

NSF CDSE DRAFT 02

Thor, Gibbs, Zeus, the guy who invented sticky notes, Santa Claus*

*North Pole department of ice and snow Fwding address - Department of Chemical and Biochemical Engineering,
Rutgers, The State University of New Jersey, Piscataway, NJ, USA 08854*

Abstract

abstract text goes here ...

Keywords: Population balance model, heteroaggregation, alginate, chitosan, oppositely charged

1. Introduction & Objectives

description of particulate processes and challenges... leads up to our "solution" or start of solution which is what this paper is about
particulate process and how they are half all chem industry
despite being important they are VERY hard to model and study bec of microphenomena.
strain difficulty and added costs to industry bec of this
PBM DEM have been helpful for this however but they take long time to solve
in the past when faced with comp heavy tasks scientists have used parallel computing. divide big prob into small pieces that are simultaneously solved. time to solve is time to solve small piece.
potential benefits this could have 1. unprecedeted accuracy 2.wide adoption of using these models since they are so fast 3. cheaper drugs 4. MPC accurate but in real time 5. parameter estimation for QbD 6. etc.

1.1. Objectives

1. develop 4D PBM that is parallelized spatially and internally for optimal utilization of modern HPC equipment.
2. use liggghts to accurately model micromechanics for processing in Lodgitech granulator.
3.LINK PBM-DEM for best of both worlds and optimal performance. 1-way or if possible 2-way coupling

19 2. Background & Motivation

20 2.1. Particulate Processes

pharma / particulate proceses information prevalence etc
difficult phyisics bec micro phenomena etc
as result use time consuming and expensive heuristics or inefficient operaiton protocol dotdotdot
also reason most blah done in batch mode still bec continous mode compounds complexity of these systems

*Corresponding author

Email address: **santaclaus** (Santa Claus)

26 will need to switch to continuous etc
 27 segway with need to better understand these systems from a modeling/theory point of view
 28 dotdotdot QbD etc

29 *2.2. Modeling*
 30 *2.2.1. Discrete Element Modeling (DEM)*

Discrete Element Method is a simulation technique used to monitor the behaviour of each particle as a separate entity compared to other bulk continuum models. This method tracks the movement of each of the particles with in the space, records the collisions of each particle with the geometry as well as with each other and it is also subject to other force fields like gravity ? This model is based on the Newton's laws of the motion and is expressed as in Equations 1 and 2 :

$$m_i \frac{dv_i}{dt} = F_{i,net} \quad (1)$$

$$F_{i,net} = F_{i,coll} + F_{i,ext} \quad (2)$$

31 In the above equations m_i represents the mass of the particle, v_i represents the velocity of the
 32 particle, $F_{i,net}$ represents the net force on the particle, forces on the particle due to collisions and
 33 other external forces are represented in $F_{i,coll}$ $F_{i,ext}$ respectively.

34 The distance between each particle calculated at every time step and if the distance between
 35 two particles is less than the sum of the radii (for spherical particles) a collision between the two
 36 particles is recorded. The tolerance for overlap is low in the normal as well as the tangential
 37 direction?. Microscale DEM simulations are computationally demanding and simulations may
 38 take upto several days to replicate a few seconds of real time experiments. Many methods have
 39 been implemented to increase the speed of these simulations, such as scaling by increasing the size
 40 of the particles. These approximations are good in understanding the physics of the system but
 41 are not directly applicable to process-level simulations.

42 Thus, this method for granular powder is usually replaced by Population Balance Method
 43 (PBM) which is a much quicker aapproximation as it is a bulk model.

44 *2.2.2. PBM*

45 Population balance models predict how groups of discrete entities will behave on a bulk scale
 46 due to certain effects acting on the population with respect to time (?). In the context of process
 47 engineering and granulation, population balance models are used to describe how the number den-
 48 sities, of different types of particles, in the granulator change as rate processes such as aggregation
 49 and breakage reshape particles (?). In a general form of population balance model is shown here
 50 as equation 3.

$$\begin{aligned} \frac{\partial}{\partial t} F(\mathbf{v}, \mathbf{x}, t) + \frac{\partial}{\partial \mathbf{v}} [F(\mathbf{v}, \mathbf{x}, t) \frac{d\mathbf{v}}{dt}(\mathbf{v}, \mathbf{x}, t)] + \frac{\partial}{\partial \mathbf{x}} [F(\mathbf{v}, \mathbf{x}, t) \frac{d\mathbf{x}}{dt}(\mathbf{v}, \mathbf{x}, t)] \\ = \mathfrak{R}_{formation}(\mathbf{v}, \mathbf{x}, t) + \mathfrak{R}_{depletion}(\mathbf{v}, \mathbf{x}, t) + \dot{F}_{in}(\mathbf{v}, \mathbf{x}, t) - \dot{F}_{out}(\mathbf{v}, \mathbf{x}, t) \end{aligned} \quad (3)$$

51 In equation 3 \mathbf{v} is a vector of internal coordinates. In a granulation system \mathbf{v} would commonly
 52 describes the solid, liquid, and gas content of each type of particle. The vector \mathbf{x} represents external
 53 coordinates which account for spatial variance in the granulation system.

54 talk about kernels - empirical, semi mech, and DEM informed? talking about kernels then
 55 mentioning there is DEM informed could be GREAT SEGWAY to multi-physics models dotdotdot
 56 combined PBM DEM etc.

57 *2.2.3. multi-physics models*

58 general goal of mutli physics is best of two (or more worlds) accuracy of one but the time savings
59 of another etc.

60 finish with PBM DEM goals and past works? then mention it still can take a long time dotdotdot
61 SEGWAY into parallel computing?

62 *2.3. Parallel Computing and Computer Architectures*

63 *2.3.1. Overview*

64 The goal of parallel computing is to distribute large amounts of computation across many
65 compute cores to solve problems faster (?).

