Powder Technology

Elsevier Publications
Editorial Team: L.S. Fan, A.B. Yu, C. Wu, A. Teleki, P. Mort
Interim Publisher: N. Lee
Publishing Director: C. Greenwell

P. Mort (IFPRI-Elsevier Liaison)

IFPRI 40th Annual Meeting, June 2018

Powder Technology, Journal Statistics

- Impact factor and cite scores are in top quartile of peer engineering journals.

- Manuscript submissions continue to increase
  - China leads in submissions and accepted articles.

- Rejection rate ~70%
  - Overall >50% desk rejection.

- Papers from IFPRI associates are among most highly downloaded from Powder Technology:
  - U. Zafar, V. Vivacqua, G. Calvert, M. Ghadiri, J.A.S. Cleaver, "A review of bulk powder caking," 2017.
  - He Y., Bayly A.E., Hassanpour A., "Coupling CFD-DEM with dynamic meshing: A new approach for fluid-structure interaction in particle-fluid flows," 2018.
  - Pitt K., Pena R., Tew J.D., Pal K., Smith R., Nagy Z.K., Litster J.D., "Particle design via spherical agglomeration: A critical review of controlling parameters, rate processes and modelling," 2018.
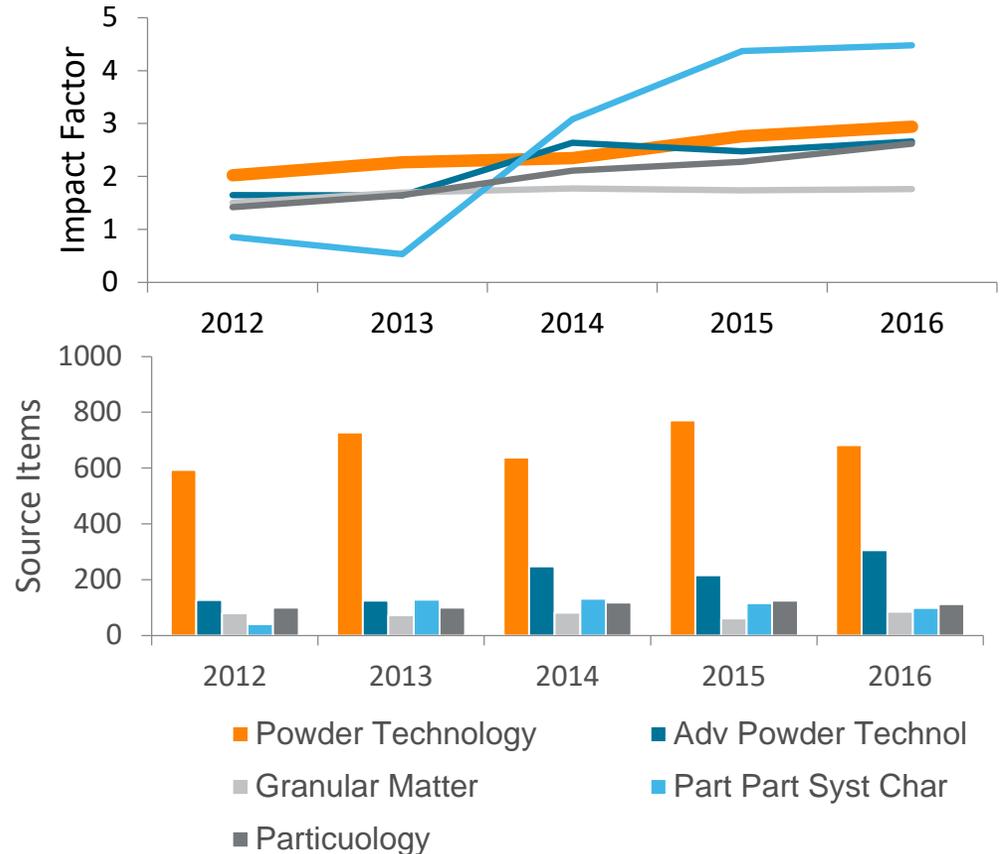
Topic: How to make Powder Technology more accessible to associate members?
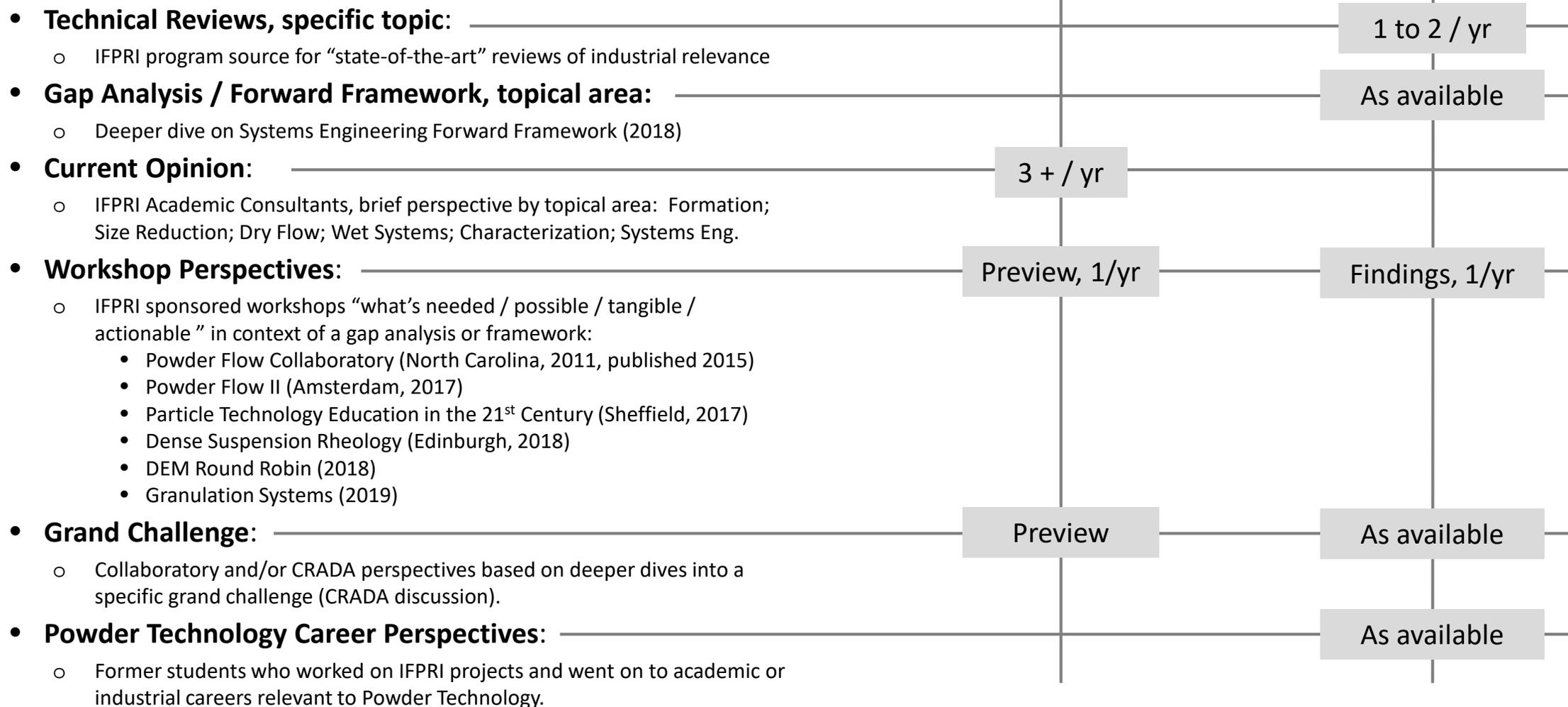
IFPRI Perspective Pipeline

Support Powder Technology's Impact with a steady stream of relevant and novel perspectives. ⟷ *Build awareness and influence of IFPRI.*

Short Communication (Perspective Brief)
About 4 pages, reporting a result likely of impact on future research; may be prescient to a planned workshop or grand challenge activity.

Review (Full Perspective)
About 10-12 pages, providing an overview of a research topic or relevant technique, with outlook and discussion of challenges and opportunities.

