantly higher at \$141MM. In other words, break-even is three years earlier, and the metric typically of even greater importance to stakeholders—the $NPV_{20}$—is \$121MM higher.

To explore this further, a more detailed Monte Carlo simulation was developed based on the scale-up of a hypothetical acrylonitrile process based on a fluidized bed. Capital costs, resource hours, and the timing of the phases are not well predefined with any scale-up process. To address the variability of the costs and timing, Monte Carlo simulations of these variabilities were employed. The path to commercialization was segmented linearly as the construction and operation of a miniplant, pilot plant, market development plant, and commercial plant based on a traditional scale-up methodology vis-à-vis the proposed scale-up methodology with a higher priority for modeling tools.

Table 1 compares the traditional versus the proposed pathways concerning capital cost (CapX), human resource requirement, and cumulative gain in delivery time. The estimates are based on a commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116] Between the two pathways, the CapX remains constant, but the human resource levels are different. For the Monte Carlo simulations, the capital costs are allowed to vary by ±20%, corresponding to the common practice for contingencies with scale-up. Human resource costs (labor and overhead) are estimated to be \$250,000 ± 20% per engineer per year, corresponding to 2000 h. This only reflects the human resources involved in scaling up, and not the researchers, chemists, and technicians involved prior to the onset of scale-up. For Stage 1 of the traditional scale-up pathway, the human resource load is set at 1 person-year. To account for the additional front-loaded modeling and engineering efforts, an additional 0.5 person-year of human resources is needed for Phase 1 of the proposed pathway. Compared to Stage 2 of the traditional pathway, Phase 2 of the proposed pathway requires an additional person-year of human resources (i.e., increased from 2 to 3). For Phase 3, human resources are increased from 10 to 12 and from 18 to 21, respectively, for the pilot and MDU operations. For commercialization, the human resource loads are similar in both scale-up pathways. In summary, the model is based on increasing the human resource loads to exploit the advanced tools, which would result in an overall reduction in the commercialization costs and time.

Of course, it would be unreasonable to expect that augmenting the additional human resources to implement to

**Table 1. CapX, Human Resource, and Cumulative Difference in Delivery Times between the Traditional and Proposed Scale-up Paths; Basis = Commercial Plant Delivering 2.06MM kg of Acrylonitrile Product Per Year[116]**

| Step Name | | | | Human Resources, person-year | |
|---|---|---|---|---|---|
| Traditional Pathway | Proposed Pathway | Primary Unit Operation | Capital Cost, $10^6$USD (2023) | Traditional Load | Proposed Load |
| Stage 1: Bench | Phase 1: Discovery | Bench Unit | 0.175 ± 0.035 | 1 | 1.5 |
| Stage 2: Lab | Phase 2: Research | Lab Unit | 0.325 ± 0.065 | 2 | 3 |
| Stage 3: Pilot | Phase 3.1: Development | Pilot Unit | 15 ± 3 | 10 | 12 |
| Stage 4: MDU | Phase 3.2: Development | MDU | 35 ± 7 | 18 | 21 |
| Stage 5: Commercial | Phase 4: Commercialization | Full-Scale Unit | 200 ± 40 | 12 | 12 |


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advanced tools would automatically reduce the commercialization time. For that reason, the time savings between 0 and 100% modeling effectiveness (i.e., how efficaciously the advanced tools are implemented) are examined. Most stages do not start up or end at full capability (i.e., square wave); instead, cost and productivity reach a maximum and decrease subsequently. Therefore, as depicted in the inset in Figure 4, a

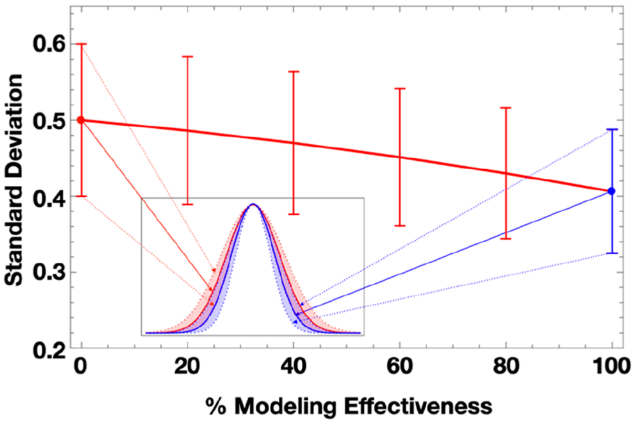


**Figure 4.** Simulated dependence of the standard deviation of a Gaussian distribution of cost with respect to duration (inset) on modeling effectiveness for each stage. Error bars indicate the ±20% in the standard deviation used for the Monte Carlo simulations.