66 *2.3.2. Computer Architecture*

67 Parallel programs are commonly run on computer clusters. Computer clusters are a collection
68 of nodes interconnected by a high speed communication network for message passing from one node
69 to another. Each node has RAM and one or more CPUs, each CPU often has multiple compute
70 cores. Commonly nodes are manufactured with two CPUs, each CPU usually has around 8-16
71 cores **maybe too big of an assumption**. CPUs have their own memory called cache which is much
72 faster than RAM which is why cache utilization should be favoured over RAM if possible **phrasing?**.
73 RAM is often split between the CPU sockets, so each CPU has a direct connection to a RAM bus.
74 This means that if there are two CPUs on a node they will not be able to access the RAM that is
75 connected to the other CPU as quickly as the RAM it is directly connected to ?.

76 Computer architectures are often classified by these memory locality dynamics. There are
77 two distinct classes, distributed memory systems and shared memory systems. A cluster is a
78 combination of the two classes. Each node operates its memory independently of the other nodes
79 and explicit message passing is needed to share memory between nodes. While the cores on a node
80 operate in shared memory with each other since message passing is not explicitly needed to update
81 the memory each core as access too. All of these aspects of the computer architecture should be
82 considered when designing a parallel program for the best performance ? **maybe reword better to**
83 **make more like CACE paper. should I state network speed much slower than RAM so try to send**
84 **few messages as possible etc? could be more explicit in these statements?**

85 *2.3.3. Parallel Application Program Interfaces*

86 Message Passing Interface (MPI) is a common parallel computing application interface standard.
87 MPI is used for distributed memory parallel computing, this is because MPI will operate every
88 MPI process as a discrete unit that does not share memory with the other processes unless explicit
89 message passing is used. Even on shared a single node where the hardware is supports shared
90 memory computing, MPI will still operate it in a distributed memory fashion ?. Operating all cores
91 as distinct units also means they each need their own copy of all variables used for computation
92 which results in a large overall memory foot print compared to a same system if it was operated in
93 shared memory.

94 Open Multi-Processing (OMP) is another application program interface stand for parallel com-
95 puting. OMP is used for shared memory and can take advantage of shared memory systems which
96 can result in much faster computation. It does not work well on distributed systems though. This
97 prevents it from being used to efficiently carry out computations across multiple nodes of a cluster
98 simultaneously ?.

99 Since MPI is best for distributed computing and OMP is better for shared computing many
100 individuals have studied the performance of MPI vs MPI+OMP methods and many studies have
101 used MPI+OMP for scientific computation for improved performance. Often times a trade off is

102 made between optimizing a program for performance and trying to make it flexible enough to run
 103 on many different computer architectures [might need reference for this](#). A summary of some works
 104 addressing MPI+OMP methods for scientific computing and architecture features and concerns
 105 can be found in ?. In the conclusion to the work by ? it was found that hybrid methods for
 106 PBM allow the code flexibility for different architectures while still maintaining good performance.
 107 [should I mention load balancing techniques of gunawan paper?](#) In the work of ? only the external
 108 coordinates of the PBM were parallelized. In this current work external and internal calculations
 109 are parallelized.

110 3. Methods

111 3.1. DEM

112 3.1.1. LIGGGHTS

113 version, compilation settings, compilers used, etc

114 compiled with intel blak mvapich balbh bec on stmapede blah blah blah run using hybrid blah
 115 with socket affinities etc this resulted in highest performance etc

116 3.1.2. Geometry

117 [check other file Charles uploaded to see if that one was more "journal ready"](#)

118 The first step in creating a DEM model is the construction of geometry (i.e. a 3D computer
 119 aided drawing of an equipment). Here, the geometry of Lödige CoriMix CM5 continuous high
 120 shear granulator has been developed using the SolidWorksTM (Dassault Systèmes). This granulator
 121 consists of a high speed rotating element enclosed within a horizontal cylindrical casing. The casing
 122 (shown in Figure 1) consists of a cylinder with diameter of 120 mm at the inlet and 130 mm at
 123 the outlet and having a total length of 440 mm. A vertical inlet port is provided at one end of the
 124 casing and an angled outlet port is provided at the larger end of the case.

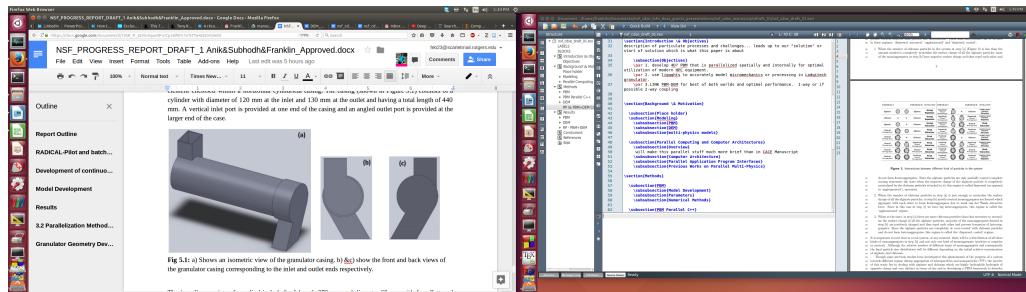


Figure 1: a) Shows an isometric view of the granulator casing. b) and c) show the front and back views of the granulator casing corresponding to the inlet and outlet ends respectively.

125 The impeller consists of a cylindrical shaft of length 370 mm and diameter 68 mm with four
 126 flattened sides 15 mm wide running along the axis. The blades are placed on these flattened sides
 127 as shown in figure 2. There are three different blade elements on the shaft (figure 2). At the
 128 granulator inlet, there are 4 paddle shaped feed elements following which there are 20 tear drop
 129 shaped shearing elements and finally 4 trapezoidal blades near the exit. All these elements are
 130 placed in a spiral configuration. The final configuration of the granulator is shown in figure 3.