- **Technical Reviews, specific topic**:
  - IFPRI program source for "state-of-the-art" reviews of industrial relevance

  1 to 2 / yr

- **Gap Analysis / Forward Framework, topical area:**
  - Deeper dive on Systems Engineering Forward Framework (2018)

  As available

- **Current Opinion**:
  - IFPRI Academic Consultants, brief perspective by topical area: Formation; Size Reduction; Dry Flow; Wet Systems; Characterization; Systems Eng.

  3 + / yr

- **Workshop Perspectives**:
  - IFPRI sponsored workshops "what's needed / possible / tangible / actionable " in context of a gap analysis or framework:
    - Powder Flow Collaboratory (North Carolina, 2011, published 2015)
    - Powder Flow II (Amsterdam, 2017)
    - Particle Technology Education in the 21st Century (Sheffield, 2017)
    - Dense Suspension Rheology (Edinburgh, 2018)
    - DEM Round Robin (2018)
    - Granulation Systems (2019)

  Preview, 1/yr — *Findings, 1/yr*

- **Grand Challenge**:
  - Collaboratory and/or CRADA perspectives based on deeper dives into a specific grand challenge (CRADA discussion).

  Preview — *As available*

- **Powder Technology Career Perspectives**:
  - Former students who worked on IFPRI projects and went on to academic or industrial careers relevant to Powder Technology.

  As available

CRADA Discussion Summary

P. Mort (IFPRI-Elsevier Liaison), J. Lechman (Sandia)

IFPRI 40th Annual Meeting, June 2018

IFPRI CRADA –

Transitioning the conversation from possibility to formulation

CRADA = Cooperative Research and Development Agreement

US Federal Technology Transfer Act of 1986 established means to form CRADA's between a US National Lab, Institute, Department and/or Agency, and:

- Industrial organizations (including corporations, schools and partnerships, and limited partnerships, and industrial development organizations);
- Public and private foundations;
- Nonprofit organizations, including universities.
- Special consideration to small business firms, and consortia involving small business firms.

Some models for IFPRI CRADA's:

1. **Collaborative supplement** to an IFPRI project or group of projects:
   - IFPRI Collaboration Grant to one or more PI's enables their engagement w/ National Lab.
   - National Lab contributes research equity and shares in the PI's research output.
   - Enables IFPRI PI['s] to go deeper w/ National Lab resources.

2. **"Jump-start"** a project of common interest to IFPRI and a National Lab:
   - IFPRI Collaboration Grant to one or more prospective PI's to engage in an exploratory CRADA with the National Lab.
   - Develop a detailed study plan, supplemented w/ National Lab resources.
   - Next step option for IFPRI to fund as a full project (e.g., graduate to model #1).

3. **LDRD + IFPRI:** Link an IFPRI project with the Sandia National Laboratory Directed Research & Development (LDRD) program. This brings additional funding and resources from Sandia.
   - Combination of IFPRI and LDRD resources can be substantial.
   - Enables broader and/or deeper scope.
   - Sandia LDRD's are focused on their Academic Alliance Universities (New Mexico, Illinois, Purdue, Texas, Georgia Tech).

4. **Multi-party** CRADA's aimed at a substantial technical challenge (e.g., a Grand Challenge) requiring substantially greater resources:

   a. A sub-set of interested IFPRI companies pool supplemental company resources toward a specific CRADA topic, with additional matching funds from the National Lab.

   b. IFPRI joins with other entities (e.g., external companies, foundations, working parties, etc.), each entity providing funds to a study a specific CRADA topic, with additional matching funds from the National Lab.

What's next?

Transitioning the conversation from formulation to action.

