

Multiscale Modelling of a Twin Screw Granulator



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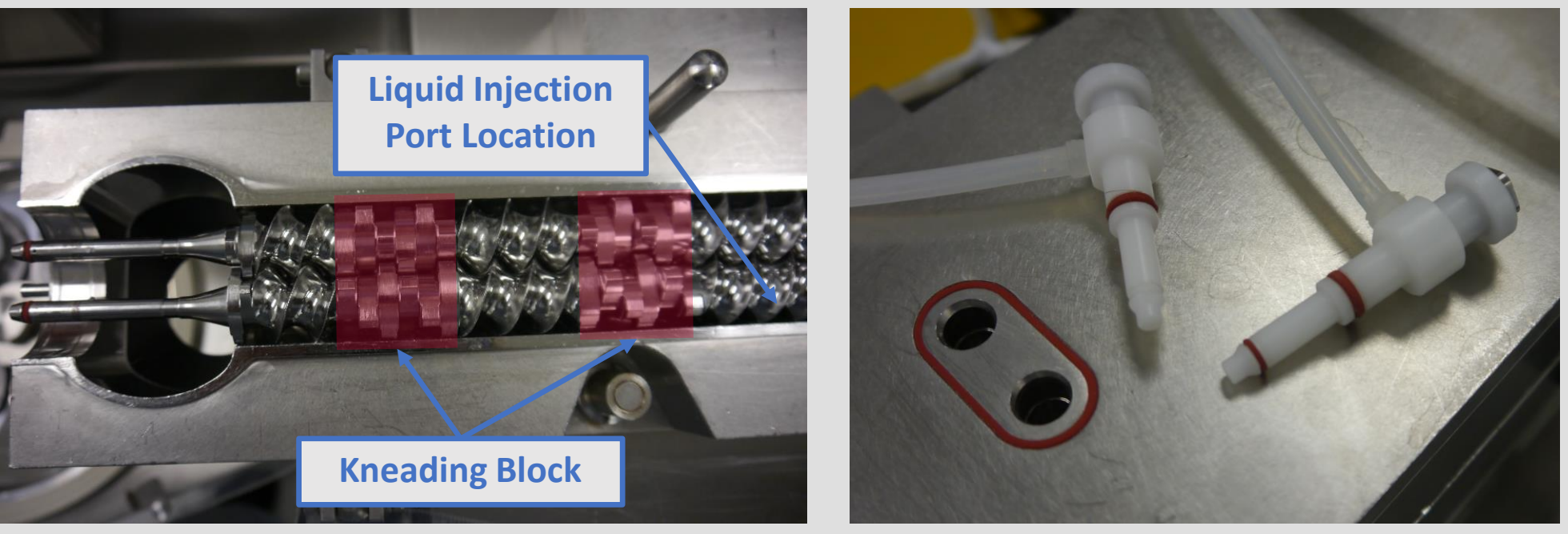
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Case study - Twin Screw Granulation

Wet granulation is a process used to create larger stable agglomerates (granules) from fine powders. However, despite wide adoption, it is often **inefficiently operated**, with **high recycle ratios** in continuous processes and **high rejection rates** in batch processes.