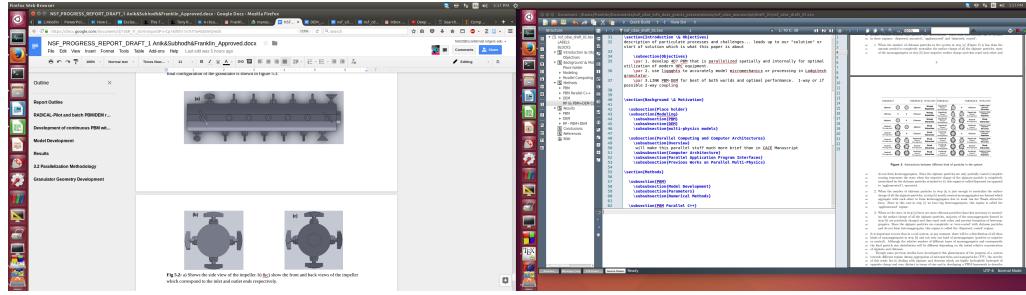


Figure 2: a) Shows the side view of the impeller. b) and c) show the front and back views of the impeller which correspond to the inlet and outlet ends respectively.

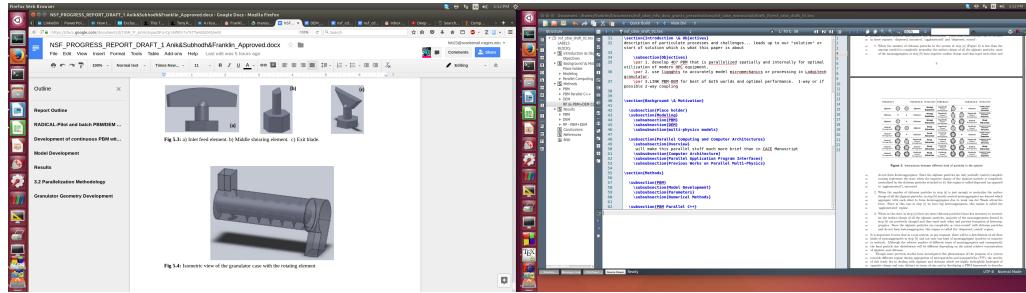


Figure 3: a) Inlet feed element. b) Middle shearing element. c) Exit blade. blah blah Isometric view of the granulator case with the rotating element

131 3.1.3. Meshing

132 After the geometry was built in solidworks the shell and impeller were exported as **non-binary**
 133 **STL files**. The coarsest output options(**include settings even if they were automatic may change**
 134 **from one version to another of SW**) were used to keep the STL files small and simple for faster
 135 computations times (**needs a citation? or is common knowledge?**). They were also exported not
 136 keeping there original coordinates (**1.too much info 2. what was option in SW for that so I can**
 137 **use that wording**) This resulted in the impeller having x-number-faces and y-number-points with
 138 approximately a file size of number KBs. The shell had x-number-faces and y-number-points and
 139 approx number KBs.

140 Meshlab was used to align the STL files for importing into LIGGGHTS. No mesh treatments
 141 were used on the STLS.

142 The meshes were then imported into LIGGGHTS using the write command (**more specific com-**
 143 **mand that we actually used?**). This resulted in 50 elements of the impeller file having "highly
 144 skewed elements angles | 0.5 deg?" that according to LIGGGHTS would degrade parallel perfor-
 145 mance. The shell did not have any skewed elements (**FUTURE SOLUTION?** - perhaps we can use
 146 **the output from liggghts exclusion list to find exact elements of issue. then we can use meshlab to**
 147 **exclude those peices or remesh thos individual pieces into better shapes with less skewed elements.**
 148 **might be better for a letter paper though**

149 3.1.4. DEM settings (input script, eqn param and relations used etc)

150 3.1.5. DEM Post data analysis

151 matlab script to check for constant flow/ steady state talk about the methods it uses etc?

152 matlab script to check for particles leaving etc make sure all good

153 3.2. PBM

154 3.2.1. Model Development

The main PBM equation developed for this work can be expressed as shown below:

$$\frac{d}{dt}F(s_1, s_2, x) = \mathfrak{R}_{agg}(s_1, s_2, x) + R_{break}(s_1, s_2, x) + \dot{F}_{in}(s_1, s_2, x) - \dot{F}_{out}(s_1, s_2, x) \quad (4)$$

155 citation?

156 where, $F(s_1, s_2, x)$ is the number of particles with an API volume of s_1 and an excipient volume
 157 of s_2 in the spatial compartment x . The rate of change of number of particles with time in
 158 different size classes depend on the rate of aggregation $\mathfrak{R}_{agg}(s_1, s_2, x)$ and the rate of breakage
 159 $\mathfrak{R}_{break}(s_1, s_2, x)$. Also, the rate of particles coming into, $F_{in}(s_1, s_2, x)$ and going out, $F_{out}(s_1, s_2, x)$
 160 of the spatial compartment due to particle transfer affect the number of particles in different size
 161 classes. The rate of change of liquid volume is calculated using the equation:

$$\begin{aligned} \frac{d}{dt}F(s_1, s_2, x)l(s_1, s_2, x) &= \mathfrak{R}_{liq,agg}(s_1, s_2, x) + \mathfrak{R}_{liq,break}(s_1, s_2, x) + \dot{F}_{in}(s_1, s_2, x)l_{in}(s_1, s_2, x) \\ &\quad - \dot{F}_{out}(s_1, s_2, x)l_{out}(s_1, s_2, x) + F(s_1, s_2, x)\dot{l}_{add}(s_1, s_2, x) \end{aligned} \quad (5)$$

162 where, $l(s_1, s_2, x)$ is the amount of liquid volume in each particle with API volume of s_1 and
 163 excipient volume of s_2 in the spatial compartment x . $\mathfrak{R}_{liq,agg}(s_1, s_2, x)$ and $\mathfrak{R}_{liq,break}(s_1, s_2, x)$ are
 164 respectively the rates of liquid transferred between size classed due to aggregation and breakage.
 165 $l_{in}(s_1, s_2, x)$ and $l_{out}(s_1, s_2, x)$ are respectively the liquid volumes of the particles coming in and
 166 going out of the spatial compartment. $l_{add}(s_1, s_2, x)$ is the volume of liquid acquired by each
 167 particle in the compartment at every time step due to external liquid addition.