CRADA models:

- Collaborative supplement
- Jump start
- LDRD link
- Multi-party Grand Challenge

× IFPRI:

- Full project
- Collaboration
- New brief

→

Some ideas to consider (climbing a tree w/ Jeremy & Paul)…

1) Collaborative Supplements and/or Jump Starts in Dry Powder Flow, extending current and/or proposed dry powder flow project[s]:
    - Develop rheology models accounting for effects of *fluctuations* in flow and stress fields, in both bulk and boundary layer conditions, e.g., a statistical physics approach.
    - Characterize boundary-layer *fluctuations* of critical interest for a range of forming processes and types of materials. Focus areas:
        - Particulate materials processing science for high-consequence, small-lot precision manufacturing (e.g., Additive Mfg.);
        - Process-structure-property relations and their relationship to variability in heterogeneous particulate materials (e.g., energetic or energy-storage materials).

2) LDRD Link w/Sandia proposal on computer-aided design and optimization of Compaction/Tableting processes. Elements include:
    - Enabling deformable particles (including yield/fracture/ fragmentation) within DEM.
    - Explore solving the inverse problem to optimize a desired property of the compact.

3) "Jump-start" IFPRI Systems Engineering, exploring tools for process-structure-function integration, especially in ways that facilitate inverse solutions (i.e., specifying structure and process models based on functional performance requirements).
    a. Do we have sufficient models to solve inverse problems, i.e., for a desired product performance, what must be true of product structure, processing, and materials used in that process? Are solutions amenable to multi-objective optimization?
    b. Describe many-to-many relations between blocks in figure below, e.g., mapping relations among processes, materials and achievable structures or specifications.

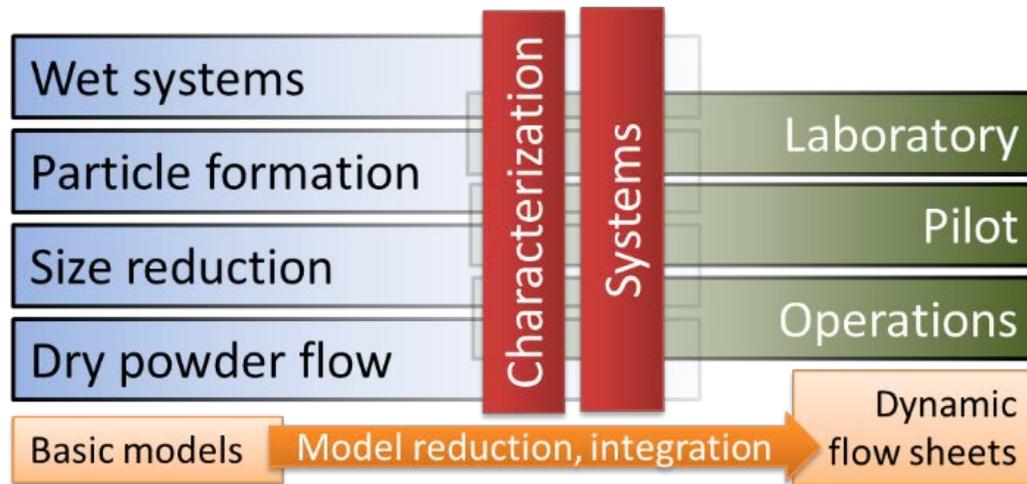| Raw materials | Particulate Processes | Product structures (particle specs) | Product function (performance) |

Systems Engineering Forward Framework

P. Mort (IFPRI-Elsevier Liaison), S. Watano (Osaka Prefecture Univ), Z. Nagy (Purdue Univ)

IFPRI 40th Annual Meeting, June 2018

IFPRI SE: Context

IFPRI perspective diagram on Systems as a means to integrate other focus areas (Van der Voort Maarschalk, Bermingham, Diemer and Mort, IFPRI 2015 AGM)

- Systems Engineering (SE) was added to the IFPRI program structure in 2015.

- SE integrates modeling and operational control frameworks over processes that encompass elements from other IFPRI focus areas.

- Models are inherent to the systems approach. Ideally, basic models developed in conjunction with IFPRI projects are translatable to dynamic flowsheets that are useful for process integration, control and optimization.

