Multi-scale modeling of powder processes:
Bi-directional coupling of population balance models in gPROMS with discrete element models in STAR-CCM+

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ENGINEERING RESEARCH CENTER FOR

STRUCTURED **O**RGANIC **P**ARTICULATE **S**YSTEMS

RUTGERS UNIVERSITY
PURDUE UNIVERSITY
NEW JERSEY INSTITUTE OF TECHNOLOGY
UNIVERSITY OF PUERTO RICO AT MAYAGÜEZ

Introduction

Objective: to develop a multi-scale, mechanistic model for wet granulation processes.

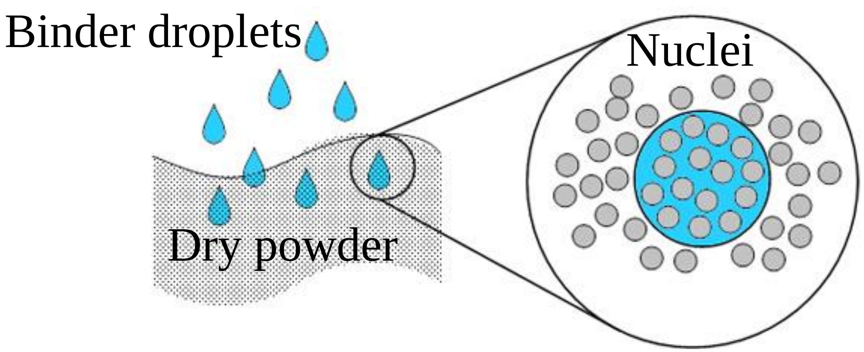
- *Process understanding and Quality-by-Design*
- *Existing approaches are insufficient*

- Outline
  - *Background and approach*
  - *Mechanistic PBM development in gPROMS*
  - *PBM-DEM coupling strategy and demonstration*
  - *Summary and future work*

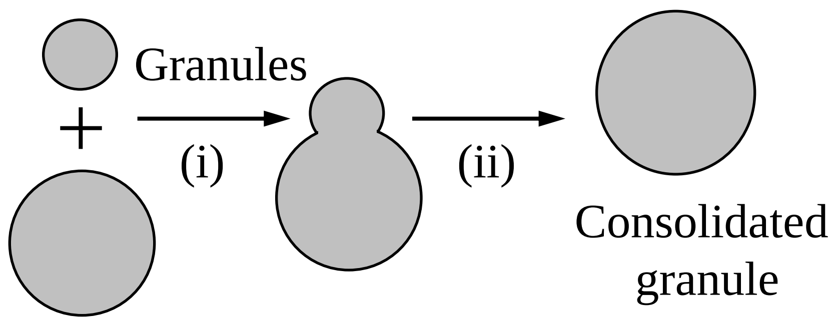
- Ongoing collaboration between Rutgers University (ERC-SOPS), Process Systems Enterprise, and CD-adapco.

Wet granulation

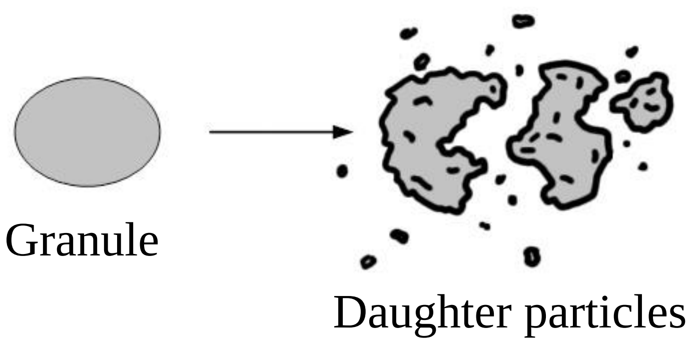
1 Wetting & Nucleation



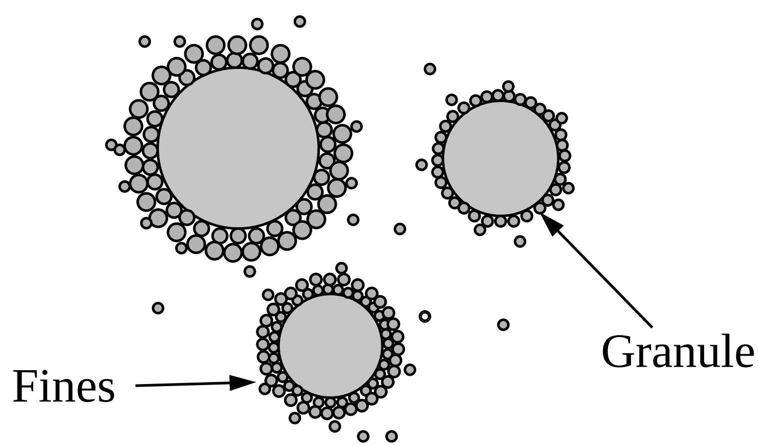
2 Aggregation & Consolidation



3 Breakage & Attrition



4 Layering



(Iveson *et al.*, 2001)

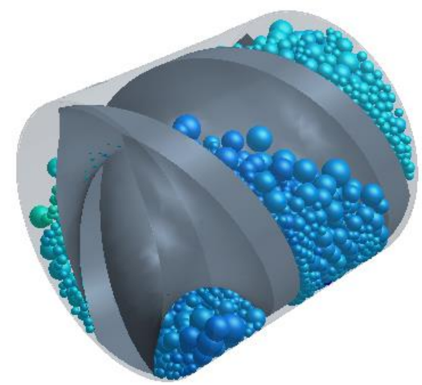
PBM vs. DEM

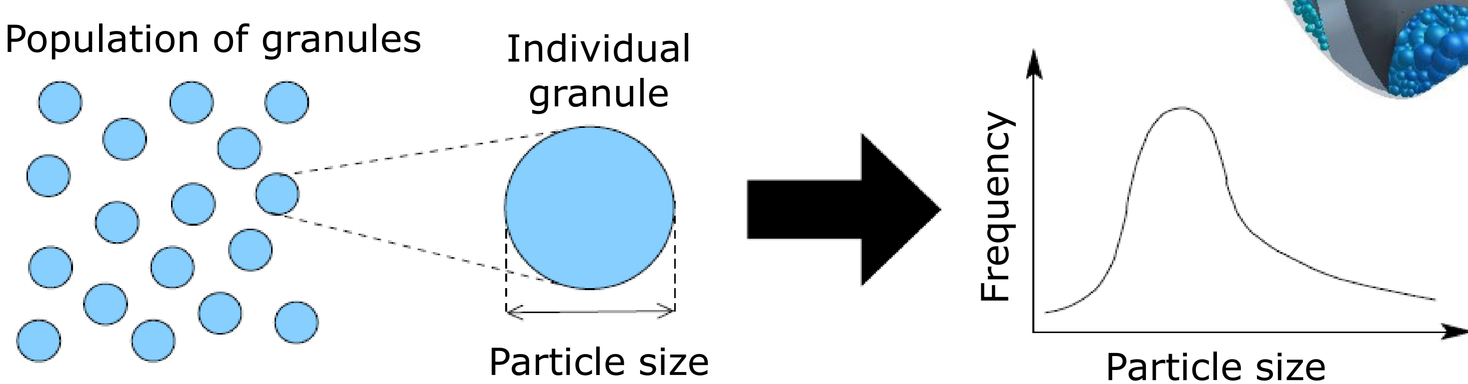
Population balance modeling:

- Tracks number of particles in each size class based on rate expressions for sub-processes
  - *Typically empirical or semi-empirical*
  - *Effects of many process parameters and material properties are not accounted for*
- Spatial information is not inherent
  - *Compartmental PBMs need transfer rate data/assumptions*
  - *Inhomogeneous liquid distributions*
- Many unknown parameters must be estimated with experimental data