Similarly, the rate of change of gas volume is calculated using the following equation:

$$\begin{aligned} \frac{d}{dt}F(s_1, s_2, x)g(s_1, s_2, x) &= \mathfrak{R}_{gas,agg}(s_1, s_2, x) + \mathfrak{R}_{gas,break}(s_1, s_2, x) + \dot{F}_{in}(s_1, s_2, x)g_{in}(s_1, s_2, x) \\ &\quad - \dot{F}_{out}(s_1, s_2, x)g_{out}(s_1, s_2, x) + F(s_1, s_2, x)\dot{g}_{cons}(s_1, s_2, x) \end{aligned} \quad (6)$$

168 citation?

169 where, $g(s_1, s_2, x)$ is the gas volume of each particle with API volume of s_1 and excipient volume
 170 of s_2 in the spatial compartment x . $\mathfrak{R}_{gas,agg}(s_1, s_2, x)$ and $\mathfrak{R}_{gas,break}(s_1, s_2, x)$ are respectively
 171 the rates of gas transferred between size classed due to aggregation and breakage. $g_{in}(s_1, s_2, x)$
 172 and $g_{out}(s_1, s_2, x)$ are respectively the gas volume of the particles entering and leaving the spatial
 173 compartment. $g_{cons}(s_1, s_2, x)$ is the volume of gas coming out of each particle in the compartment
 174 at every time-step due to consolidation of the particles.

The rate of aggregation, $\mathfrak{R}_{agg}(s_1, s_2, x)$ in Equation 4 is calculated as

$$\begin{aligned} \mathfrak{R}_{agg}(s_1, s_2, x) &= \frac{1}{2} \int_0^{s_1} \int_0^{s_2} \beta(s'_1, s'_2, s_1 - s'_1, s_2 - s'_2, x) F(s'_1, s'_2, x) F(s_1 - s'_1, s_2 - s'_2, x) ds'_1 ds'_2 \\ &\quad - F(s_1, s_2, x) \int_0^{s_{max_1} - s_1} \int_0^{s_{max_2} - s_2} \beta(s_1, s_2, s'_1, s'_2, x) F(s'_1, s'_2, x) ds'_1 ds'_2 \end{aligned} \quad (7)$$

175 citation?

where, the aggregation kernel, $\beta(s_1, s_2, s'_1, s'_2, x)$ is expressed as

$$\begin{aligned} \beta(s_1, s_2, s'_1, s'_2, x) &= \beta_o * (V(s_1, s_2, x) + V(s'_1, s'_2, x))^\gamma * (c(s_1, s_2, x) \\ &\quad + c(s'_1, s'_2, x))^\alpha \left(1 - \frac{(c(s_1, s_2, x) + c(s'_1, s'_2, x))^\delta}{2} \right)^\alpha \end{aligned} \quad (8)$$

176 citation?

177 where, β_o , α , δ and γ are aggregation rate constants, $V(s_1, s_2, x)$ and $V(s'_1, s'_2, x)$ are the
178 volumes of the aggregating particles. $c(s_1, s_2, x)$ and $c(s'_1, s'_2, x)$ are the external liquid fraction of
179 the aggregating particles.

180 Similarly, the breakage rate is expressed as-

$$\mathfrak{R}_{break}(s_1, s_2, x) = \int_0^{s_{max1}} \int_0^{s_{max2}} K_{break}(s'_1, s'_2, x) F(s'_1, s'_2, x) ds'_1 ds'_2 - K_{break}(s_1, s_2, x) F(s_1, s_2, x) \quad (9)$$

181 citation?

182 where, the breakage kernel $K_{break}(s_1, s_2, x)$ is formulated as

$$K_{break}(s_1, s_2, x) = \left(\frac{4}{15\pi} \right)^{\left(\frac{1}{2}\right)} G_{shear} \exp \left(-\frac{B}{R(s_1, s_2, x)} \right) \quad (10)$$

183 citation?

184 where, G_{shear} is the shear rate exerted by the impeller on the granules. $R(s_1, s_2, x)$ is the
185 radius of the granule that breaks and B is the breakage kernel constant. G_{shear} is calculated as
186 $\frac{\nu_{impeller} * D_{impeller} * PI}{60}$ where $\nu_{impeller}$ and $D_{impeller}$ are respectively the rotational speed and diameter
187 of the impeller.

188 The rate of increase of liquid volume of one particle, $\dot{l}_{add}(s_1, s_2, x)$ is expressed as $\frac{(s_1 + s_2)(\dot{m}_{spray}(1 - c_{binder}) - \dot{m}_{evap})}{m_{solid}(x)}$
189 where, $(s_1 + s_2)$ is the total solid volume of the particle; \dot{m}_{spray} is the rate of external liquid ad-
190 dition, c_{binder} is the concentration of binder in the external liquid (which is assumed to be zero
191 in this case as pure liquid is added); \dot{m}_{evap} is the rate of evaporation of liquid from the system
192 (which is also assumed to be zero in this case) and m_{solid} is the total amount of solid present in
193 the compartment.

194 The rate of decrease in gas volume per particle due to consolidation is calculated using the
195 following expression:

$$\dot{g}_{cons}(s_1, s_2, x) = c * (\nu_{impeller})^\omega * V(s_1, s_2, x) \frac{(1 - \epsilon_{min})}{s} [g(s_1, s_2, x) + l(s_1, s_2, x) - (s_1 + s_2) \frac{\epsilon_{min}}{1 - \epsilon_{min}}] \quad (11)$$

196 where, c and ω are the consolidation constants; $\nu_{impeller}$ is the impeller rotational speed;
197 $V(s_1, s_2, x)$ is the volume of particle, ϵ_{min} is the minimum porosity; $g(s_1, s_2, x)$ and $l(s_1, s_2, x)$
198 are respectively the gas and liquid volume of the particle.

