

## **A Scoping Review of Tools for Teaching Particle Science Engineering & Technology**

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## Introduction

Particle science, engineering, and technology (PSET) is an essential part of engineering across various industrial sectors—as nearly all engineering fields rely on the effective and efficient use of granular and powder materials. Particles and powders are present in many fields, including but not limited to materials and chemical engineering (e.g., in-line process sensors, additive manufacturing), consumer products (e.g., food processing, paints), agriculture, pharmaceuticals, energy and pollution (e.g., air pollution and microplastics) [1], [2]. Particle science plays a crucial role in product quality, material transport and storage, manufacturing processes and advancement of materials science [3]. For example, understanding particle behavior (i.e., dry flow, aggregation and agglomeration) at a mass scale is crucial to the safety and improvement of storage, transport and manufacturing processes [3].

Despite calls since the 1990's to increase the availability of a uniform particle science curriculum, little progress has been made in integrating particle science into the current engineering curriculum—resulting in a limited number of engineers trained in the field [1]. Within the United States, particle science courses are sparse and lack uniformity within the materials and chemical engineering curriculum [3]. Currently, only around 15-20 programs offer particle science courses, and within these programs, there lacks common curriculum and learning objectives [1], [2], [3]. As a result, the United States has become increasingly out-of-date with cutting edge particle technologies and potential impacts to the economies of particle and powder-based products [1]. Additionally, the lack of formal education available often results in a shift in responsibility from the institutions to the companies and engineers to learn fundamental particle concepts through continuing education programs.

Educational tools, specifically virtual and remote tools, are one avenue for integrating fundamentals of particle science into engineering classrooms and reaching engineering professionals. While virtual and remote laboratories are not new to engineering education, there is an increasing need for these alternate methods of teaching due to decreased availability of lab time (from increased undergraduate classes) and the rise of remote higher education programs, such as remote graduate degrees and continuing education [4], [5].

In this study, we perform a scoping literature review to explore the tools and labs available to PSET educators. Specifically, we focus on virtual and remote tools that might aid in the education of continuing education students and programs with rigid curriculums that do not allow for additional lab time. We were guided by the two following research questions, *what pedagogical tools are available to educators to teach particle science*, and *what tools are available to teach remote and in person students the fundamentals of particle science?*

## **Methods**

### ***Positionality***

Adrian Nat Gentry (they/them) is both a master's student in materials engineering and a PhD candidate in engineering education, having completed their materials engineering bachelor's degree from a large R1 institution in 2020. Having experience in both materials engineering and engineering education has encouraged my interest and supported my understanding of materials engineering pedagogies. Because of the duality of my experience, I am able to determine an appropriate literature review method for this study and analyze the papers in this study from a materials engineering and educational perspective, while my co-author, Langdon, leveraged his particle science expertise to increase the rigor of the technical content.

Langdon Feltner is a PhD candidate in materials engineering, completing his bachelor's in materials engineering at a large R1 institution in 2022. My expertise is in particle science and technology and computational science, with my current research focuses on methods for building Finite Element Analysis (FEA) informed machine learning models and implementing these models in a digital twin framework. My passion for teaching and research was one of my motivations for performing this literature review, specifically using my rich understanding of particle science to add technical nuance to the analysis and discussion of the tools purpose and use.

Together, we leverage both of positionalities to analyze and disseminate this review in a way that would be of interest to both the materials engineering community and the engineering education community. Specifically, we engaged each other in reflexivity to ensure the study would be accessible to both communities.

### ***Literature Review Methods***

We utilized a combination of a systematized review and scoping review methodology to examine engineering tools available to teach particle science fundamentals. Our research questions reflected a scoping review and the querying and reviewing method reflected a systematized review, all established by Borrego et al. [6] and Grant & Booth [7]. As recommended, we utilized a similar search string when querying two databases, Inspec and Compendex, chosen through Engineering Village for its focus on engineering-based journals. Our search string used variations of the words "particle science," "tool" and "education" (see Table I). This yielded 301 full length, peer-reviewed journal and conference articles. We conducted additional "snowballing" sampling, where we directly searched for literature using well-aligned studies as a starting point. Through this process we added twelve additional papers. Once duplicates were removed (42 articles), we reviewed titles, abstracts then full articles using inclusion and exclusion criteria. The process of eligibility and inclusion is displayed in Figure 1. Following these criteria, we had 22 articles for analysis. Articles were coded based on the research questions.