Gaussian distribution is presumed to represent the cost versus duration of each stage. Figure 4 illustrates two concepts. First, as the modeling effectiveness (which is an independent variable for the Monte Carlo model) increases, the stage duration (i.e., Gaussian distribution width) shrinks to represent the decrease in time needed for that stage, which reflects the benefits of more effective modeling. Second, the Monte Carlo simulation varies this standard deviation by 20% (i.e., to account for a 20% contingency factor) to represent such variability common with most scale-up programs. The duration of each stage and the resulting resource costs changes by modifying the predefined standard deviation of the Gaussian distribution. At 0% modeling effectiveness, the standard deviation is set at 0.5, but at 100%, the standard deviation is reduced to 0.4 (Figure 4). While the standard deviation values may appear arbitrary, the resulting stage durations are reasonable based on experience. For any given simulation case, some stages will happen faster than that predicted by the curve, while others will happen slower. Each stage, represented by a Gaussian distribution, is allowed to overlap by 15%. In other words, Stage 2 starts at 85% of the Stage 1 peak in terms of duration. Similarly, Stage 4 starts at 85% of Stage 3 and Stage 5 starts at 85% of Stage 4.

Table 2 shows the estimates of the modeling costs at each step. The costs are a composite of minimal central processing unit (CPU) architecture and software licensing. Network infrastructure and IT support are outside the scope of this model. The present value product price is assumed at \$32/kg (based on acrylonitrile[116]) and operating costs are set at \$7/kg, including taxes.

Figure 5 depicts representative Gaussian cost profiles for a single stage, in this case the Pilot stage, to understand the impact of modeling effectiveness on cost. Specifically, each stage is assessed in terms of the capital, resources, and CPU/licensing costs as a Gaussian distribution to represent the typical delay in starting up and conclusion. Production and operating costs are modeled to a sigmoidal distribution, assuming that full capacity takes one year. This is to account for the fact that projects rarely start and end at full productivity. The tax rate is set at 25%. Note that 0% effectiveness represents the traditional pathway. As modeling effectiveness improves, the leftward shift in the peak is due to the corresponding reduction in the time to commercialization. Of course, the cost (and revenue) needs to be standardized with respect to the time value. Figure 5 shows the cost in USD of the present value in 2023. To account for the real cost of earlier delivery, peaks are corrected for the average for the U.S. inflation rate at 2.47% (averaged over the past five years), as apparent in the decreasing peaks with increasing years (i.e., discounting). For this pilot stage analyzed, Figure 5 indicates a time savings of two years between 0 and 100% modeling effectiveness, which is quite significant for a single stage.

**Table 2. CPU and Licensing Costs (Human Resource Costs Not Included)**

| Step Name | | | | |
|---|---|---|---|---|
| Traditional Pathway | Proposed Pathway | Primary Unit Operation | CPU Architecture Costs, $10^3$USD (2023) | Licensing Costs, $10^3$USD (2023) |
| Stage 1 | Phase 1 | Bench Unit | 25 ± 5 | 30 ± 6 |
| Stage 2 | Phase 2 | Lab Unit | 50 ± 10 | 60 ± 12 |
| Stage 3 | Phase 3.1 | Pilot Unit | 100 ± 20 | 120 ± 24 |
| Stage 4 | Phase 3.2 | MDU | 100 ± 20 | 120 ± 24 |

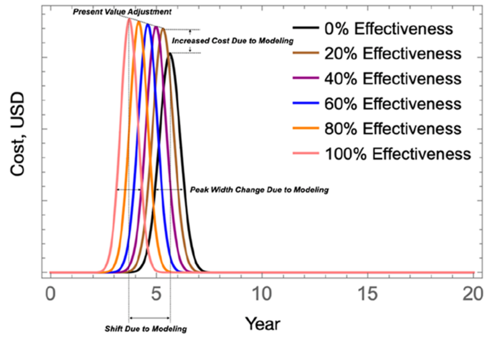


**Figure 5.** (a) Representative Gaussian cost profiles for various modeling effectiveness for a stage (in this case the Pilot stage) during scale-up. With increasing modeling effectiveness, the peak shifts leftward (i.e., less time) and the width narrows (i.e., decreases in duration) in accordance with Figure 4. Profiles are corrected to the present value (2023).