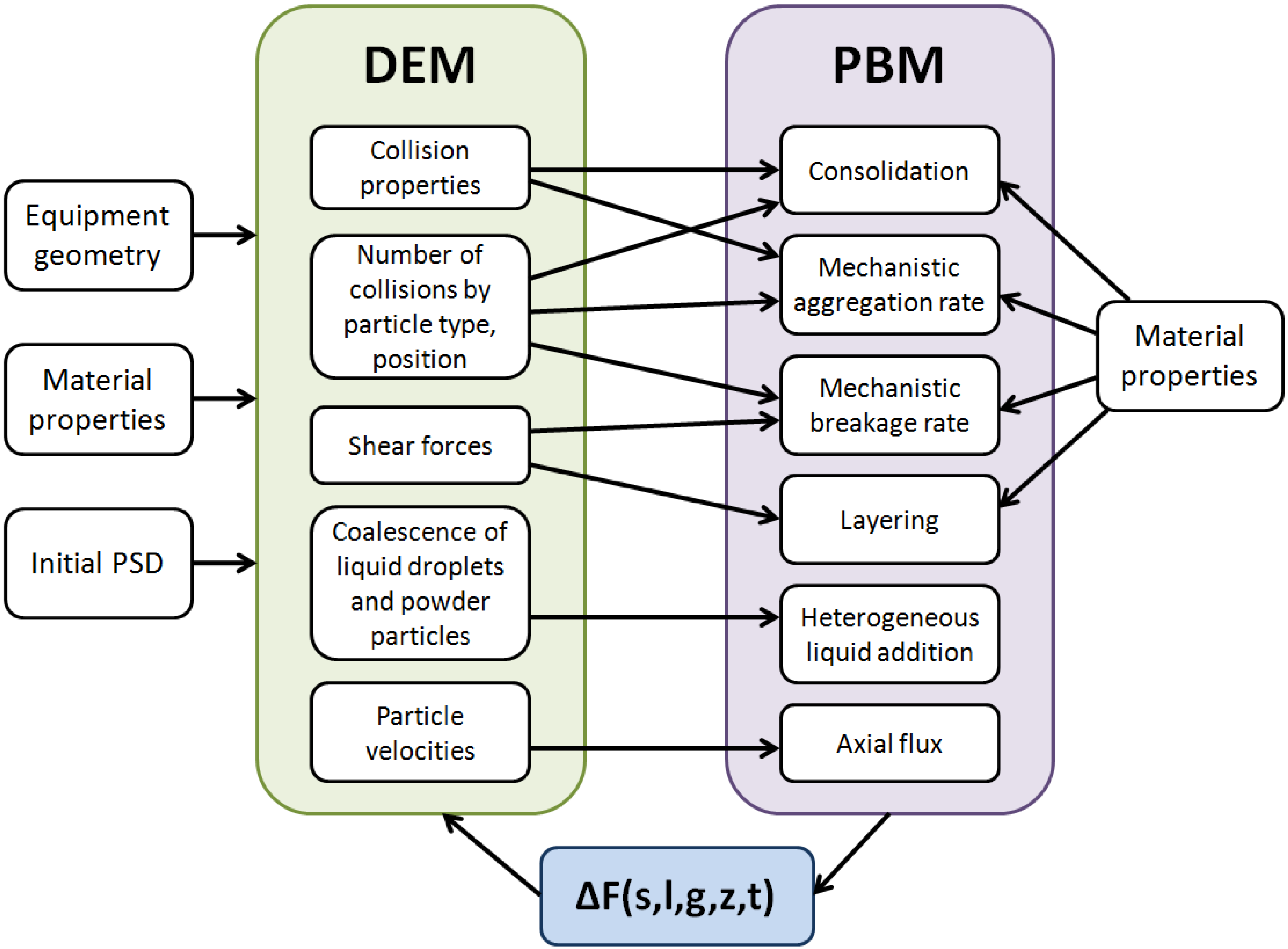
Discrete element modeling:

- Tracks each particle in space using laws of physics
- Can output collision, velocity, force, and spatial data at the particle scale.
- Does not inherently simulate rate processes, such as aggregation.
- Computationally intensive

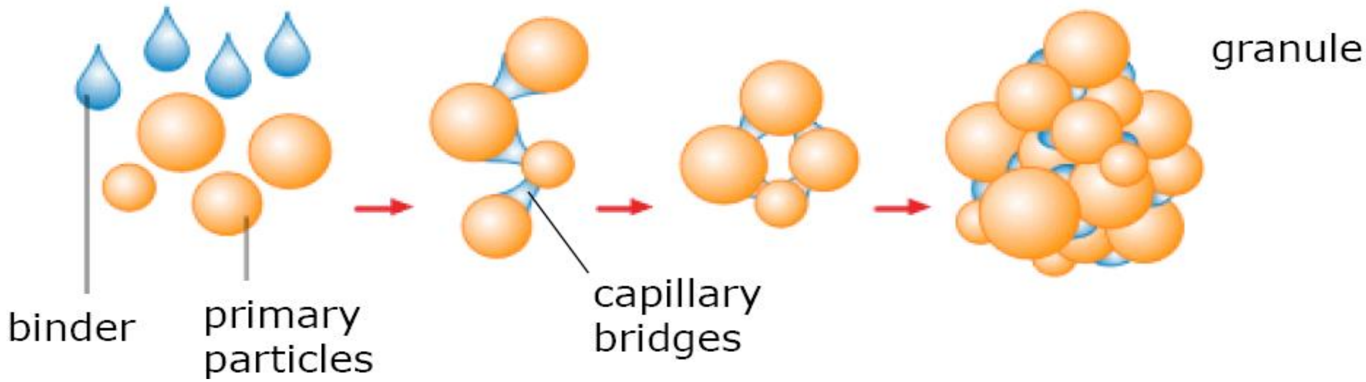




PBM & DEM: a multi-scale approach



Mechanistic PBM development

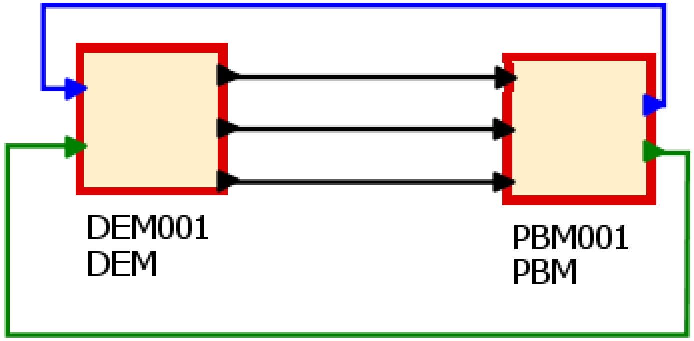


- Objective:
  - *Incorporate mechanistic and spatial details into multi-scale model.*

- Features:
  - *Mechanistic aggregation rate*
  - *Liquid addition*
  - *Porosity and consolidation*
  - *Internal vs. external liquid*
  - *Spatial compartments and particle/liquid transfer*

Detailed gPROMS Model

- UNIT: Population balance model
  - *Number and properties of particles of each volume class in each spatial compartment*
  - *Number of free liquid droplets in each compartment*
  - *Uses DEM results in rate expressions for sub-processes*