IFPRI within broader SE Context*

SE Transformation Metrics, (3 E's)	IFPRI Perspective, Particle Technology
• **Efficacy**: is the system producing the desired result?	Assess pre-competitive tools for Product Quality, Process Systems Integration and Optimization.
• **Efficiency**: is the system using the minimum of resources relative to the output produced?	Identify and develop fundamental capabilities needed to enable "Hard Systems" approach. **A**
• **Effectiveness**: is the system doing the right thing - contributing to higher-level industry-wide or societal goals?	Consider post-competitive IFPRI purposes relevant to higher order systems, e.g., sustainability, safety, life-cycle analyses. **B**

Consider…

A. Consistent with the original IFPRI Gap Analysis brief, identification of gaps in sensor, process actuation and/or modeling can be useful to the goal of enabling Hard System Methodologies.

   Can IFPRI better utilize Soft System Methods to identify new opportunities, e.g., for identifying and spanning said gaps?

B. Going forward, should IFPRI focus only on *pre-competitive* content at the SE base-level, or extend scope to appropriate *post-competitive* topics (e.g., safety, sustainability, LCA) at higher SE levels?

SE Levels:

1. Process systems engineering, control and optimization – focus on technology integration: sensors, actuators, control models, etc.

2. Project systems -- Product systems engineering with cross-discipline and human integration.

3. Business systems – Enterprise systems engineering, service systems engineering, continuous improvement and quality management for business operations.

4. Industry systems – Long-term economic and environmental sustainability of an overall industry.

5. Societal systems – Analysis and improvement of associated societal issues.

SE Methodologies:

• Hard System Methods – means to achieve a well-defined and agreed objective; complex yet are solvable using available SE tools.

• Soft System Methods – interactive and participatory approaches to assist diverse participants to alleviate a complex, problematic situation of common interest; rather than guaranteeing a solution to a problem, SSM provides a systematic way of organizing and exploring complex problems as learning systems.

• Critical Thinking – combination of hard and soft approaches applied situationally.

SE Transformation Metrics: Efficacy, Efficiency, Effectiveness.

Two IFPRI SE frameworks…

Particulate Products and Processes

- Particulate products have distributed characteristics, e.g., particle size, shape, composition, porosity or other structural attributes.

- Efficacy (quality, performance) of products comprising particulates depends on these characteristics and structural attributes.

- Efficient processes are required to transform raw materials into particulates to meet specifications.

- Consider tools for process/structure/performance integration, especially in ways that enable inverse solutions.

- Describe many-to-many relations between blocks in figure below, e.g., mapping relations among processes, materials and achievable structures or specifications.

```
Raw        →  Particulate  →  Product structures  →  Product function
materials      Processes       (particle specs)       (performance)
```

Process System Integration

- Process flowsheet models are useful for development and execution of control and optimization.
  - Flowsheet modules (e.g., unit ops) are connected with material streams having distributed attributes.
  - Specification of attributes is important to quality.

- In practice, issues with startup, reliability, operating efficiency, and throughput capacity are often traced to solids handling problems (build-up, plugging, uneven flow, etc.). Handling issues may be compounded with recycle streams.

- Are transport and handling models sufficiently developed relative to consequential process efficiency, reliability, etc.? Are such models sufficient for use in flowsheets?

- Recognizing cost, operational and quality implications of solids handling, consider how advances in unit operations and close-coupled integration thereof can be advantageous:
  - What are the priorities for advancing unit operations with control capability for multiple transformations?
  - How can measurement and modeling of internal (unit-op) solids flow and stress fields promote and enable such developments?

Case Study: Process systems engineering in pharmaceutical industry

QbD (Quality by Design) embeds quality attributes in the initial product design along with quality risk assessments and lifecycle analyses. Steps include:
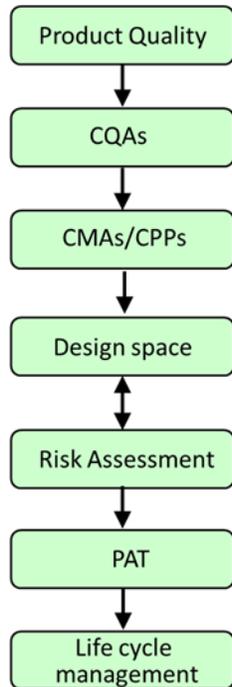
1) Define product quality target profile (QTPP) based on the clinical performance and identify the critical quality attributes (CQAs) of the drug products;
2) Identify critical material attributes (CMAs) and critical process parameters (CPPs) based on the process design and experiments;
3) Develop a design space which links CMAs and CPPs to CQA;
4) Conduct risk assessment for better design space;
5) Design and implement a control strategy using PAT (Process Analytical Technology) and design of experiments (DoEs);
6) Conduct product life cycle management including continual improvement.