Figure 6 overviews one simulation scenario, showing the cost at each stage, operational cost, and the revenue stream. As noted above, scale-up costs are modeled as Gaussian distributions. The commercial plant costs are modeled as a sigmoidal distribution spanning 10 years with a 10 year loan payout at an interest rate of 12%. Operating costs include the feedstock costs, which also have a sigmoidal profile, allowing for one year to reach the design capacity of the commercial operation. The revenue stream is also sigmoidal, with the same profile as the operating cost. The variability in the operating cost and revenue stream reflects the historical (5 year) market pricing variability for the feedstock and the product pricing.

Ideally, the pinnacle of modeling efforts would enable confidently eliminating or reducing the need for an MDU unit


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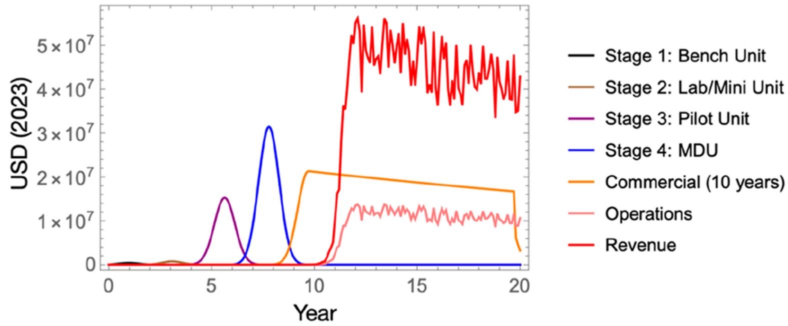


**Figure 6.** Representative costs and revenue for scale-up and operations for the case of 0% modeling effectiveness. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

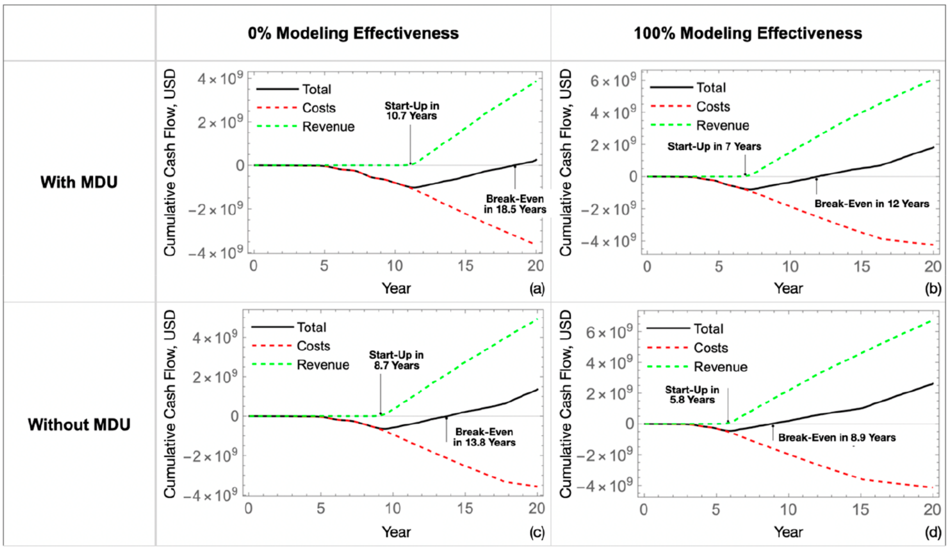


**Figure 7.** Cumulative costs, revenue, and total cash flow with and without an MDU in the Development Phase and with 0 and 100% modeling effectiveness. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