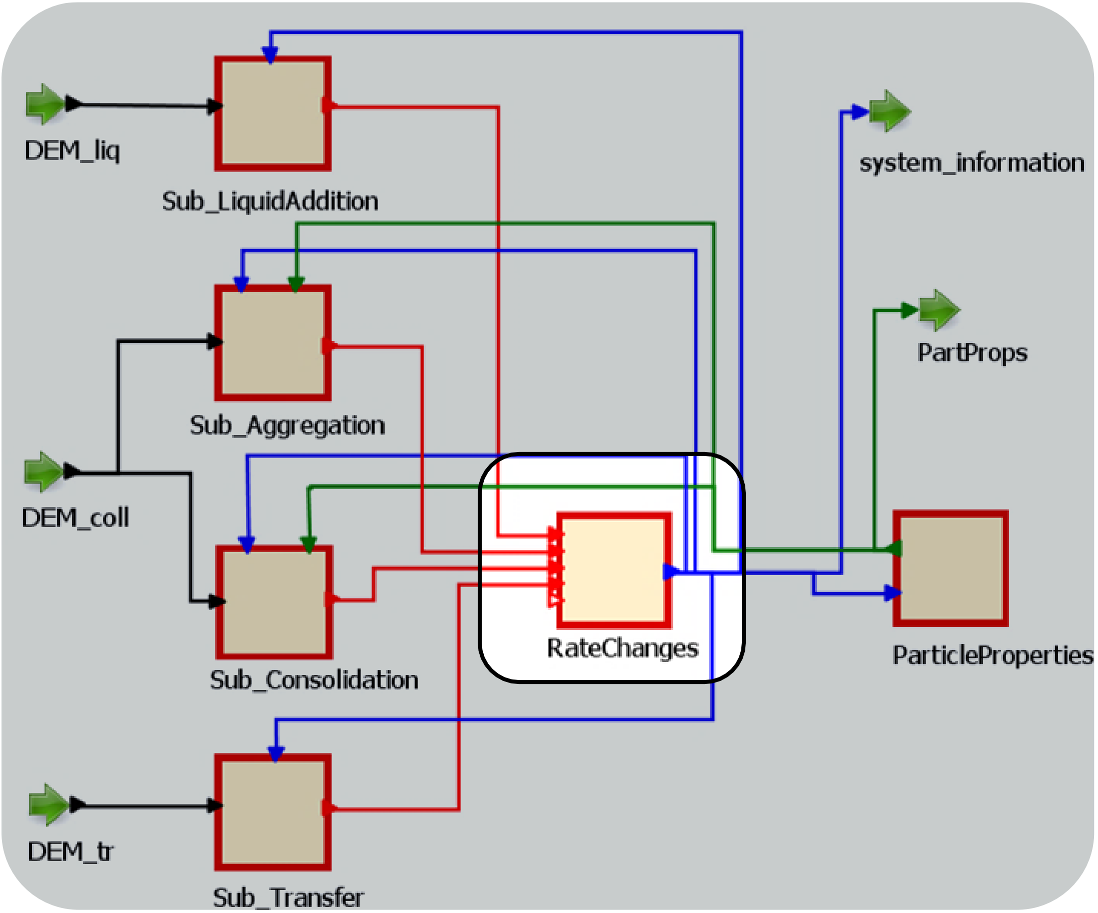


- UNIT: Discrete element model
  - *Uses current PBM results to determine collision rates, relative velocities, and transfer between compartments.*

- UNIT: Universal parameters
  - *All user input settings*

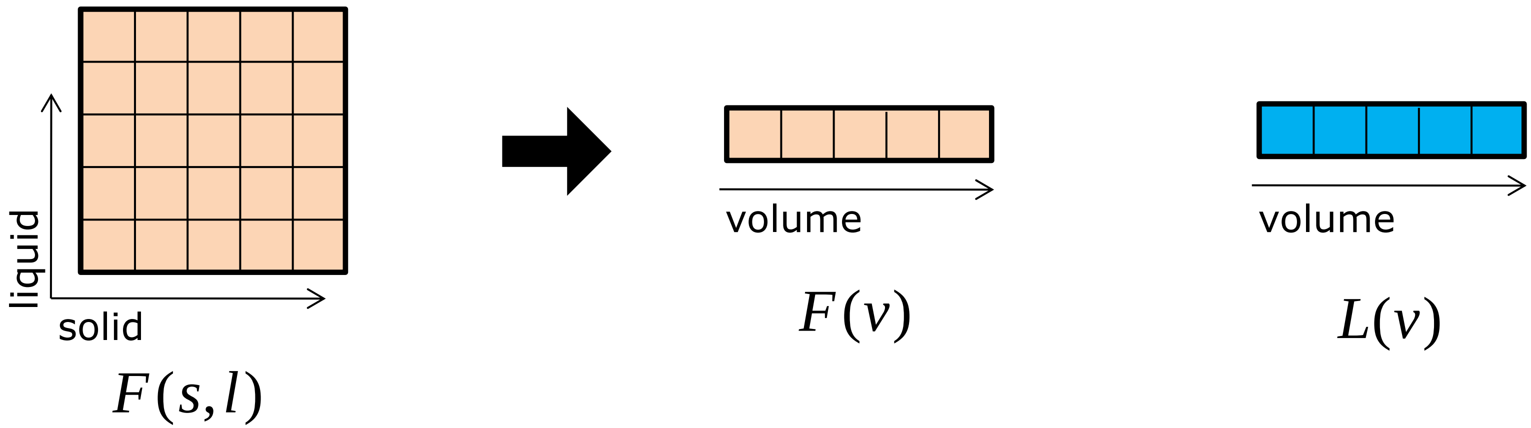
- UNIT: Volume domain
  - *Sets volume grid for PBM.*
  - *Calculates cell location for colliding particles.*

PBM with lumped parameters



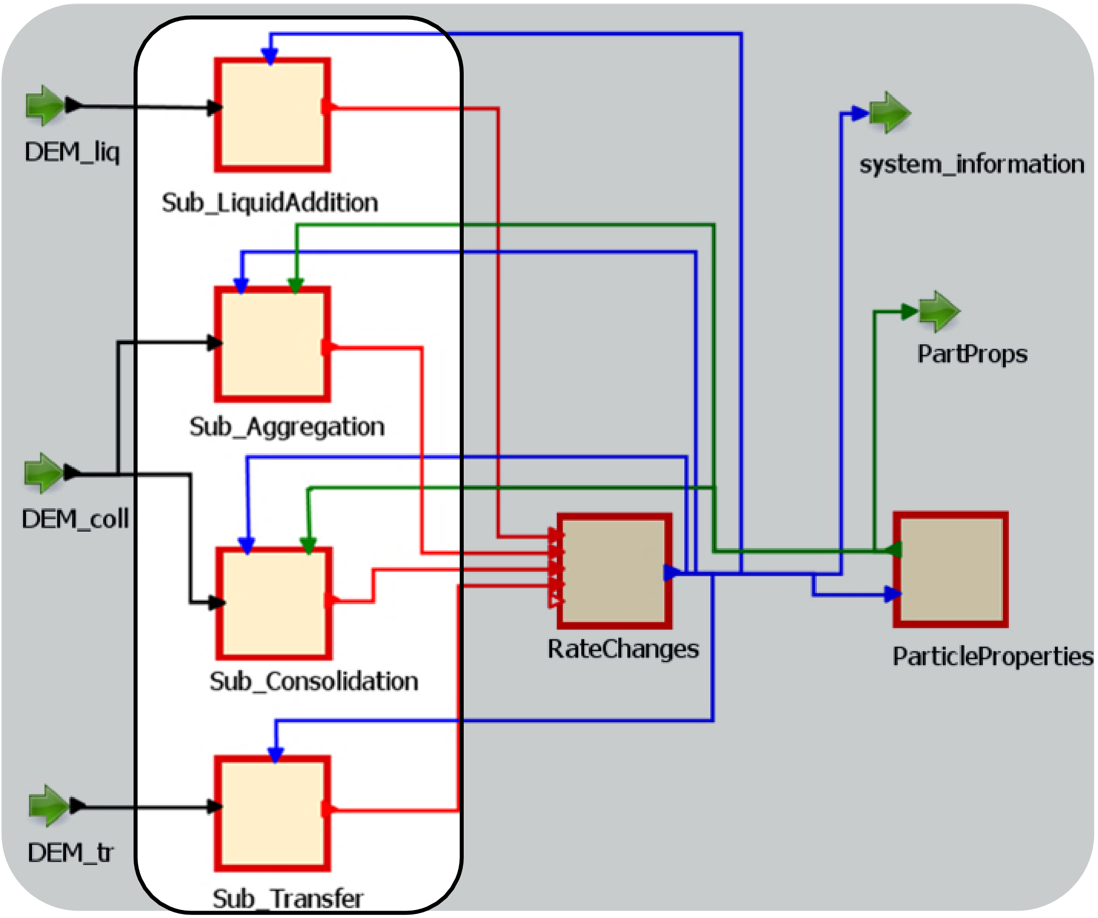
- RateChanges
  - *Determines rates of change in each compartment of*
    - *Number of particles in each bin*
    - *Total liquid and pore volumes in each bin*
    - *Free liquid droplets*
  - *Net rates of four sub-processes*