To be included:

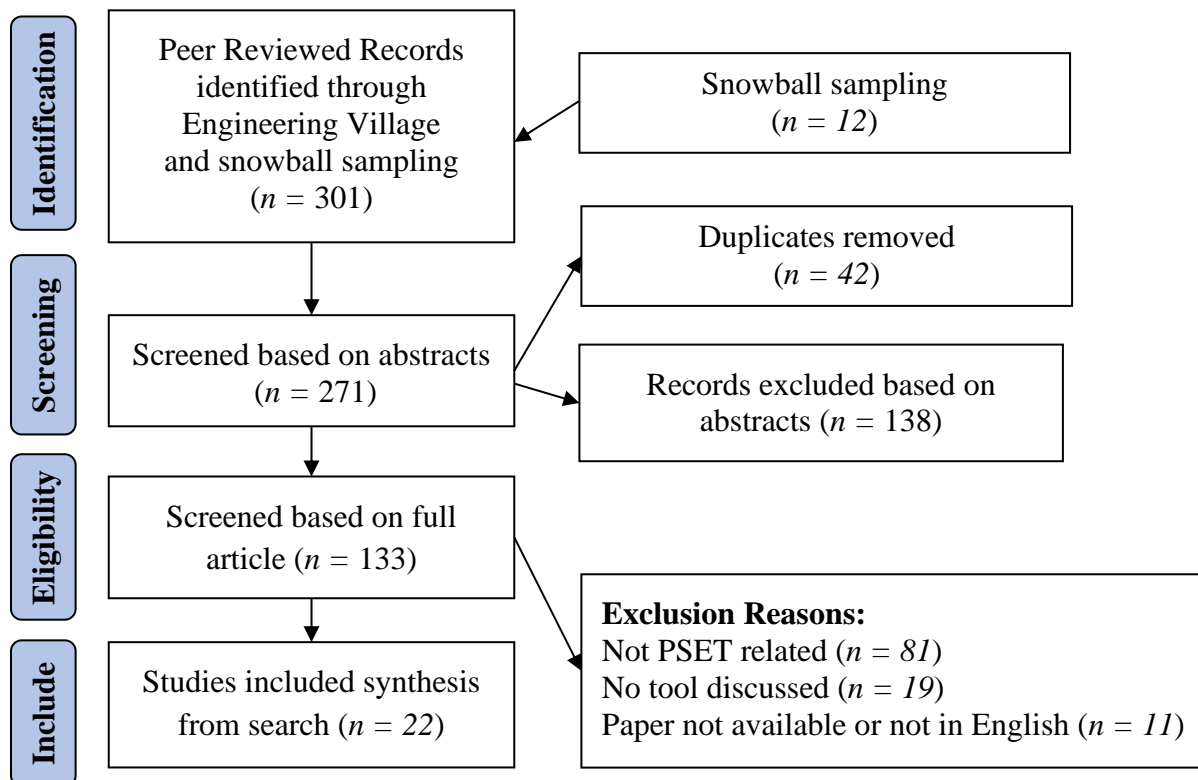
- Articles must include topics relevant to the field of particle science, engineering and technology.
- Articles must discuss a tool available for use.
- Articles must provide detail on the tool so that it can be utilized or be replicated to be used for educational purposes.

Articles were excluded if:

- No full-length paper available or paper not accessible in English.
- The tool or lab was not available or described in enough detail to replicate.