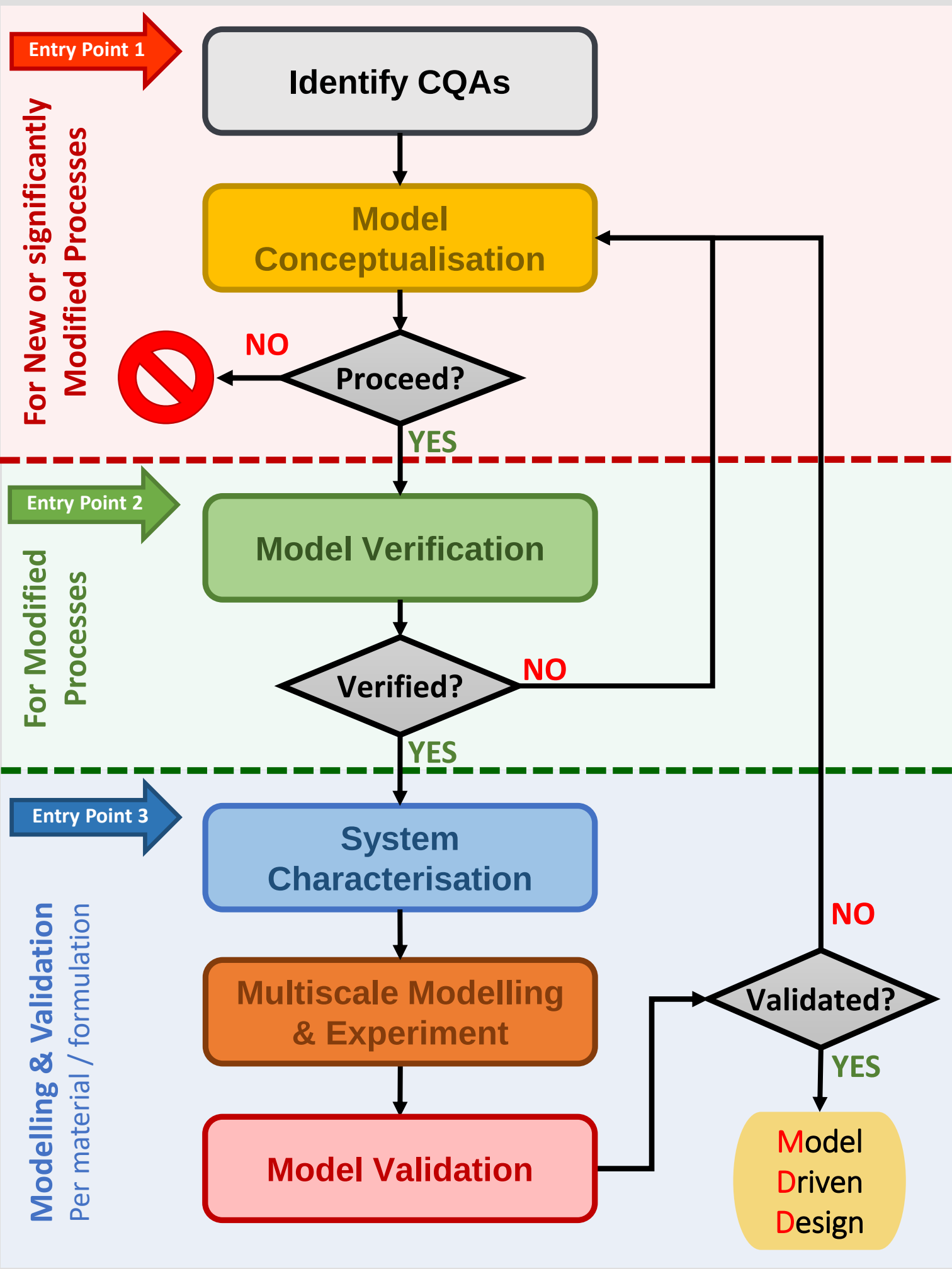
This numerical study simulates a **GEA ConsiGma™ 1** Twin Screw Granulator (**TSG**), following a standard framework for model-driven design.