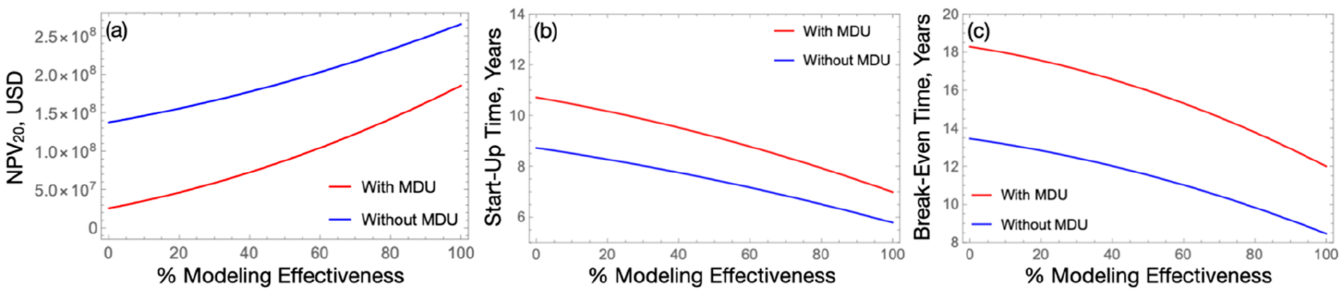


**Figure 8.** Estimates for the hypothetical fluidized bed acrylonitrile plant: (a) $NPV_{20}$, (b) start-up time, and (c) break-even time with respect to modeling effectiveness. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

during scale-up. The cumulative cost and revenue for the proposed scale-up pathway are shown in Figure 7 for cases with and without an MDU in the Development Phase, as well as for 0 and 100% modeling effectiveness. Expectedly, as scale-up progresses, the cumulative cost curves become increasingly negative with time, the cumulative revenue curves tick upward only after successful operation of the commercial unit, while the total cash flow curve (i.e., revenue minus cost) reflects the break-even time (i.e., the number of years needed for the revenue to offset the total costs). Clearly, the total revenue curve is relatively less negative without the MDU and relatively less negative with 100% modeling effectiveness.

Figure 8a presents the resulting net present value over 20 years ($NPV_{20}$). It should be noted that any economic model showing an $NPV_{20}$ of less than zero would not proceed further. In practice, the critical $NPV_{20}$ value that warrants a green light to proceed is typically much higher at \$100MM or more. As Figure 8a shows, $NPV_{20}$ increases with modeling effectiveness, reflecting the economic benefits of leveraging modeling tools. Also, the $NPV_{20}$ values are a few-fold higher for the case without the MDU, reflecting the significant advantage. With 0% modeling effectiveness and the use of a MDU, the $NPV_{20}$ is approximately \$25MM. For most, it is a value that would be considered economically unattractive. As for 0% modeling


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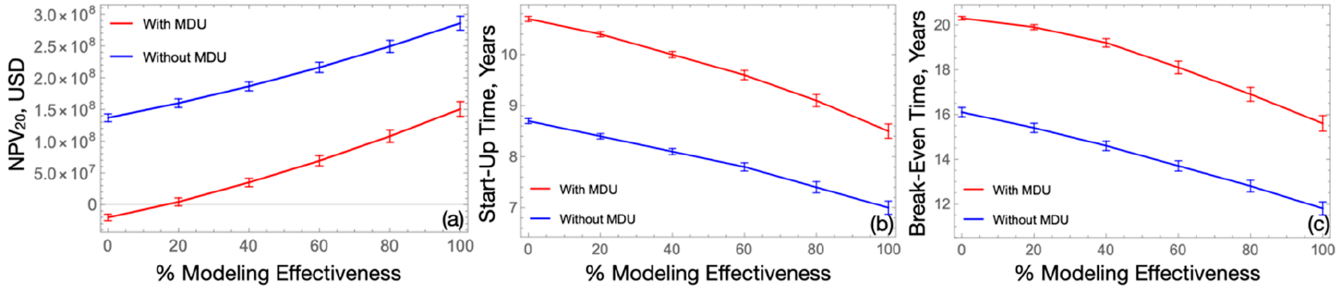


**Figure 9.** Monte Carlo simulation of the hypothetical fluidized bed acrylonitrile plant: (a) $NPV_{20}$, (b) start-up time, and (c) break-even time with respect to modeling effectiveness. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