**Figure 1**

*Adaptation of the PRISMA flowchart based on Moher et al.'s [8] work on reporting items for systematic reviews.*



## Findings

Overall, the 22 articles were categorized by the fundamental of particle science covered and the pedagogical delivery method. First, each paper was categorized by the pedagogical delivery method, such as in-person, virtual and remote labs and tools. Within virtual and remote tools,

two sub-categories are used: code-based tools that rely on beginner to advanced coding skills to perform the analysis and simulation-based tools that utilize easy-to-use user interfaces to perform the analysis. Second, each paper was categorized by fundamental topics in particle science curriculum as recommended by Litster et al. [1] from their outcomes from the 2017 the International Fine Particle Research Institute (IFPRI) sponsored workshop. The curriculum overview recommended included topics such as characterization, design and analysis of particles creation, design and analysis of processing operations for formation, transport, separation and mass transfer, and synthesis and analysis of flowsheet for manufacture using simulations and models [1, p. 147].

### *Tools available for continuing education and in-person students*

Table 1 provides an overview of the virtual, remote and in person labs and tools introduced the articles.

**Table 1**

*Overview of pedagogical modes of PSET tools.*

<b>Type of lab/tool</b>	<b>Definition</b>	<b>Citations</b>
<b>Code-based tools (7)</b>	<i>Virtual lab that requires coding knowledge, may contain user interface-based design</i>	Casas-Orozco et al., 2021; Goicochea et al., 2015; Jha et al., 2021; Kozicki & Donze, 2009; Skorych et al., 2020; Weinhart et al., 2020; Windows-Yule et al., 2023
<b>User interface-based tools (8)</b>	<i>Virtual lab that has easy-to-use user interface-based design, little to no coding skills needed</i>	Adler et al., 2018; Dosta & Skorych, 2020; Hartge et al., 2006; Kozicki & Donze, 2009; Rodríguez et al., 2019; Skorych et al., 2020; Tassieri et al., 2016; Wagner & Huang, 2021
<b>Remote labs (2)</b>	<i>Labs that utilize automated or robotic equipment</i>	Frerich et al., 2014; Kruse et al., 2016*
<b>Virtual Reality tool (1)</b>	<i>Virtual lab that uses augmented reality through accessing devices</i>	Trentsios et al., 2020
<b>In-person labs (7)</b>	<i>Labs that have in-person elements</i>	Dave et al., 1997; Durak et al., 2023; Jacobson et al., 2008; Reynolds et al., 2019*; Rodríguez et al., 2019; Scholz et al., 2016; van Wie et al., 2021*

\* Some papers queried discussed the same tool. Papers covering a duplicate tool were kept in the analysis to represent changes to the tool over time.

### *Virtual tools*

The most common tool found was virtual user-interface-based and code-based tools (15 articles). Nearly all the user-interface and code-based tools performed 3D discrete particle mechanics simulations (e.g., agglomeration, segregation, mixing and breakage) or processing flow sheet analyses.

Eight articles featured virtual *user interface-based* tools, that required no to very little coding experience in order to run simulations [9] - [16]. Three of the user interface-based tools require knowledge of downloading software using command lines, however thorough instructions on implementing these tools were provided [9], [13], [14]. Two tools, Wagner & Huang [16] and Adler et al. [15], were no longer available on the web, however instructions of how the tools were made and the corresponding learning objectives are documented in the articles.

Seven articles featured *code-based* tools, requiring varying levels of C++ and Python coding knowledge. Based on the coding language required, the tools found ranged in difficulty of implementation—where some programs provide beginner level coding modules and others provide in-depth, lengthy code to model complex simulations [13], [14], [17] – [22]. Solvers, found in three articles, are generally written in low-level compiled languages, such as C++, to optimize the computational efficiency of the program. Languages like C++ are more challenging for beginners since they are statically typed and have a difficult to read syntax. Many low-level tools are written with an object-oriented organization strategy, making contributing and changing the code approachable for intermediate level users. On the one hand, work by Jha et al. [17] and Goicochea et al. [18] required extensive coding knowledge. While not any less valuable, these coding tools may be more suitable for upper-level undergraduate and graduate level students. On the other hand, some tools aim to reduce barriers to entry; for example, work by Weinhart et al. [19] provided comprehensive, easy to follow documentation for projects with differing level of difficulty (i.e., simulation/code complexity).