Generic Framework for Model Driven Design

A **generic framework** for translating particle models of industrial relevance into industrial practice:

- Significant input from industry to inform the work flow
- **Structured** process for **conceptualising**, **characterisation** and **modelling** of large scale industrial processes
- **Decision support tool** for commercial exploitation

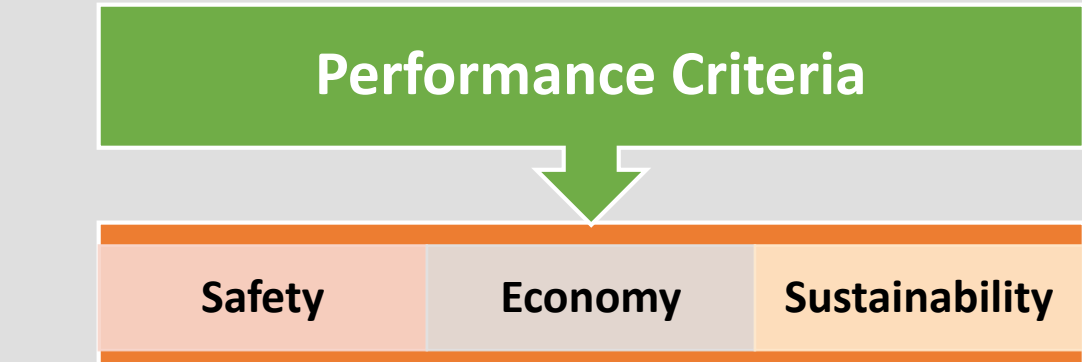


The proposed framework provides a platform for both:

- **Developing best practice** in model driven design
- **Progressively replacing empiricism** in particle based models

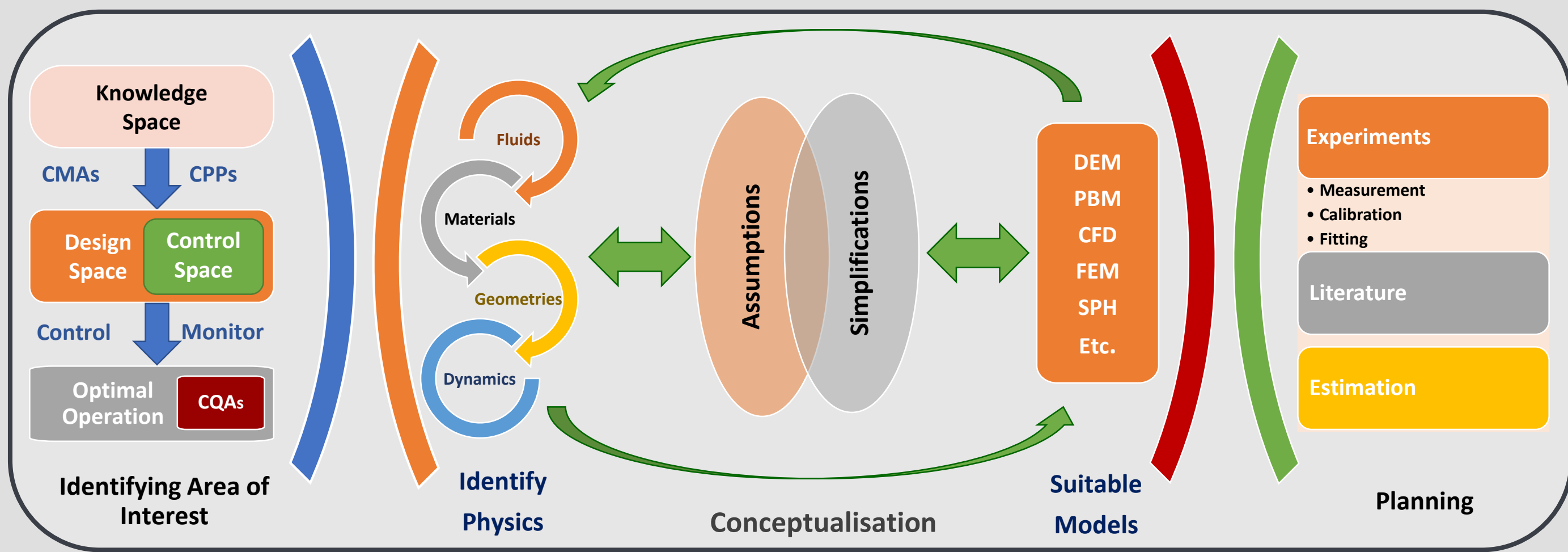
Defining the computational model requires **knowledge and understanding** of the system being studied.