Lumped parameter approach



- Multi-dimensional PBM tracks simultaneous distributions in multiple attributes (such as size and liquid content)
- Lumped parameter approach reduces dimensionality of distribution
  - *Assumes every particle in the same bin has the same amount of lumped parameter.*
  - *Each lumped parameter creates an additional PBM to track volume of that component in each bin.*
  - *Lumped property can change over time due to aggregation, liquid addition, and other rate processes.*
  - *Lumped property can also depend on particle size.*
  - *Using compartments, spatial inhomogeneities can still exist.*

Sub-processes



- Sub-processes
  - *Aggregation*
  - *Liquid addition*
  - *Consolidation*
  - *Transfer*

Mechanistic aggregation rate

Frequency

$$\beta(v,v') = C(v,v')\Psi(v,v')$$

Efficiency

$$\Psi(v,v') = \begin{cases} 1 \ for \ St \le St^* \\ 0 \ \ for \ St > St^* \end{cases}$$

- Collision rate can be directly provided by DEM

- Collision efficiency depends on Stokes criterion
  - *Critical stokes number a function of thickness of surface liquid and particle surface asperity*

$$St^* = \ln \frac{\lambda_{12}}{h_a} \qquad St = \frac{8\tilde{m}u_0}{3\pi\mu\tilde{d}^2}$$

  - *Stokes number depends on particle masses and diameters, relative velocity, and binder viscosity*
  - *Critical velocity*

$$u_{cr} = \frac{3\pi\mu\tilde{d}^2}{8\tilde{m}} \ln \frac{\lambda_{12}}{h_a}$$

  - *Average relative collision velocity provided by DEM*

Liquid addition

$$\dot{L}(v,x) = f_{drop}(v,x)F(v,x)N_{drop}(x)v_{drop}$$

- 1-D PBM with liquid volume as “lumped” parameter
- Rate of liquid addition to any bin (v) and compartment (x) is proportional to:
  - *Fractional rate of liquid droplet uptake*
  - *Total particles in that bin and compartment*
  - *Total number of free droplets in compartment*
  - *Droplet volume*

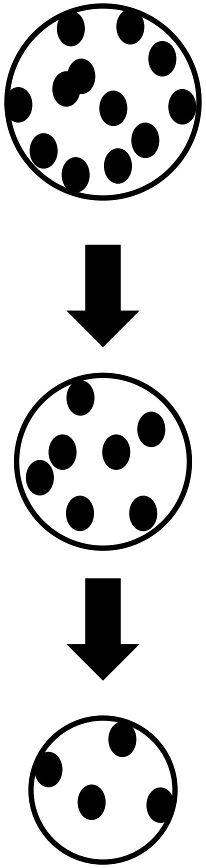
$$f_{drop}(v,x) = \frac{n_{drop}(v,x)}{N_{drop}(x)F(v,x)\Delta t}$$

- Fractional rate of liquid droplet uptake can be estimated using DEM
  - *Create droplets that disappear upon collision with a particle.*
  - *Count these collisions over a time interval, by particle size and compartment.*
  - *Calculate rate, per particle, per droplet, per second.*
- Liquid volume is transferred during other rate processes, such as aggregation.

Porosity and consolidation

$$\varepsilon(v) = \frac{p(v)}{s + p(v)}$$

- Particle pore volume consists of internal space occupied by air or liquid.
  - *Lumped parameter approach to track pore volume of each particle in each bin and spatial compartment*
  - *As particles collide and deform, porosity decreases*



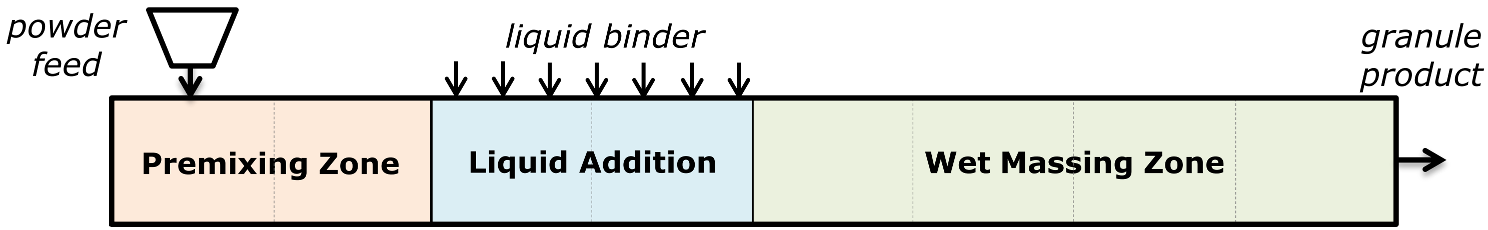
- Consolidation rate:
  - *Exponential decay in porosity approaching a minimum value*

$$\dot{p}_{cons} = -c\left(\frac{1 - \varepsilon_{min}}{1 - \varepsilon}\right)\left(p - \frac{s\varepsilon_{min}}{1 - \varepsilon_{min}}\right)$$

  - *Unknown rate coefficient*
  - *Collision frequency (total per bin) can be included*

$$c = c_0 \dot{N}_{coll}(v)$$

Spatial compartments



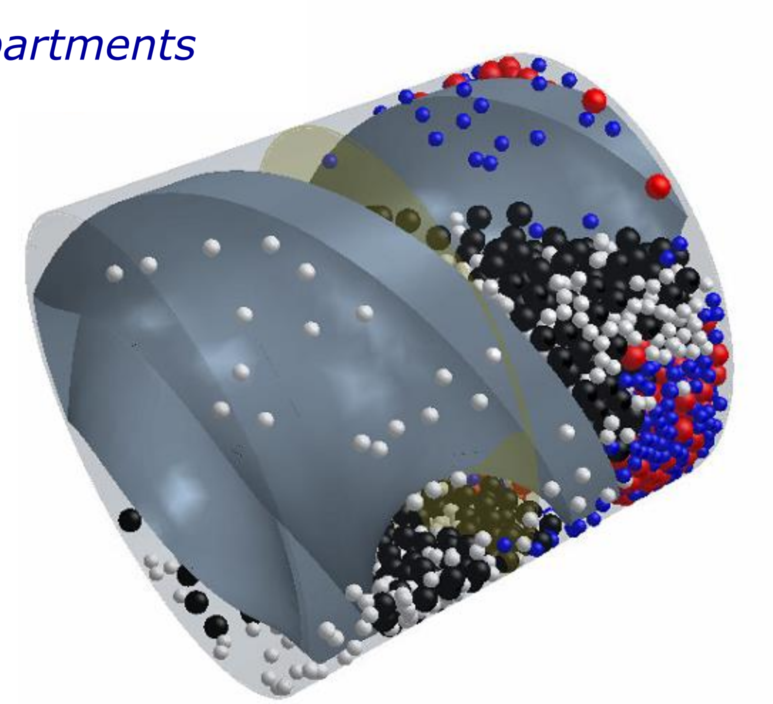
- PBM solved in each compartment
- Liquid addition region specified by user
- Transfer between compartments
  - *Fraction of particles transferred*
  - *Number of particles crossing boundaries provided by DEM, converted into rate per particle*
  - *Particles transfer can occur into and out of compartments at the same time*
  - *Compartments can be arbitrary size, shape, and position.*
- Strategy needed to define compartments

$$\frac{dF(v,x)}{dt} = \Re_{agg,net}(v,x) - \sum_{x'} F(v,x)\alpha(v,x,x') + \sum_{x'} F(v,x')\alpha(v,x',x)$$