One strategy to develop beginner friendly tools is to use object-oriented coding and a high-level interface to interact with a low-level program, seen in Windows-Yule et al. [20] and Casas-Orozco et al., 2021 [21]. Utilizing Python to pass commands to LAMMPS greatly reduced the complexity and allows the user to focus on the problem they are simulating rather than syntax. Python's advantages include dynamic types (i.e., the Python interpreter will automatically cast data into the correct type as it passes into a function), a readable code structure that makes the language approachable for beginners, and libraries of pre-built functions for common tasks, at the expense of computational efficiency. Pharma-Py [21] is an example of a tool built entirely in Python. Lastly, two articles, Kozicki & Donze [13] and Skorych et al. [14], provided the option of utilizing a user-interfaces or coding; specifically, the programs provided pre-established simulations and analysis or the opportunity to adapt provided modules for the users specific needs.

### *Remote and virtual reality labs*

Two articles proposed a remote laboratory, located at Ruhr-University Bochum in Germany, available for educational purposes. As described by the articles, Frerich et al. [22] and Kruse et

al. [23], users can check out the lab equipment, live stream the experiment, perform analysis on a LabVIEW interface controlling the equipment, and learn through provided educational modules. The BEETbox and iLab project, in the past referred to as the ELLI (excellent teaching and learning in engineering) project, has remote labs available for performing flow measurement through flowsheet analyses in addition to rotary draw bending, tensile testing, and sheet metal testing.

Additionally, one article, Trentsios et al. [24], proposed a virtual reality flow measurement tool to be used in conjunction with Beetbox's remote lab—specifically designed for educational purposes. The proposed virtual reality tool includes a model of the flow measurement equipment that students can virtually “move around” and interact with while they perform their experiments. Accomplishing this level of integration between the remote lab equipment, the LabVIEW software, and the virtual reality is truly impressive.

### *In person labs*

Seven articles featured in person labs developed for entire particle science courses or low-cost laboratory equipment for a single lab. Three articles, Durak et al. [25], Reynolds et al. [26], and van Wie et al. [27], described the development and implementation of “low-cost desktop modules,” including a fluidized bed module. Scholz et al. [28] described the development of a Mie scattering lab using 3D printed and programmed equipment developed for less than one-hundred dollars (probably more in 2024!). Three articles, Dave et al. [20], Jacobson et al. [30] and Rodríguez et al. [11], provided an overview for a real and/or hypothesized particle and powder science course including labs. Rodríguez et al. [11] proposed a course structure, including virtual and in person labs, that have been specifically designed to engage Generation Z students. Proposed virtual labs include the use of Aspen Solids, previously SolidSim, a flow sheet analysis program. Dave et al. [29] and Jacobson et al. [30] proposed labs that require a large amount of specialized equipment, which is less feasible for most educators.

### *Fundamental tools to teach particle science*

Fundamental particle science categories were based on recommendations for curriculum by Litster et al. [1] from the 2017 the International Fine Particle Research Institute (IFPRI) sponsored workshop. Tools on the left side of Figure 2 (i.e., modeling particles and characterization) are best for teaching fundamental physics topics that model particle-particle interactions. Tools on the right side of Figure 2 (i.e., modeling powder flow and flow measurement) are useful for teaching process dynamics as these tools focus on large scale processes.