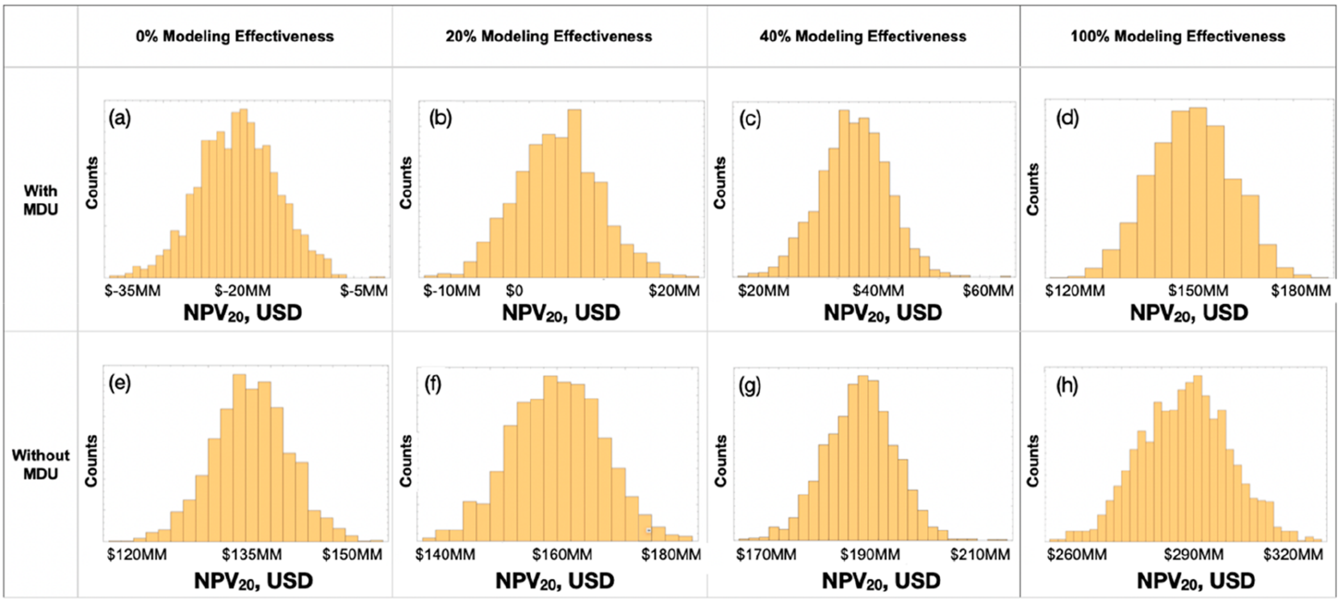


**Figure 10.** Histograms of $NPV_{20}$ values from the Monte Carlo simulations at varying modeling effectiveness and with or without an MDU. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

without the MDU, the $NPV_{20}$ increases to \$135MM, which is much more economically attractive. At 100% modeling effectiveness, the $NPV_{20}$ is an attractive \$190MM with an MDU and becomes a compelling \$265MM if the MDU is eliminated. If an MDU swings the economics into unfavorable economics, perhaps a more model-based scale-up path may be even more prudent. Clearly, the benefit of a scale-up program with a strong emphasis on more modeling and repetitive risk analysis (much of which is supported by modeling) is value-added.

Panels b and c of Figure 8 show the start-up and break-even times, in the presence and absence of the MDU, with respect to modeling effectiveness. With 0% modeling investment (i.e., 0% modeling effectiveness) and an MDU, the start-up time is determined to be 10.7 years and break-even point is at 18.3 years. Arguably this economic driver is too unattractive for most to consider it a worthwhile investment. On the other hand, in the ideal case of 100% modeling effectiveness and no MDU, the start-up time and break-even point are approximately halved to 5.8 years and 8.5 years, respectively. This is now a much more reasonable economic driver.

Notably, Figure 8 is based on fixed cost, revenue, and duration with a predefined reduction in that duration due to modeling efforts. In order to better rationalize the cost and time benefits of advanced modeling tools,[1] Monte Carlo simulations are performed. Specifically, the capital costs are allowed to vary by 20%, corresponding to the common practice for contingencies with scale-up (Figure 4). Thus, for each step, a random number generator via Mathematica 13.2 is used to discern the resource cost, modeling CPU and licensing costs, bench and lab units capital costs, pilot plant capital costs, MDU capital costs, commercial construction costs, commercial operating costs, and product revenue. Similarly, all other costs and revenue are constrained to the ±20% variability limits. The present value of the human resource costs (labor and overhead) is estimated to be in the range of \$250,000 ± 20% per engineer per year. The present value product price is assumed at \$32/kg ± \$4/kg. Operating costs are set at \$7/kg ± \$1/kg and include taxes. Pricing variability of up to ±20% is applied at 0.1 year intervals. The stage durations are also allowed to vary up to ±20%, as indicated by the error bars in Figure 4. Thus, even if the modeling effectiveness is at 100%, a stage duration has a probability of either showing no decrease in the project duration or exceeding that indicated by the curve by 20%. For each simulation pass, it is possible for the start-up time to be the same or be reduced by an assumed maximum of five years. Thereby, the simulation results will give a start-up time between the two limits. The Monte Carlo simulations require 2000 steps to reach a 95% confidence level (i.e., Student *t* test) in significance, but 10000 steps are used.