199 Particle transfer rate, $F_{out}(s_1, s_2, x)$ in Equation 4 is calculated as $F(s_1, s_2, x) * \frac{\nu_{compartment(x)} * dt}{d_{compartment}}$
200 where, $\nu_{compartment(x)}$ and $d_{compartment}$ are respectively the average velocity of particles in com-
201 partment x and the distance between the mid-points of two adjacent compartment, which is the
202 distance particles have to travel to move to the next spatial compartment. dt is the time-step. The
203 values of various parameters used in the model are provided in Table 1.

204 3.2.2. Parameters

205 3.3. PBM Parallel C++

206 3.3.1. Discretization & Parallelizing PBM

207 To solve the PBM numerically it was discretized using a finite element method type solution. To
208 obtain the most optimal parallel performance, when solving the PBM, work loads were distributed

Table 1: Parameters for PBM from Anik's hetero. agg. paper. currently place holder

Parameter	Symbol	Value	Units
Boltzmann constant	k	$1.3806488 \times 10^{-23}$	$m^2 \text{ kg s}^{-2} K^{-1}$
Charge of electron	e	$1.60217657 \times 10^{-19}$	Coulombs
Avogadro Number	N_A	6.0221413×10^{23}	—
Hamaker constant	A_H	3×10^{-21}	J
Hydration force constant	F_0	10^{-2}	$N m^{-1}$
Temperature of the medium	T	298	K
Viscosity of the medium	μ	0.8999×10^{-3}	Pa.s
Permittivity of the medium	$\epsilon_0 \epsilon_r$	6.93×10^{-10}	$C^2 N^{-1} m^{-2}$
Valence of ions in medium	z	1	—
Bulk concentration of ions in medium	C^b	1×10^{-2}	$kg m^{-3}$
Debye length	$\frac{1}{\kappa}$	1.3581×10^{-7}	m
Decay length	δ_0	6×10^{-10}	m
Density of alginate	$\rho_{Alginate}$	1050	$kg m^{-3}$
Density of chitosan	$\rho_{Chitosan}$	1000	$kg m^{-3}$
Surface potential of alginate	$\Psi_{Alginate}$	-46×10^{-3}	Volts
Surface potential of chitosan	$\Psi_{Chitosan}$	56×10^{-3}	Volts
Volume of the system	V	10×10^{-6}	m^3
Volume of the smallest alginate bin	a_1	1.5×10^{-17}	m^3
Volume of the smallest chitosan bin	c_1	0.3×10^{-17}	m^3
Aggregation kernel constant	K_0	5×10^9	—
Simulated Process Time	t	10	s
Simulation Time-Step	dt	0.01	s

in a manner which took into account the shared memory and distributed memory aspects of the clusters the PBM was being run on. To parallelize the model in a way which could use shared and distributed methods of OMP and MPI were used.

One MPI process was used per CPU socket and one OMP process was used per CPU core, as authors (?) found it resulted in the best performance. MPI was used for message passing from one node to another while OMP was used for calculations on each node that could be efficiently solved using a shared memory system i.e. calculations were inter-dependent but could be computed simultaneously.

Pseudo code is presented below illustrating how the calculations are distributed and carried out during the simulation. For each time step the MPI processes are made responsible for a specific chunk of the spatial compartments. Then each OMP thread, inside of each MPI process, is allocated to one of the cores of the multi-core CPU the MPI process is bound too. The OMP processes divide up and compute \mathfrak{R}_{agg} and \mathfrak{R}_{brk} . (include more detail about how they do it? last paper reviewer complained that could not understand figure by JUST reading what I wrote about it in meat of paper)

After \mathfrak{R}_{agg} and \mathfrak{R}_{brk} are calculated the MPI processes calculate the new PSD value for their chunk at that specific time step, $F_{t,c}$. The slave processes send their $F_{t,c}$ to the master processes which collects them into the complete $F_{t,all}$. The master process then broadcasts the $F_{t,all}$ value to all slave processes.

228 A crucial feature of the PBM is that the current PSD ($F_{t,all}$) value is used to compute a new
 229 time step size for the next iteration. This means all of the MPI processes need to have the same
 230 dynamic time step size at each iteration for the calculations to be properly carried out in parallel.
 231 Since the completely updated $F_{t,all}$ value is shared before calculating a new time step each process
 232 will have the same $F_{t,all}$ value. As a result each process calculates the same size for the new time
 233 step. **Did not include the liquid and gas PBMs in this but hoping they will be some what assumed?**
 234 **Also the Ragg omp distributed work is an a what about private OMP vars specified that has impact**
 235 **on how model is solved etc. Should look into this. might change based on locking/blocking tests**
 236 **that need to be implemented still.**

Algorithm 1 Pseudo code

```

while  $t < t_{final}$  do
    // the spatial domain is divided into equal chunks (with in 1 bin size)
    // each MPI process is assigned on chunk of spatial domain shown as  $c_{low}$  to  $c_{up}$ 
    // sum all  $c_{low_i}$  to  $c_{up_i}$  is = to [0,numCompartments]
    for each MPI processes do  $c = c_{low_i}$  to  $c_{up_i}$ 
        // each MPI process is further divided with OMP to take advantage of multi-core CPU
        // each OMP process is allocated to a single compute core
        //  $\Re$  integrals (i1)  $\int_0^{s_2}$ , (i2)  $\int_0^{s_{max2}-s_2}$ , and (i3)  $\int_0^{s_{max2}-s_2}$  are divided into smaller integrals
        //  $\int_{i_1 low_n}^{i_1 up_n}$ ,  $\int_{i_2 low_n}^{i_2 up_n}$ , and  $\int_{i_3 low_n}^{i_3 up_n}$  which are solved by the "n" OMP processes
        // allocated to that MPI process (CPU)
        for each OMP process do

            
$$\Re_{agg}(s_1, s_2, c) = \frac{1}{2} \int_0^{s_1} \int_{i_1 low_n}^{i_1 up_n} \beta(s'_1, s'_2, s_1 - s'_1, s_2 - s'_2, c) F(s'_1, s'_2, c) F(s_1 - s'_1, s_2 - s'_2, c) ds'_1 ds'_2$$

            
$$- F(s_1, s_2, c) \int_0^{s_{max1}-s_1} \int_{i_2 low_n}^{i_2 up_n} \beta(s_1, s_2, s'_1, s'_2, c) F(s'_1, s'_2, c) ds'_1 ds'_2$$


            
$$\Re_{break}(s_1, s_2, c) = \int_0^{s_{max1}} \int_{i_3 low_n}^{i_3 up_n} K_{break}(s'_1, s'_2, c) F(s'_1, s'_2, c) ds'_1 ds'_2 - K_{break}(s_1, s_2, c) F(s_1, s_2, c)$$


        end for

        
$$F_{t,c} = \frac{\Delta F(s_1, s_2, c)}{\Delta t} \Delta t + F(s_1, s_2, c)_{t-1}$$

        
$$= (\Re_{agg}(s_1, s_2, c) + \Re_{break}(s_1, s_2, c) + \dot{F}_{in}(s_1, s_2, c) - \dot{F}_{out}(s_1, s_2, c)) \Delta t + F(s_1, s_2, c)_{t-1}$$


    end for
    MPI Send  $F_{t,c}$  to Master MPI process
    MPI Recv  $F_{t,c}$  from MPI all slave processes
    Master consolidate all  $F_{t,c}$  chunks into a complete  $F_{t,all}$ 
    Master does inter-bin particle transfers (updates  $F_{t,all}$ )
    MPI Broadcast  $F_{t,all}$  to all slave processes
     $t_{new} = t + timestep$ 
end while