The **Critical Quality Attributes (CQAs)** are the quality attributes to ensure product quality. They inform the product and process development.



Granule size distribution and **granule porosity** are granulation CQAs for TSG.

1. Defining the Model



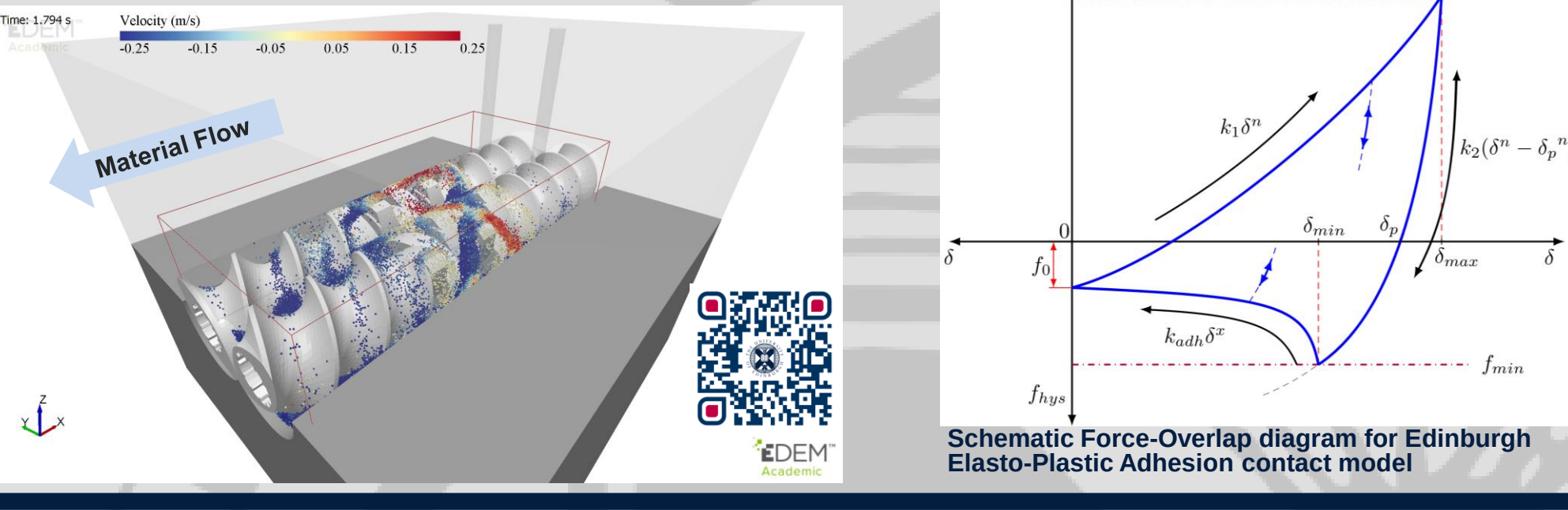
- What are the **key physics** for the **intended purpose**?
- Are current models **fit for purpose**?
- What are **reasonable** assumption/simplifications that could be made in these models?

The process may lead to **new physics** (models) being implemented or developed if **existing models** are deemed **unsatisfactory or lacking**.