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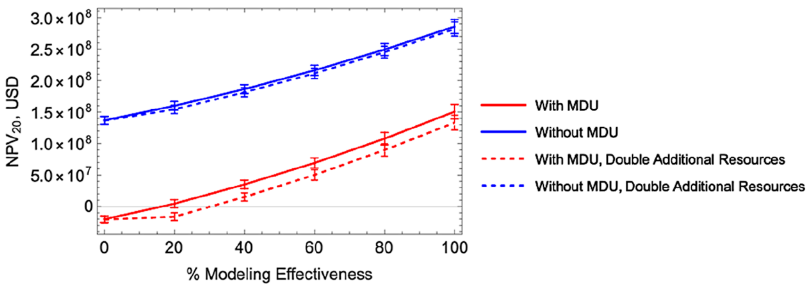


**Figure 11.** $NPV_{20}$ values from Figure 9a vis-à-vis $NPV_{20}$ values from a similar simulation but whereby the number of additional resources needed for modeling was doubled. Basis = commercial plant delivering 2.06MM kg of acrylonitrile product per year.[116]

Figure 9 shows the $NPV_{20}$, start-up time, and break-even time for the Monte Carlo simulations accounting for modeling effectiveness from 0% (traditional pathway) to 100% (idealized proposed pathway) with and without an MDU. The extremes (i.e., 0 versus 100% modeling effectiveness) clearly show the benefits of a more model-based scale-up pathway. The $NPV_{20}$ results in Figure 9a show the benefit of the Monte Carlo simulations that account for variability. While Figure 8a indicates 0% modeling effectiveness and an MDU gives an $NPV_{20}$ value of \$25MM for fixed cost and duration, the Monte Carlo simulations with up to ±20% variability in costs, revenue, and stage durations give an $NPV_{20}$ of less than zero (i.e., not financially feasible) in Figure 9a. In fact, as shown in Figure 10a, the histogram plots of the $NPV_{20}$ results from the Monte Carlo simulations suggest that $NPV_{20}$ values are less than zero in most cases. Even at 20% modeling effectiveness, with an MDU, 25% of the cases give $NPV_{20}$ values of less than zero (Figure 10b). At 40% modeling effectiveness and an MDU, the best cases are still well below the critical \$100MM $NPV_{20}$ (Figure 10c). At 0% modeling effectiveness, eliminating the MDU augments the $NPV_{20}$ to \$138MM (Figure 9a), which is slightly higher than that shown in Figure 8a. At 100% modeling effectiveness, Figure 9a shows that the $NPV_{20}$ values are \$150MM and \$285MM respectively for cases with and without the MDU, while panels d and h of Figure 10 present the corresponding spread of expected values that are all above the critical \$100MM value. Clearly, $NPV_{20}$ increases with higher modeling effectiveness.

For the start-up times at 0% modeling effectiveness, Figure 9b shows that the Monte Carlo simulation results are similar to that in Figure 9b. This suggests that it is the variability in the costs and revenue, rather than the duration, that lower the $NPV_{20}$ values. At 100% modeling effectiveness, the start-up times increase by 1−1.5 years compared to that in Figure 9b, suggesting that variabilities in costs, revenues, and stage durations need to be duly accounted for. As for the break-even results in Figure 9c, the consideration of variability in cost, revenue, and stage duration increases the break-even time for all modeling effectiveness. Since no difference in the start-up time is determined for the 0% modeling effectiveness case, the break-even trend further suggests that cost variability needs to be considered with any economic analysis on fluidized bed scale-up.

Considering the beneficial impact of modeling on cost and time, the effect of increased investment on modeling efforts is assessed. Figure 11 shows the $NPV_{20}$ results for similar Monte Carlo simulations, except the resources needed for modeling (i.e., human resources, CPU costs, and licensing) are doubled at each modeling effectiveness above 0%. If an MDU is included, the additional costs for the additional resources have negligible impact (i.e., within the error bar) on the $NPV_{20}$. If the MDU is omitted, the $NPV_{20}$ values drop only about 2 ± 1% with the additional modeling resources. This suggests that doubling modeling resources has minimal effect on the bottom line.