```

237 3.4. RP & PBM+DEM Communication

238 4. Results

239 4.1. PBM

240 4.1.1. PBM Validation

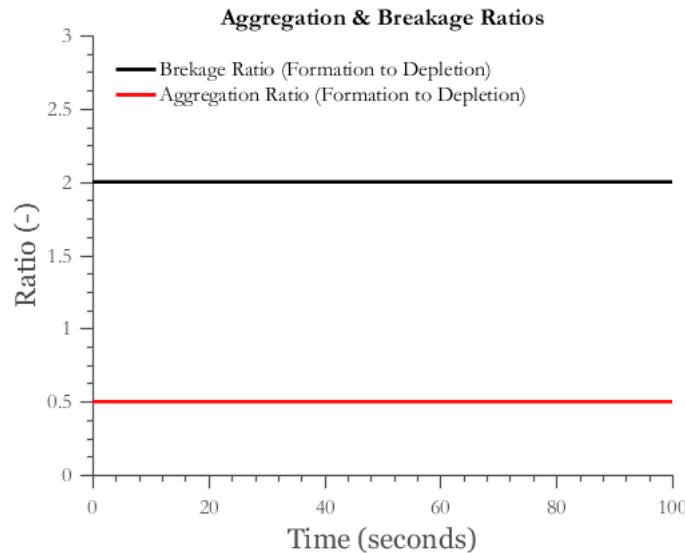


Figure 4: Ratio of formation-to-depletion through aggregation and breakage over time. Breakage ratio of 2 and aggregation ratio of 0.5 indicate mass conservation in the model. **NOTE DID NOT HAVE .fig file for this figure so it is in as JPG will need to replace**

241 The ratio between the number of particles formed due to aggregation and the number of particles
242 depleted due to aggregation and the ratio of the number of particles formed due to breakage to the
243 number of particles depleted due to breakage are plotted. In aggregation two particles agglomerate
244 to form one particle and in breakage one particle breaks to form two particles. So, these ratios
245 are expected to be 0.5 and 2 respectively. As can be seen from Figure 4, these ratios are accurate
246 confirming that mass is conserved accurately in the model.

247 The granulator was divided into 3 compartments spatially and the total volume, solid volume
248 and pore volume and the median diameter d_{50} in each compartment were plotted to study the
249 granulation behaviour and are shown in Figure 5.

250 It can be seen from Figure 5a that the total volume starts to increase first in compartment 1
251 followed by compartment 2 and then compartment 3. This happens as gradually particles entering
252 compartment 1 moves to the other compartment due to particle transfer from compartment 1 to
253 compartment 2 and then compartment 3. In Figure 5b it is observed that the solid volume similar
254 to the total volume increases first in compartment 1 and last in compartment 3. The solid volume
255 becomes constant and equal in all the compartments at around 30-50 seconds and steady state is
256 reached when the rate of particle volume being transported through the compartments and leaving
257 the system is equal to the rate of particles entering the system. Although, as seen in Figure 5c
258 the pore volume which is the sum of the gas and the liquid volume is highest in compartment 3
259 and lowest in compartment 1. This happens due to the external liquid addition to the system. As
260 the particles move from compartment 1 to compartment 3, they gradually acquire a higher amount
261 liquid, thereby increasing the pore volume. In Figure 5d, the D_{50} is seen to be increasing from

262 compartment 1 to 3. This happens because of the size enlargement of large particles coming in
 263 from the previous compartment because of the external liquid added to each compartment and a
 264 longer residence time in the granulator.