2. Defined Model

A compartment-based **DEM-PBM** model is developed where the **residence time τ** is obtained from **DEM** with the following PBM assumptions:

- That material only flows in one direction
- The inlet flow rates are equal to the outlet flow rates of the previous compartments
- Kernels are chosen for each compartment based on the assumed phenomena occurring within

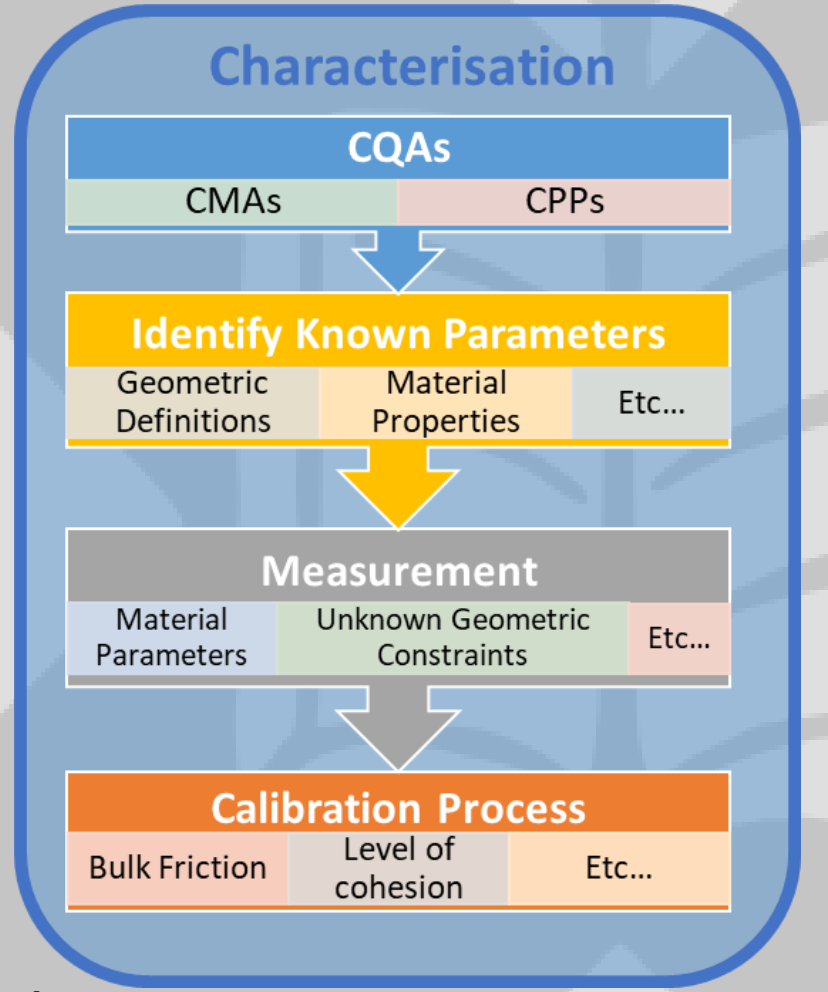


4. System Characterisation

Using the **CQAs** and the identified **CMA**s and **CPP**s the range of operating conditions and, thus, the likely parameter range can be identified.

Unknown parameters (e.g. cohesion) can be **measured** or **calibrated** from experiments.

Experiments used to **derive** model input parameters **CANNOT** be later used to **Validate** the model.