### *Modeling: Particles*

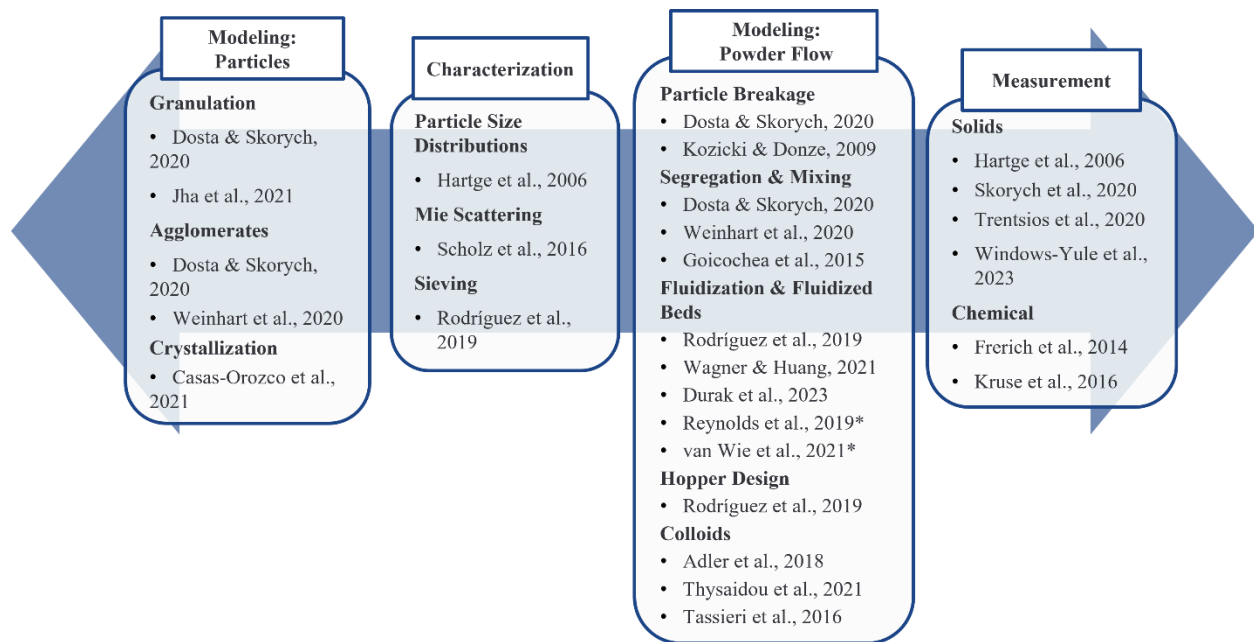
Four articles, Jha et al. [17], Weinhart et al. [19], Casas-Orozco et al. [21] and Dosta & Skorych [9], proposed tools to model the process of making particles and powders, specifically crystallization, granulation and agglomeration. Jha et al. [17] proposed the tool “PeriDEM,” capable of simulating particle-particle and particle-wall breakage of particles of various shapes (e.g., non-sphere). MercuryDPM, a DEM simulation for modeling granular phenomena by

Weinhart et al. [19], can simulate deformable or breakable particle agglomerates. Pharma-py [21] is a Python based population balance model (PBM) tool for designed for industrial-scale simulation of pharmaceutical processes. Population balance models set up and solve a set of differential equations that track the state and locations of particles within a system over time, allowing for users to see the process scale effects of changing the operations of individual steps.

One tool, MUSEN, may be of particular interest to educators. MUSEN, by Dosta & Skorych [9], is an open-source framework for DEM simulations with an intuitive user interface. The discrete element method is an essential tool for particle science and technology education, as it allows users to visualize the dynamics of discrete particle systems by explicitly simulating them. DEM solvers perform a momentum update loop over a short time step for large numbers of particles and can handle both surface and body force computations. The flexibility of the DEM approach, coupled with a natural scale independence, make DEM a tool of choice for studies ranging from atomic to industrial scale. Unlike other open source DEM tools (e.g., LAAMPS by Thompson et al. [31]), MUSEN has an intuitive GUI, such that novice users can investigate critical physics of particle systems, varying initial conditions and visualizing the effect on the outcome, all for free within the MUSEN application.

**Figure 2**

*Overview of articles covering fundamental topics in particle science.*



### *Characterizing particles and powders*

Three articles discuss tools capable of characterizing particle and powder size. Hartge et al. [10] introduced SolidSim, now a part of Aspen Solids, as a tool to teach flow analysis with respect to particle size distributions. SolidSim was an opensource flow sheet software developed specifically for solving problems in solid particle processing. SolidSim contained pre-built



modules for classification, size reduction, crystallization, phase separation, and agglomeration among others. To do this, SolidSim utilized an equation-oriented approach that allows for multiple subprocesses to be efficiently simulated in series and in parallel and offers a friendly user interface. While SolidSim offered these features to users in an open-source software, Aspen Solids may provide additional features in their license. Rodríguez et al. [11] provided multiple labs capable of teaching characterization, such as a sieving lab using brown sugar, performing shape analysis from images and a flow process lab using Aspen Solids. Scholz et al. [28] developed a low-cost Mie scattering device, capable of determining particle size in dilute monodisperse colloidal suspensions.