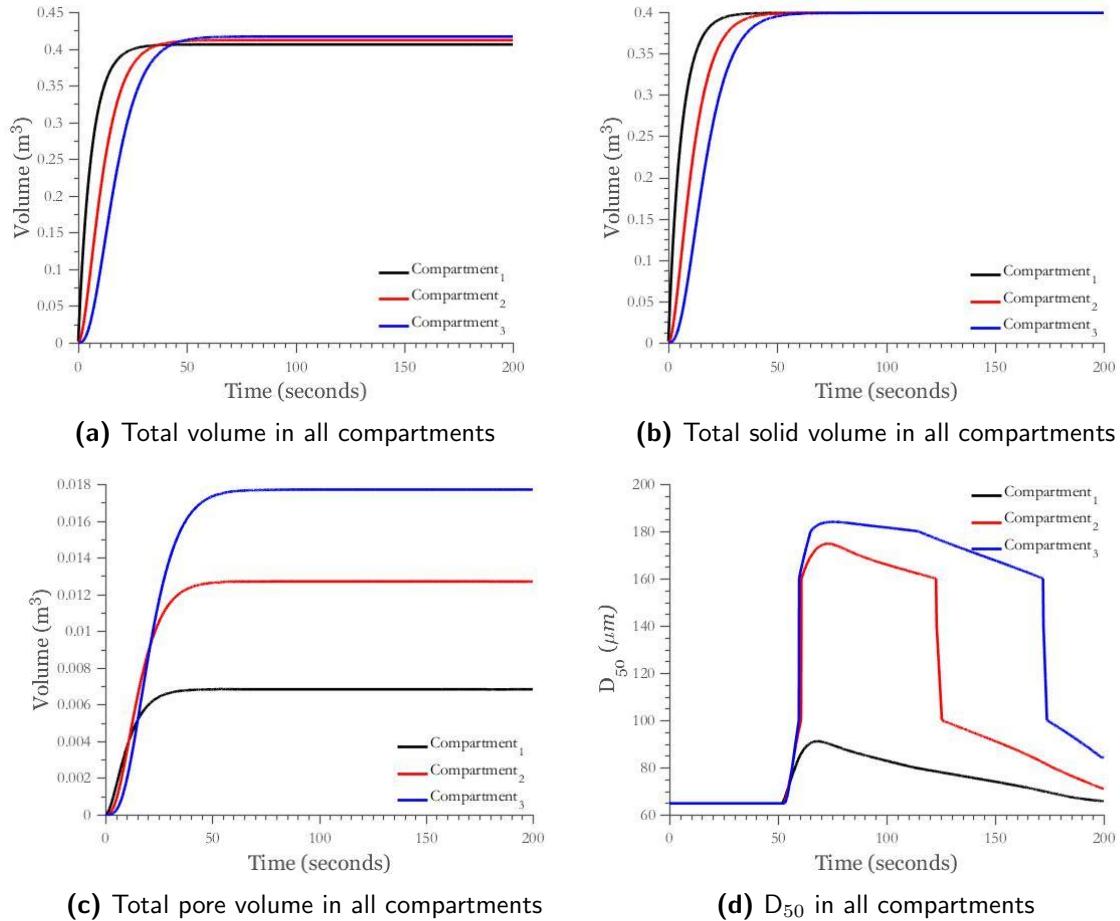


Figure 5: Volume and D_{50} in all compartments over time. Volumes become constant as steady state is reached. Median diameter increases and then decreases as bigger particles leave the system and smaller particles occupy that volume.