3. Multiscale Model Verification

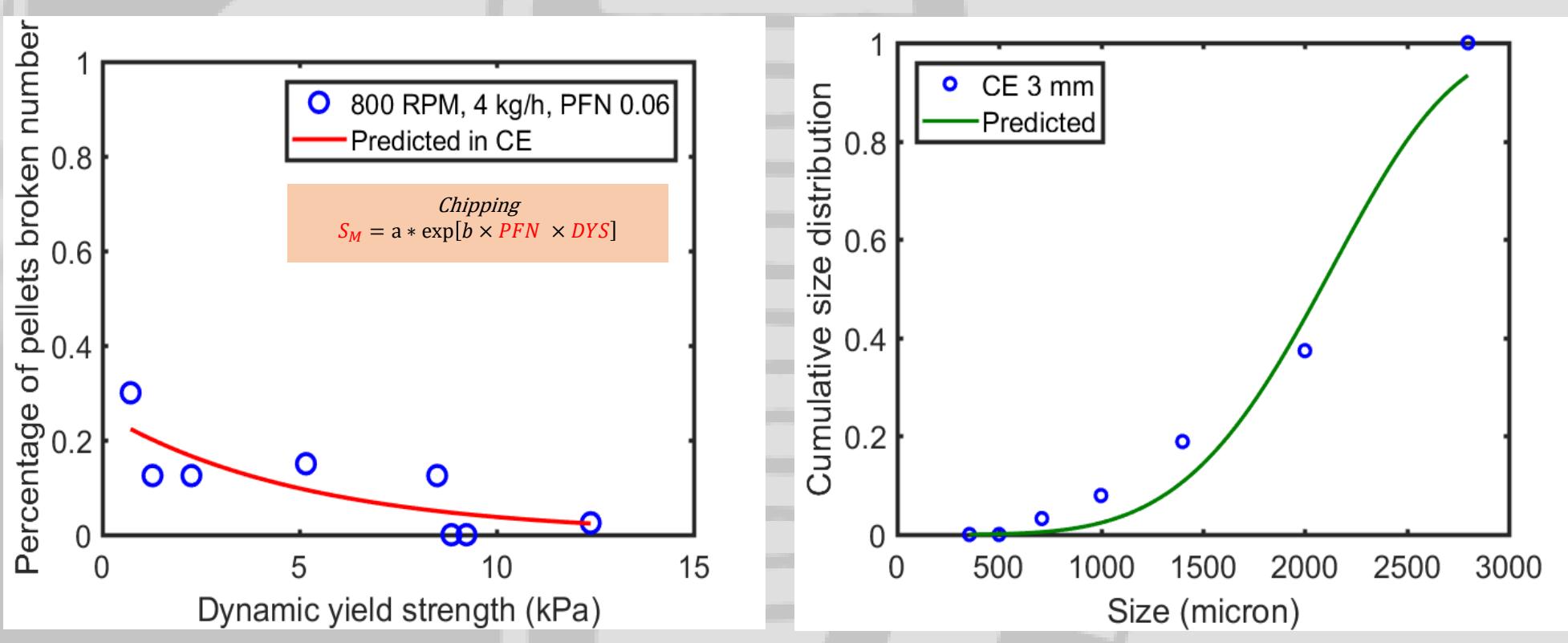
Considering three levels of verification: **Code** verification, **Calculation** verification and **Model system** verification.

Bottom-up approach starting with the **sub-models** to identify components of the multiscale model that may not be performing as expected. This provides **early check on the appropriateness** of the model.

Full-sized DEM Models are **computationally expensive**. Simplified **Compartmental models** have been verified as providing equivalent results.