Spatial compartments

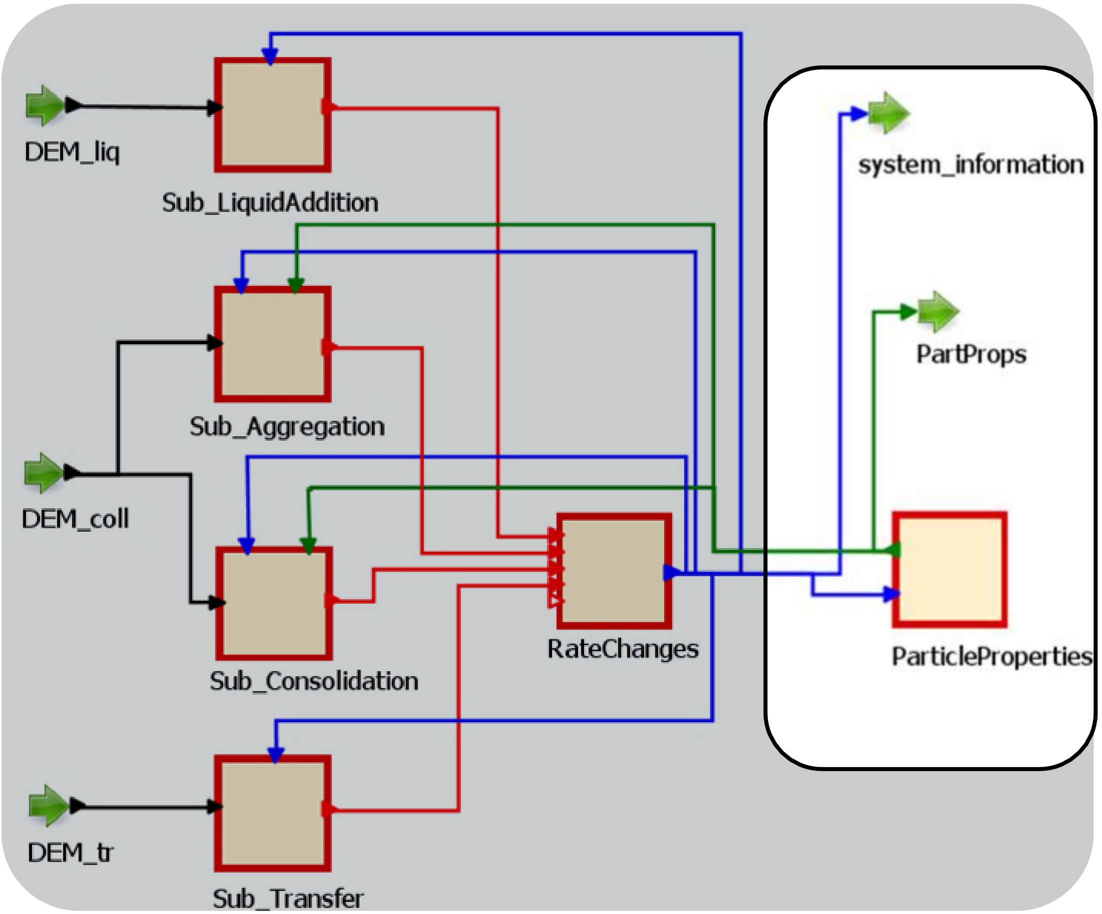
- Compartments
  - *Create compartments in STAR-CCM+*
  - *Track particle transfer between compartments*

Size	Initial Region	Color
Small	Left	White
Small	Right	Blue
Large	Left	Black
Large	Right	Red



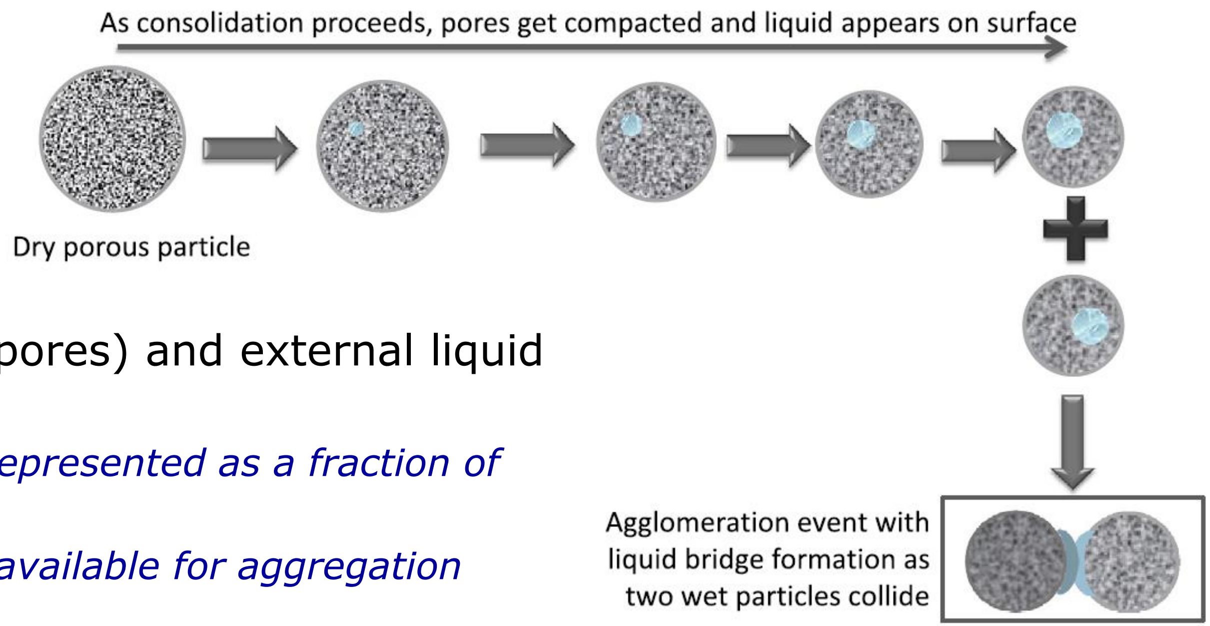
- End goal for user:
  - *Define compartments as regions of arbitrary size and shape in STAR-CCM+*
  - *Specify total the number of regions in gPROMS*
  - *Turn on or off sub-processes in each region (liquid addition, inflow/outflow)*

Particle and bulk properties



- Main granulation model
  - *Mass and volume balances*
  - *Bulk properties in each compartment and overall (d4,3, mass distributions)*
- Particle Properties model
  - *Per-particle volumes in each bin, compartment (pore, liquid)*
  - *Internal and external liquid*
  - *Total volume and diameter, wet and dry masses*
  - *Aggregation information (surface asperity, surface liquid thickness, critical Stokes number)*