#### *Modeling: Powder flow*

Twelve articles proposed tools that could be used model powder flow phenomena (i.e., process dynamics) such as particle breakage, segregation and mixing, fluidized beds, hopper design, and colloids. Dosta & Skorych [9], Kozicki & Donze [13] and Weinhart et al. [19] presented DEM models capable of simulating particle-particle interactions, specifically for modeling breakage and deformation. Kozicki & Donze [13] proposes the tool “YADE,” which can be used to model particle-particle dry flow, deformation, and compaction. Peri-DEM, by Jha et al. [17], and YADE were developed in an object-oriented framework that can make development of the code more approachable for users with intermediate coding skills and an interest in learning the fundamentals of particle sciences.

As part of an International Fine Particle Research Institute sponsored study to determine how DEM is used within industry and national laboratories, Windows-Yule et al. [32] developed a set of digital twin models for the popular “Granutools” set of particle flow measurement instruments. Digital twin models are simulations meant to recreate a physical process or experiment. In this case, Granutools are designed to characterize flow and packing behaviors of particle systems. Based on model building insights from industry experts and experimental measurements from positron emission particle tracking, the digital twin models are built using LAMMPS and have a Python interface that streamlines simulation setup, submission, and data reduction. These are great educational tools since Granutools instruments are built to study the basic physics of flow of particle systems. The Python interface allows for the details of the simulation, such as particle size, orifice size, cohesion between particles, etc., to be tweaked and its effect quickly observed.

Four papers discussed colloids as a part of particle science, engineering and technology. i-Rheo, a web-based and code-based tool for modeling complex shear modulus of materials by Tassieri et al. [12], can be used to model the rheology of highly concentrated suspensions of colloidal particles. Adler et al. [15] proposes a theoretical model for colloidal behavior in liquid crystals, and Thysiadou et al. [33] proposes a course on simple colloids in an interactive learning management system. Goicochea et al. [18] proposes a DPD model to simulate the viscosity and rheology of colloid dispersions. DPD (dissipative particle dynamics) tools proposed by Goicochea et al. [18] are capable of simulating particle-particle and colloidal interactions including segregation and mixing. Dissipative particle dynamics differ from DEM approaches by including a dissipative force, effectively adding a viscous effect. For this reason, DPD methods are popular when investigating suspensions and can be coupled with other solvers, DEM for example, to model viscous fluid phases in multiphase systems.