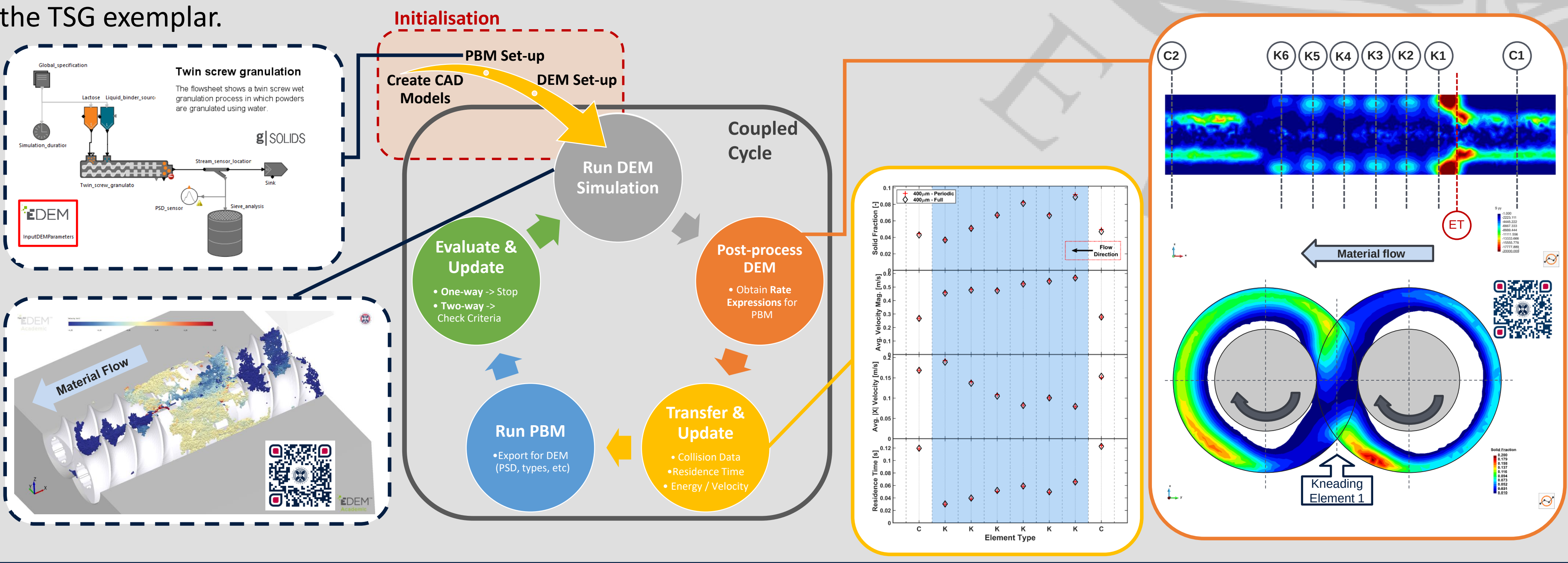
RTD's (Residence Time Distributions) have been compared against results in literature to establish if observed results are within expected range.

Experimental studies highlighted the need for TSG appropriate **breakage kernels** for **chipping** and **fragmentation**. These were implemented and verified in g|FORMULATE.



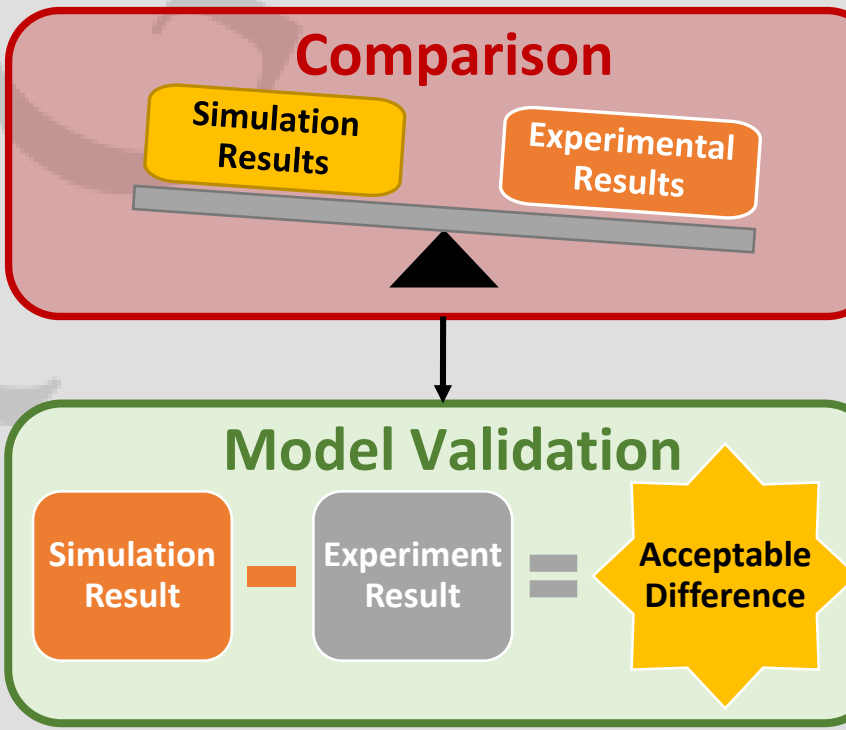
5. Multiscale Modelling: DEM-PBM Coupled System

A **bi-directional coupling framework** is implemented with information shared between the two simulation tools. The **DEM** simulation is conducted using the commercial code **EDEM** while the **PBM** simulation is carried out with the commercial code **g|FORMULATE**, which is built on top of the **g|PROMS** advanced modelling platform. A one-way coupling was utilised for the TSG exemplar.