Internal and external liquid



Chaudhury, et al. (2014)
Chemical Engineering Science

- Total liquid volume, per particle, calculated using lumped parameter

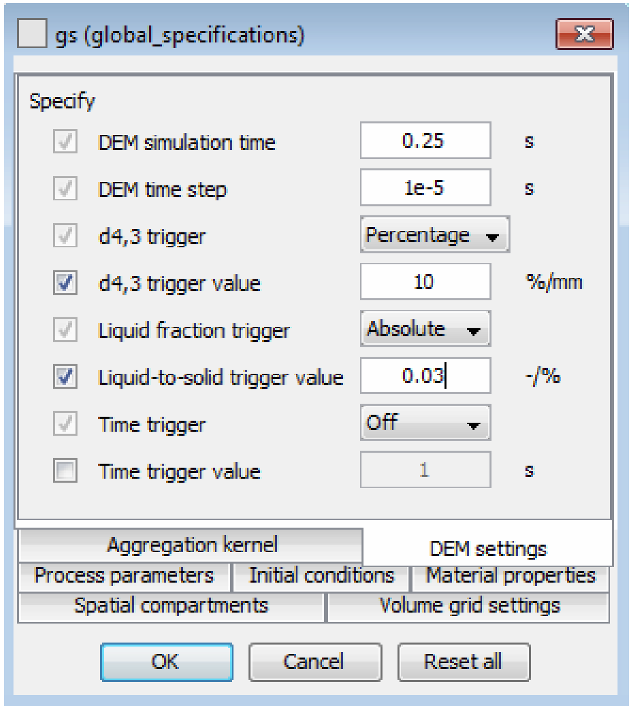
- Distinction between internal liquid (trapped in pores) and external liquid (on the surface)
  - *Maximum internal liquid represented as a fraction of the total pore volume*
  - *Remainder is on surface, available for aggregation*

- As porosity decreases, surface liquid increases, resulting in greater aggregation rates

- Drop penetration time
  - *Based on Washburn equation for capillary flow*
  - *Droplet volume, effective porosity and pore radius, binder viscosity, surface tension, and contact angle*
  - *Order of magnitude for small amounts of liquid: 1e-4 s*

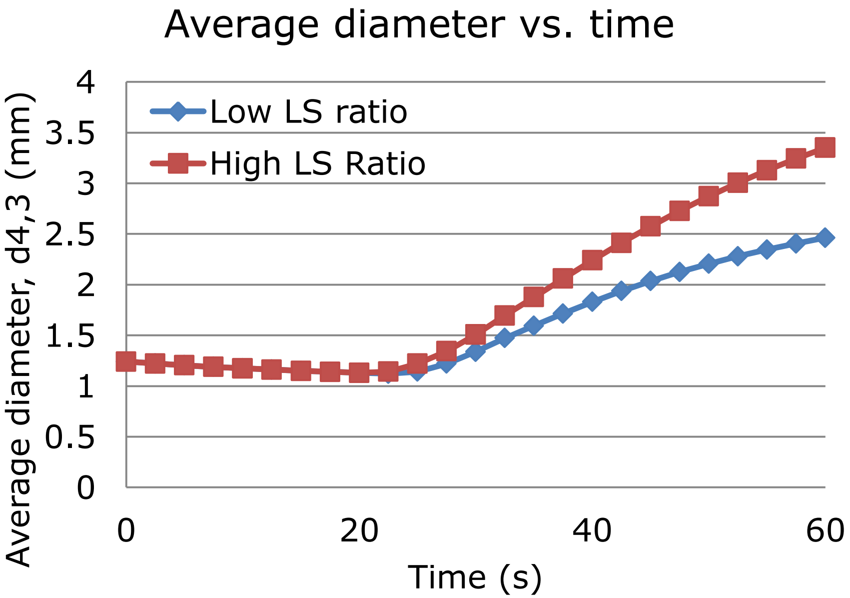
Summary of model

- User inputs
  - *Initial conditions*
  - *Material properties (including DEM parameters)*
  - *Process parameters (batch time, L/S ratio, screw speed)*
  - *Model settings (compartments, volume grid, kernel selection)*
  - *DEM settings (simulation time, time step, trigger)*
- From gPROMS to DEM
  - *PSD in each compartment*
  - *Particle properties*
  - *Liquid addition details*
  - *Process parameters*
  - *DEM settings*
- From DEM to gPROMS
  - *Collision rate between bins*
  - *Average relative velocity of collisions*
  - *Collision rate for each bin*
  - *Liquid uptake rate*
  - *Particle transfer rate between compartments*



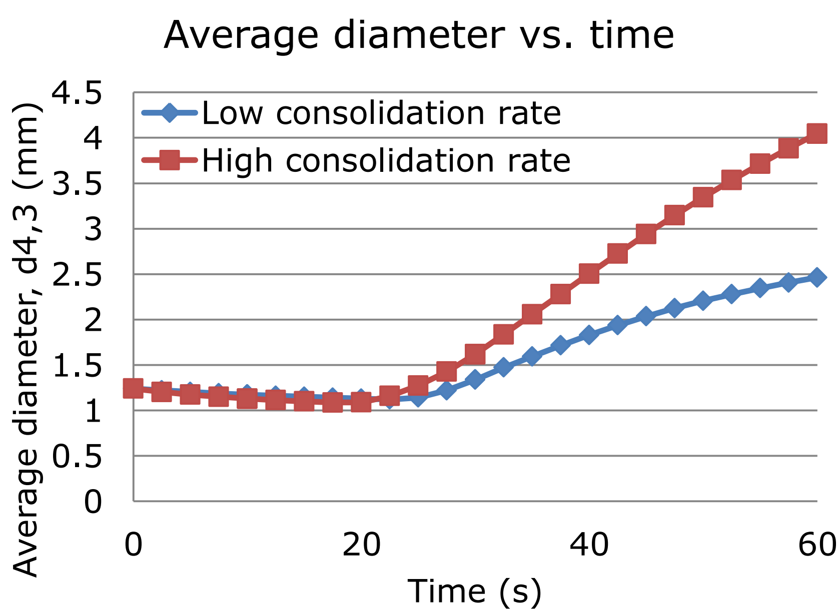
Results of uncoupled gPROMS model

- Higher liquid-to-solid ratio results in larger granules.
  - *High: 0.35*
  - *Low: 0.3*