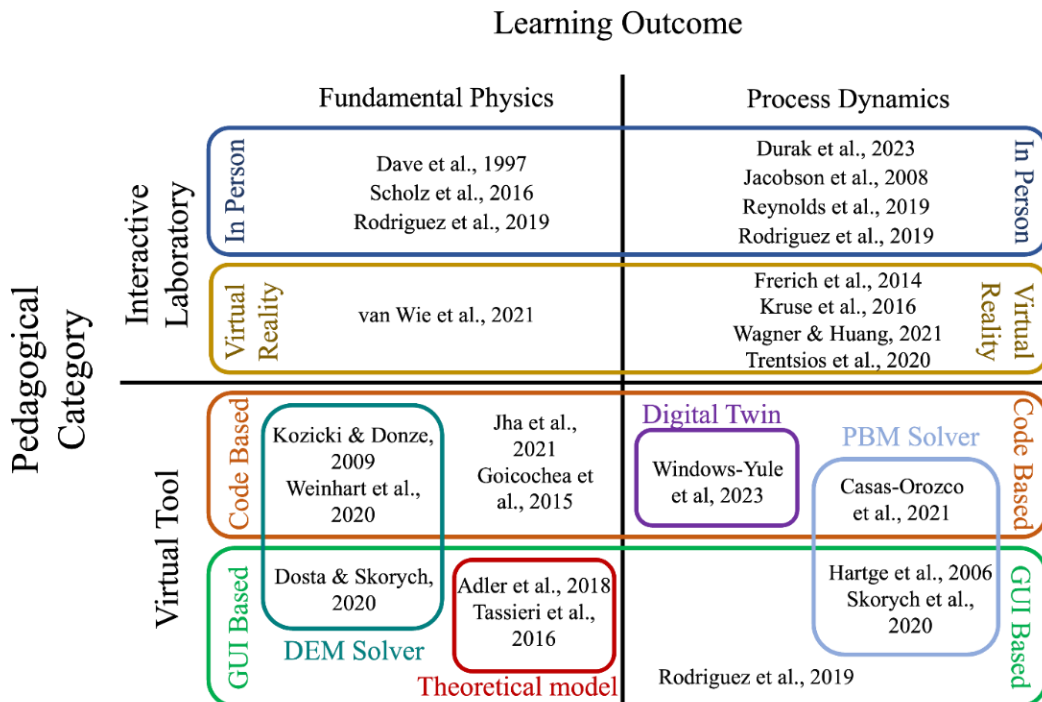
Five articles proposed tools for teaching fundamental processing concepts, such as fluidized beds and fluidization velocity. While these tools and labs do not specifically use particles or powders, the labs conceptually teach the purpose of and utilization of fluidized beds. Three of the articles proposed a low-cost desktop module for teaching fluidized beds, Durak et al. [25], Reynolds et al. [26], van Wie et al. [27], Rodríguez et al. [11] conceptualized a fluidization velocity in a fluidized bed. Wagner & Huang [16] proposed a tool for modeling fluidized bed data, including a model for experimental data and the Ergun equation. Lastly, Rodriguez proposed labs to teach students about hopper design [11].

*Flow Measurement*

Five articles, Hartge et al. [10], Frerich et al. [22], Kruse et al. [23], Trentsios et al. [24], and Skorych et al. [14], propose virtual and remote tools for performing flow analysis using interactive flowsheets. Skorych et al. [14] present Dyssol, an open-source process flowsheet software with a well-developed user-interface capable of modeling complex, multistep industrial processes. In Dyssol, the user provides physical information about the materials and subprocesses at play, (e.g., particle size, moisture content, and mass fraction of the initial particles). The user can define the set of processes that can occur in series and in parallel and each one's time-dependent effect on the product. Dyssol sets up and solves a population balance model for each of the subprocesses by solving a differential equation that describes the process dynamics. The state of all mass in the system is continually tracked and updated on short time increments. Finally, based on the findings from the study, we present an overview of the pedagogical and fundamental concepts discussed in the review (Figure 3).

**Figure 3**

*Overview of the pedagogical and fundamental concepts covered by each tool.*



## Conclusion

This scoping literature review queried two engineering specific databases to find tools available for teaching in person and continuing education students the fundamentals of particle science, engineering and technology. Findings include multiple code-based, user interface-based and remote tools on fundamental topics in particle science (e.g., characterization, aggregation, particle flow and flow measurement process sheets available) for educators to utilize in their chemical and material engineering courses (Figure 3).

As authors, we propose a guide for PSET educators to selecting in-person and remote tools from three main fundamental categories: fundamental physics (e.g., discrete particle interactions), process dynamics (e.g., effects on bulk powders), and the type of model used (e.g., digital twin and population balance model). We categorized our tools based on the fundamental concept that could be most easily aligned with pre-existing learning objectives. For example, a learning objective that includes identifying inter-particle forces (e.g., Coulombic and van der Waals forces) could be taught using tools that model discrete particle interactions from the *fundamental physics* section. Educators should select tools from this list based on the difficulty of implementation in their course and appropriate challenge-level for their students. Limitations of this work, like all qualitative work, stem from the researcher as the instrument. One author is new to the field of particle science and analyzed the content and difficulty of implementation based on articles and tool webpages (e.g., GitHub). Future work could include a case study of implementing various tools into current materials and chemical engineering curriculum.

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