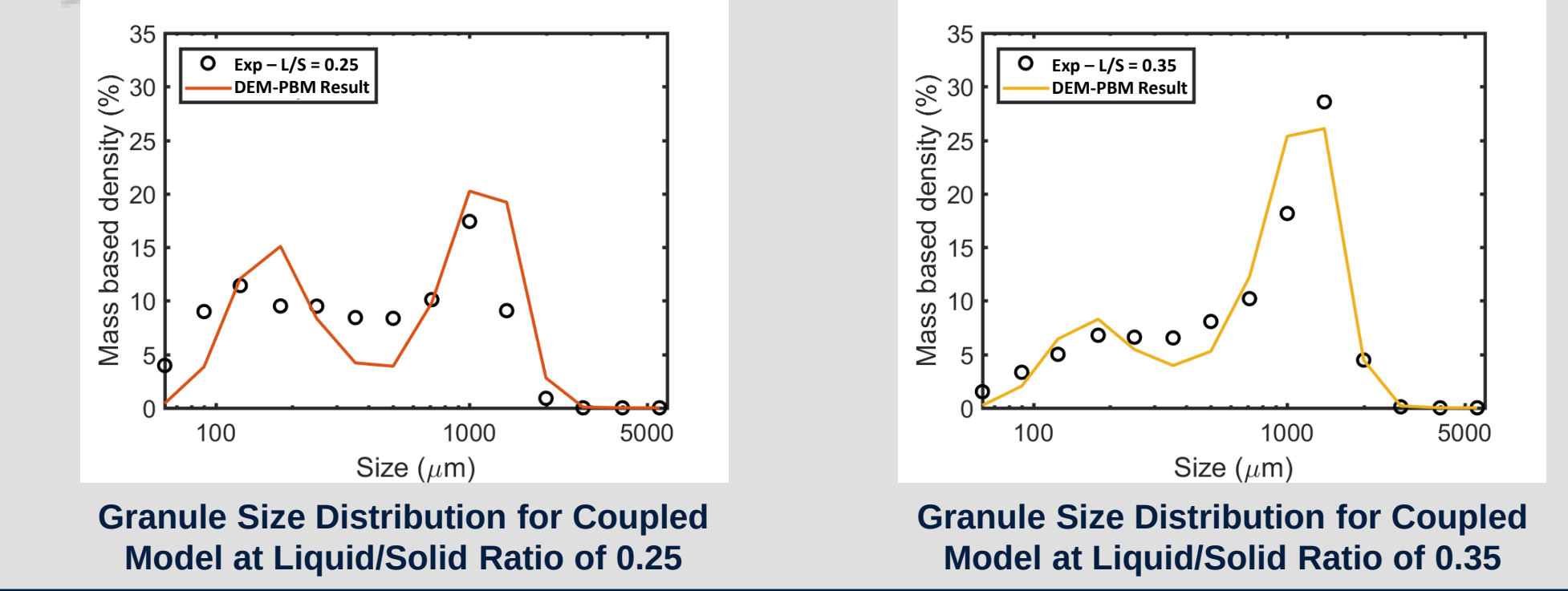


6. Validation for TSG

Validation is concerned with **establishing the predictive capability** of the computational model in relation to the real system with **independent experimental results**.



This acceptable difference must be evaluated against the degree of **uncertainty in both** the **validation experiment** and the **multiscale model**.



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