Collectively, the analysis highlights how advanced scale-up tools can turn an economically unfeasible scale-up project into a feasible and even attractive project. As Figure 10c shows, even at only 40% modeling effectiveness and with MDU, all cases have $NPV_{20}$ values above zero, although none attain the critical \$100MM value. If \$100MM is used as a cutoff for determining the feasibility of the project to move forward, then modeling effectiveness needs to be at least 80%. In addition, with an MDU, panels b and c of Figure 9 demonstrate that the incorporation of advanced scale-up tools can reduce the start-up and break-even times by 20 and 23%, respectively. If the MDU can be eliminated, then all cases of modeling effectiveness give attractive economics of well above the critical \$100MM (Figure 10e−h). Without the MDU, relative to the case of 0% modeling (i.e., traditional pathway), having 100% modeling effectiveness more than doubles the $NPV_{20}$ to almost \$290MM, along with a 20% reduction in the start-up time and 27% reduction in the break-even time (Figure 9). Compared to the worst case (i.e., 0% modeling and an MDU), the optimal case (i.e., 100% modeling effectiveness and excluding the MDU) gives an $NPV_{20}$ of \$310MM higher and results in 35 and 42% reductions in the start-up and break-even times, respectively (Figure 9). Clearly, for fluidized beds to contribute toward the pressing deadlines of today's climate-neutral challenges, the scale-up focus should not only be on reducing the duration of each stage but also on the possibility of not using a MDU, both of which are achievable by efficient and judicious implementation of the advanced tools.

## ■ CONCLUDING REMARKS

Fluidized beds are important for addressing time-critical sustainability challenges, so scale-up needs to be achieved more resource-, time- and cost-efficiently. Scale-up has been done in the literal sense of progressively larger units. Specifically, traditional scale-up efforts follow a waterfall approach (i.e., linear sequence of stages) and focus almost solely on the economic analysis usually preceding each stage gate. To expedite scale-up, it is proposed to circumvent the linear constraints by focusing instead on Phases (namely, Discovery, Research, Development, and Commercialization), and incorporating risk analysis that precedes each stage gate including the initial one, as well as AI and other models (ROM, PBM, CFD, DEM, Flowsheet Synthesis, Generative Design, etc.). A scale-up of a hypothetical fluidized bed here


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demonstrates that well-designed, verified, and validated mathematical modeling can significantly improve the scale-up process with respect to time (i.e., 35% reduction in start-up time) and financial returns (i.e., 42% reduction in break-even time and \$310MM improvement in $NPV_{20}$).

In essence, a paradigm shift is needed, whereby the design, flowsheeting, risk assessment, and economics are evaluated at every step, even in the initial Discovery Phase. Experiments need to be integrated with models to capture specific physics or patterns. Well-thought-out small-scale experiments should be prioritized over the more convoluted large-scale cold-flow experiments. Small-scale experiments can be done earlier in the process and under more realistic conditions. Modeling, whether in the form of ROM, CFD, CFD-DEM, CFD Hybrid, ANN, or PINN, needs to be considered and efficiently incorporated. Such models and their applications need to be defined and targeted early in the scale-up process. It should be considered as a Day 1 activity.

It is acknowledged that some of the CFD models need further development with constitutive equations (i.e., drag, interparticle forces, etc.), while AI-based models require lots of upfront data for training and testing. Also, AI models such as the neural network models have a black-box nature, which may do little to mitigate perceived risks. PI-AI can reduce that perceived risk but still requires quite significant development efforts; yet, such efforts are only a few years off from becoming a readily available tool. Starting early with such models could add significant value, especially since costs associated with these additional modeling efforts are small compared to other costs (i.e., CapX). This is especially true if such models with reactor performance, design, and flow sheeting are integral to risk analysis and economic evaluation. This integration would streamline the workflow while mitigating stakeholder concerns with the economic risks.

In short, model development and application need to take a higher priority in the scale-up process if time and costs are to be markedly reduced. New models should be considered even if more development is needed. The increase in costs for augmenting and advancing modeling efforts is significantly less relative to the gains in the $NPV_{20}$ and time.

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### Notes

The authors declare no competing financial interest.

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