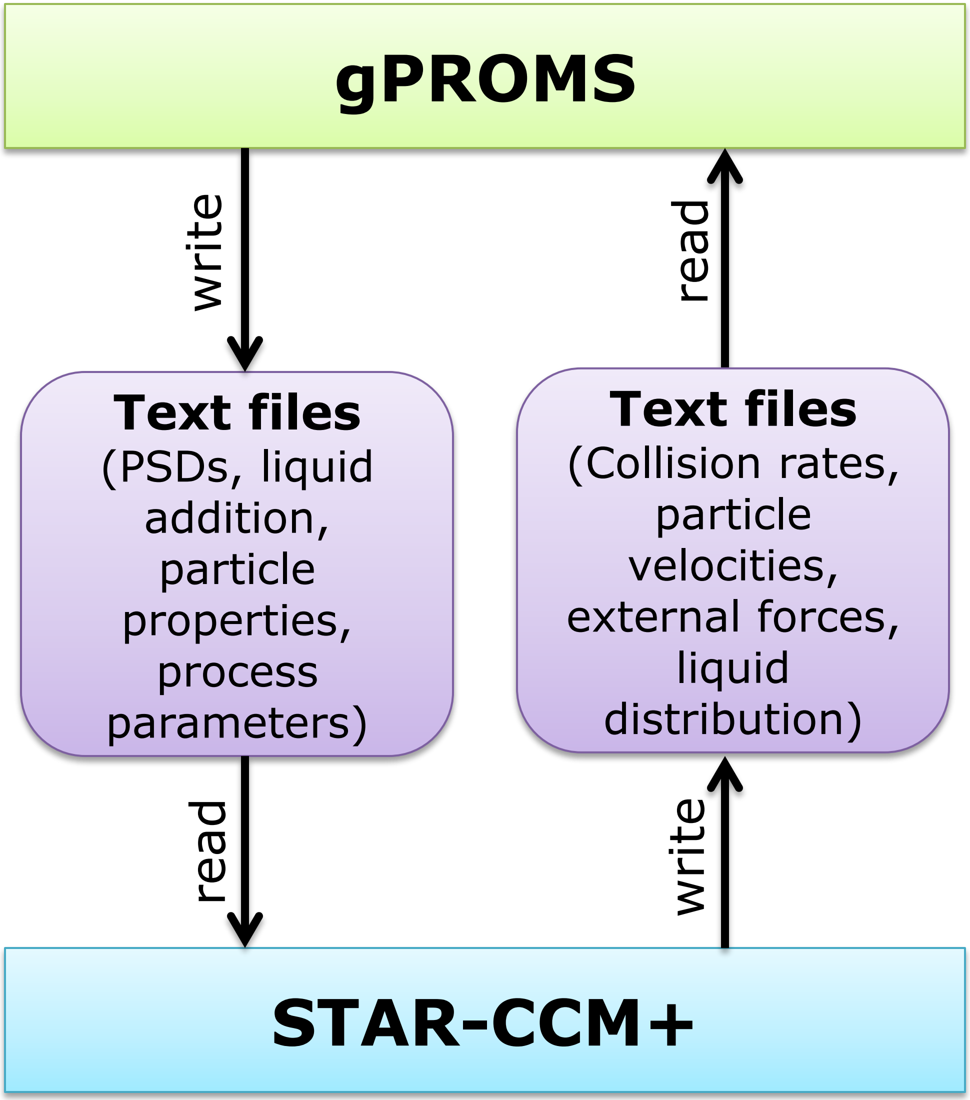
- Higher consolidation rate results in faster aggregation.

Consolidation rate constant	Percent surface liquid
5e-4/s	38%
1e-3/s	62%

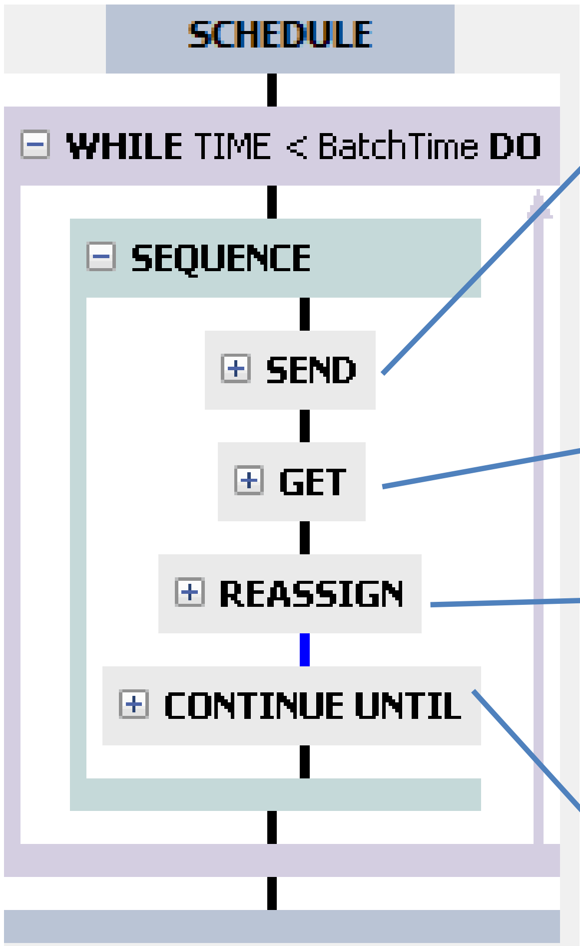


Coupling with STAR-CCM+: approach

- gPROMS
  - *Population balance, rate changes*
  - *Controls process parameters and problem set up (number and sizes of particles, liquid addition rates, rotational speeds, etc.)*
- STAR-CCM+
  - *Collision rates and forces*
  - *Flux and spatial behavior*
  - *Liquid addition*
- Data transfer
  - *Text files*
  - *DEM simulations triggered by sufficient changes to key variables*



Schedule and FPI



SEND:
- Writes particle distribution to text file.

GET:
- Runs DEM using system command.
- Reads DEM results from file, passes values to gPROMS.

STAR-CCM+ macro:
- Reads text file.
- Creates/deletes particles.
- Runs simulation.
- Exports results to text file.

REASSIGN:
- Defines criterion for next DEM iteration.

CONTINUE:
- Runs PBM until condition is met.

gPROMS/STAR-CCM+ simulation workflow

1

- Create simulation file in **STAR-CCM+**.
  - *Define geometry (Future: define compartments).*
  - *Set model physics to turn on DEM.*
  - *Specify movement of parts (impeller or screw).*
  - *Create scenes to output images.*

2

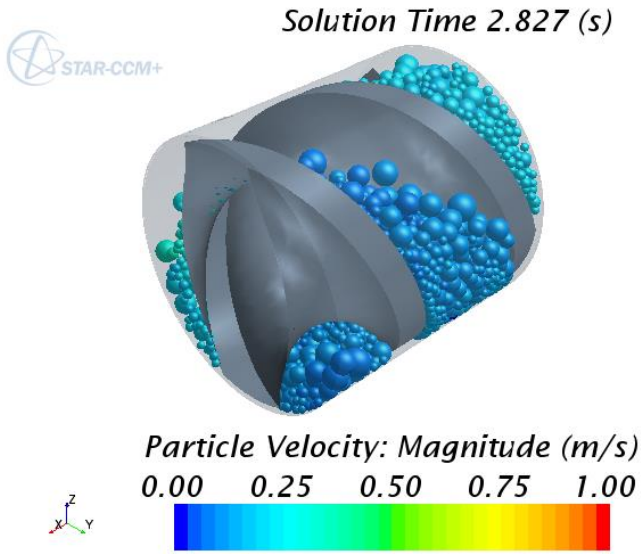
- Specify parameters in **gPROMS** model.
  - *DEM settings (time, time step, trigger)*
  - *Volume grid size and bounds*
  - *Initial PSD, porosity, and liquid content*
  - *Process parameters and material properties*

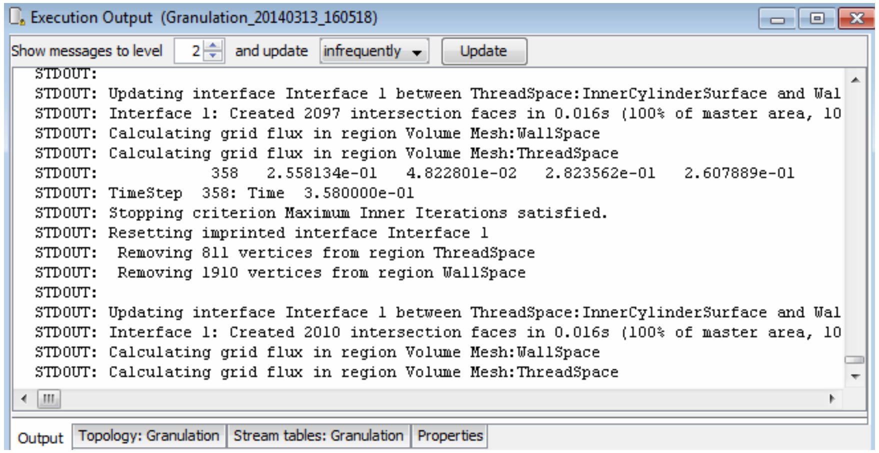
3

- Run process with **FPI** and appropriate **SCHEDULE**.
  - *Grid size and particle/collision properties are automatically read and transferred to STAR-CCM+.*
  - *STAR-CCM+ simulation is modified and executed by gPROMS during GET command.*