More recently, QbC (Quality by Control) uses closed-loop (feedback) control approaches to determine operating trajectories.

With suitable closed-loop control approaches, process disturbances can be reduced, increasing the applicable design space.

Systems Engineering (SE) is essential in the development of pharmaceutical QbD and QbC, including instrumentation of on-line monitoring and process control.

Cost and time required to obtain design space data can be significantly reduced by using smaller-scale laboratory experiments provided one has:

a) mechanistic understanding of critical quality attributes (CQAs); and
b) modeling technologies for predictive scale-up.
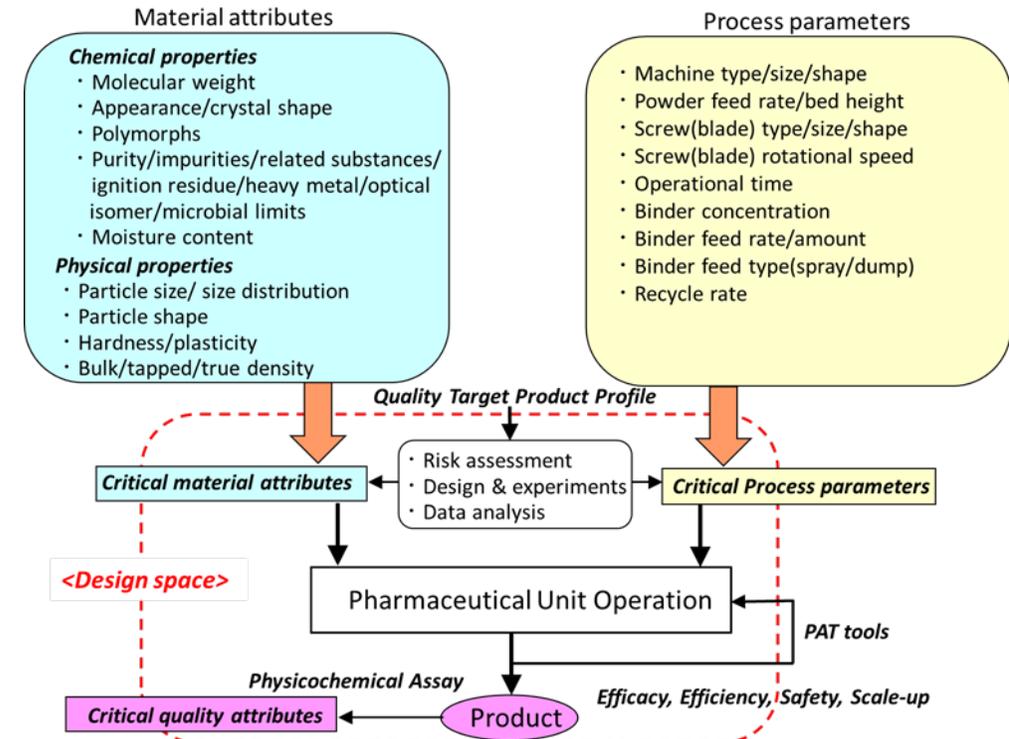
Conclusion

- IFPRI Systems Engineering started as a means collaborate across subject areas; consider using SE to extend to other organizations of complementary interest.
  - Granulation Systems Workshop, PARTEC 2019, Agreement to coordinate between IFPRI and the Working Party on Agglomeration of European Federation of Chemical Engineering (EFCE).
- CRADA's can extend depth and breath of IFPRI projects.
  - Consider using LDRD and Multi-Party options toward Grand Challenges.
- Powder Technology pipeline – IFPRI has opportunity to extend influence and create vision for the future.