gPROMS/STAR-CCM+ coupling

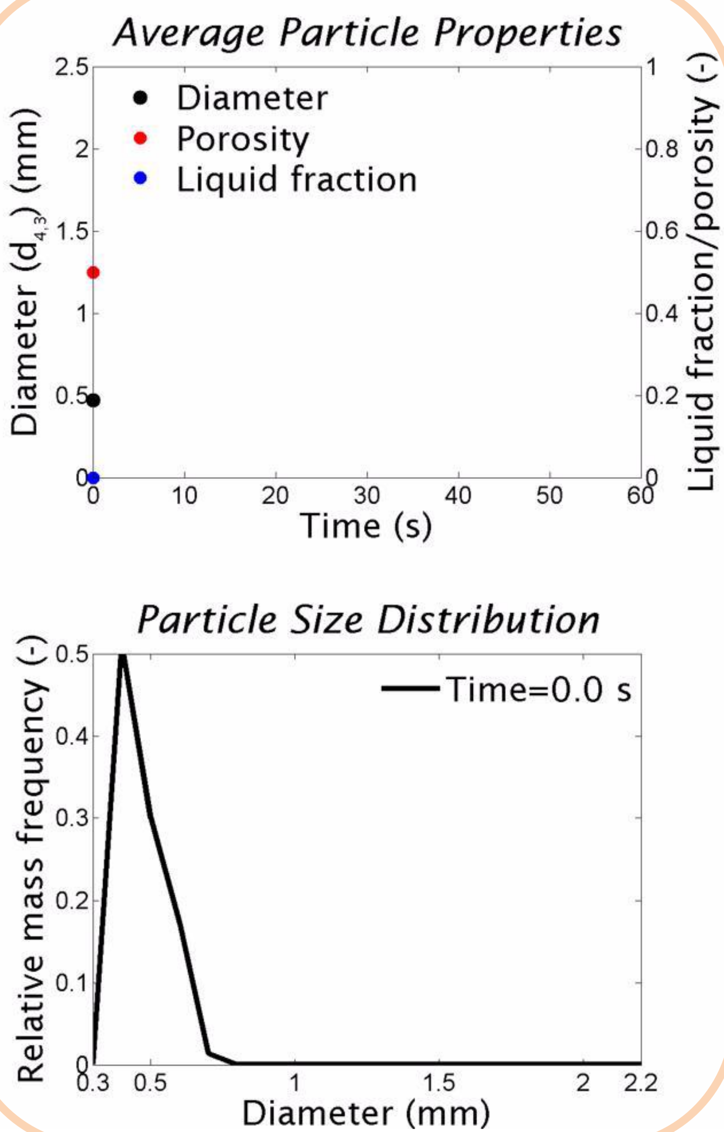
- Mechanistic model with one spatial compartment, only data transferred from STAR-CCM+ is collision rate.
- 20 bins (total volume)
  - *0.3-2.2 mm in diameter*
  - *Lumped solid/pore, liquid*
  - *Internal and external liquid*
  - *L/S=0.3, added from 2-12 seconds*
- STAR-CCM+ called when $d_{4,3}$ changes by more than 10% or liquid-to-solid ratio changes by more than 0.1.
- 60 s simulation
  - *Total simulation time: 4 hrs*
  - *CPU time: 18 s*



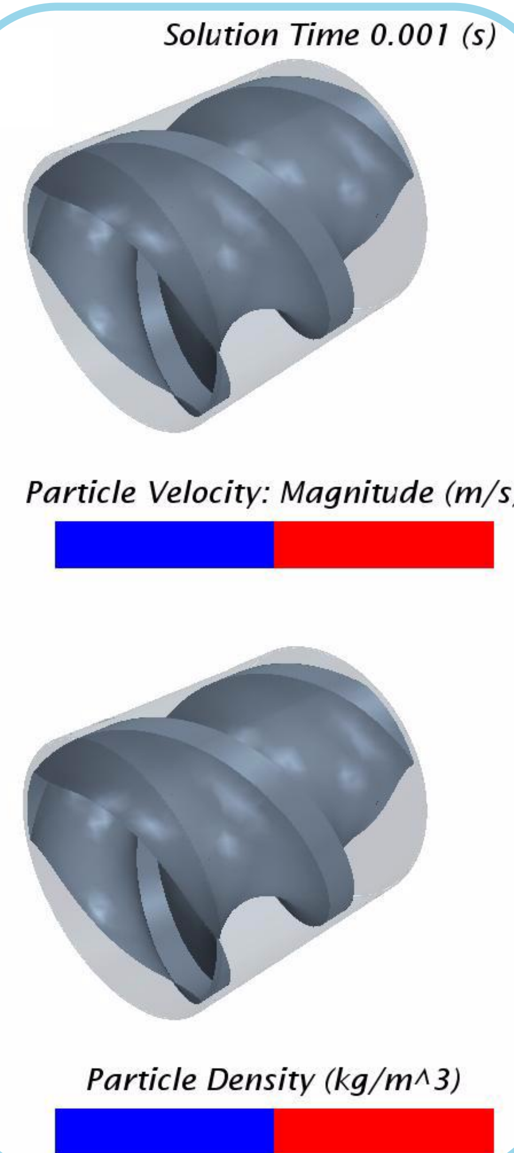


gPROMS/STAR-CCM+ results

gPROMS



STAR-CCM+



Summary and future work

- Modeling granulation is a multi-scale problem
  - *Developed a detailed, **mechanistic PBM** for wet granulation processes in gPROMS.*
  - *Established and demonstrated a **bi-directional coupling** technique with STAR-CCM+.*

- Ongoing and future work
  - *Expand **data transfer** from STAR-CCM+ to gPROMS (liquid addition, spatial compartments, relative velocity)*
  - *Include **additional rate processes**, such as breakage, nucleation, and layering.*
  - *Develop efficient solution techniques for **multi-dimensional PBMs** in gPROMS.*
  - ***Test and validate** multi-scale model.*

Acknowledgements

- National Science Foundation Engineering Research Center for Structured Organic Particulate Systems (ERC-SOPS)
- Process Systems Enterprise for providing this internship opportunity.
- Jim Litster (Purdue) for his useful feedback.
- CD-adapco for their support and guidance.

Thank you.

BACKUP SLIDES

Customizing the DEM simulation

- Java macro reads from three text files, modifies existing simulation
  - *General **simulation parameters**: total simulation time, DEM time step, number of bins, rotational speed*
  - ***Bin information**: Number of particles in each bin and their properties (size, Poisson ratio, density, Young's modulus)*
  - ***Collision information**: Contact model parameters for each bin with each other bin and the walls (coefficients of restitution, friction)*

Bin Number	Diameter (mm)	Count	Density (kg/m^3)	Poisson's Ratio	Young's Modulus (MPa)
1	0.4	500	2000	0.2	0.2
2	0.5	400	1750	0.2	0.2
3	0.6	300	1500	0.2	0.2
4	0.7	200	1250	0.2	0.2
5	0.8	100	1000	0.2	0.2
6	0.9	50	1000	0.2	0.2
7	1	25	1000	0.2	0.2

Execution of Java macro

- Before simulation:
  - *Changes **simulation parameters.***
  - *Creates **DEM phase** (particle type) for each bin.*
  - *Defines **interactions** between each pair of phases.*
  - *Checks if particles need to be removed (when F decreases), and if so, **removes particles.***
  - *Creates an **injector** for each bin.*
  - *Creates reports and monitors for key information we want to **output.***
- Runs simulation.
- After simulation:
  - *Exports contact data over time.*
  - *Parses file to approximate **number of collisions**, **relative velocity**.*
  - *Creates **text file** with number of collisions between each pair of bins, number of particles in those bins, and average collision velocity.*