265 *4.1.2. Parallel C++ PBM Validation*

266 show PSD or D_{50} is the same as Matlab or serial PBM

267 1. fig D_{50} Matlab vs Parallel

268 *4.1.3. Parallel PBM Performance*

269 show that RP has minimal impact on performance

270 show that performance is mostly unaffected by RP

271 1. fig scaling

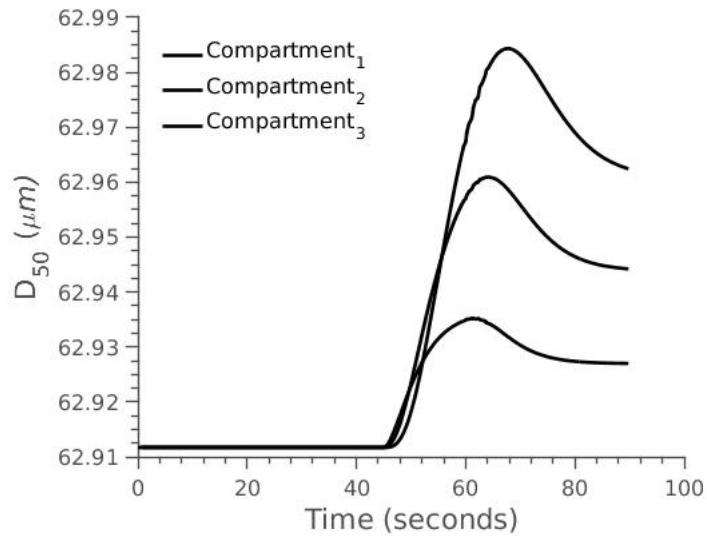


Figure 6: D_{50} of Matlab PBM vs Parallel PBM

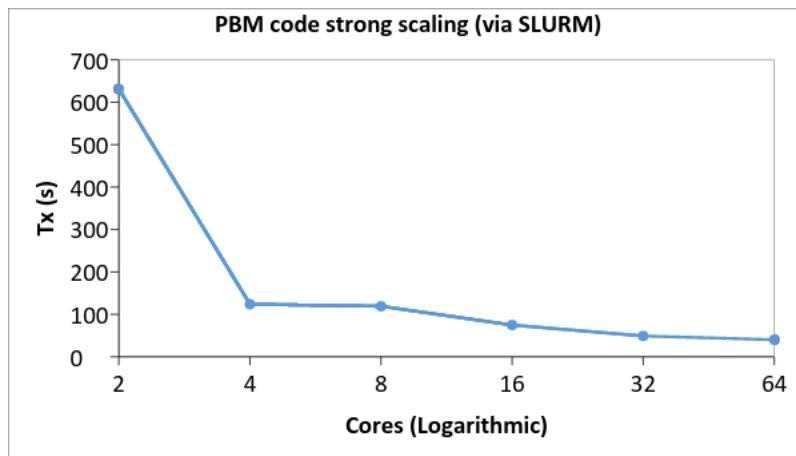


Figure 7: PBM strong scale slurm

272 2. fig scaling w/ RP

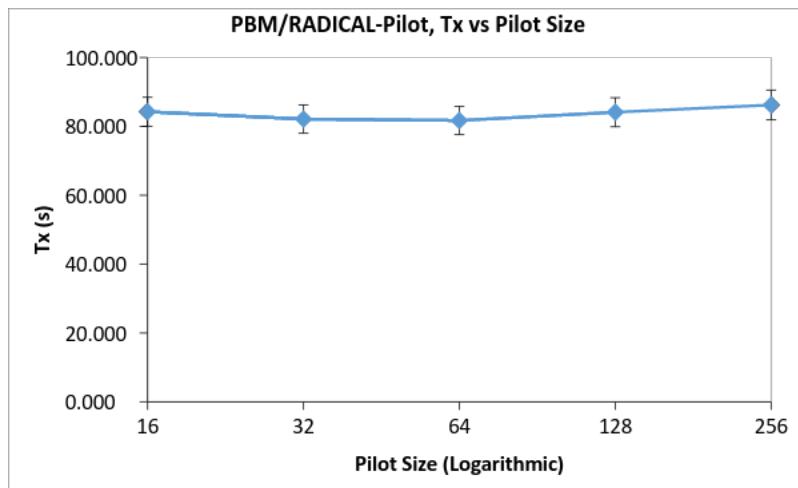


Figure 8: PBM strong scale RP

273 4.1.4. Parallel PBM Parameter space and Parameter Estimation

- 274 I. show how effective parallel pbm is for parameter estimation
 275 II. Find/ explore ranges of DEM data that PBM can use to find Critical parameters and
 276 sensitivities will be useful to us in linking and in picking best DEM parameters to vary and best
 277 parameters for PBM+DEM code
 278 1. fig range of some parameters?
 279 2. fig range of other pbm parameter ?

280 4.2. DEM

281 4.2.1. DEM Validation and Parameter Space Studies

- 282 show that DEM is somewhat behaving like a real system
 283 fig constant flow reached by end of DEM simulation

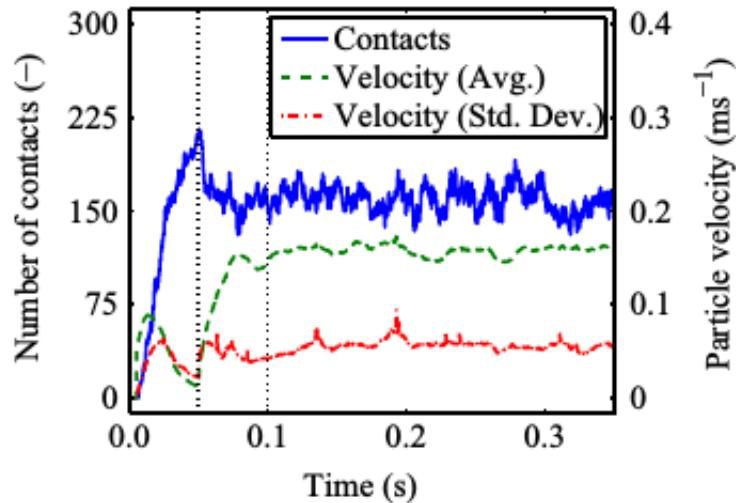


Fig. 3. Time trajectories from DEM simulation showing number of contacts between 1-mm particles with particles of the same size, and the average and standard deviation of the velocity of 1-mm particles. Particles are added at time=0 s with a median diameter of 1.5 mm and a standard deviation of 0.5 mm. Dotted lines indicate start of rotation of the screw and start of data collection, respectively.

Figure 9

284 fig RTD
 285 show affects of certain parameters on DEM and which ones are most critical to outcomes - will
 286 help decide on PBM+DEM parameters to study in later section
 287 fig vary impeller RPM see how RTD or hold up changes
 288 fig vary PSD (range and/or particle sizes) to see how C_{coll} etc will be affected - important for
 289 PBM Kernel

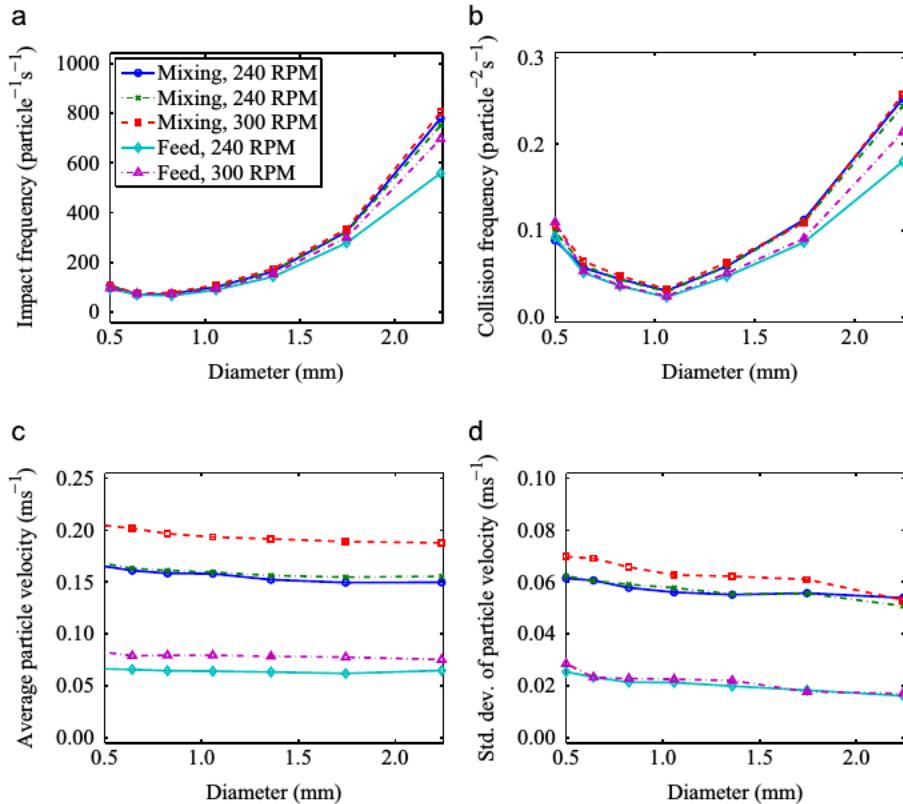


Fig. 6. DEM results showing the effects of screw element type and rotational speed on (a) impact frequency, (b) collision frequency with 1-mm particles, (c) average particle velocity, and (d) standard deviation of particle velocity for each size class.

Figure 10: fig showing sensitivity of C_{coll} and etc to RPM

290 fig vary impeller RPM see C_{coll} changes

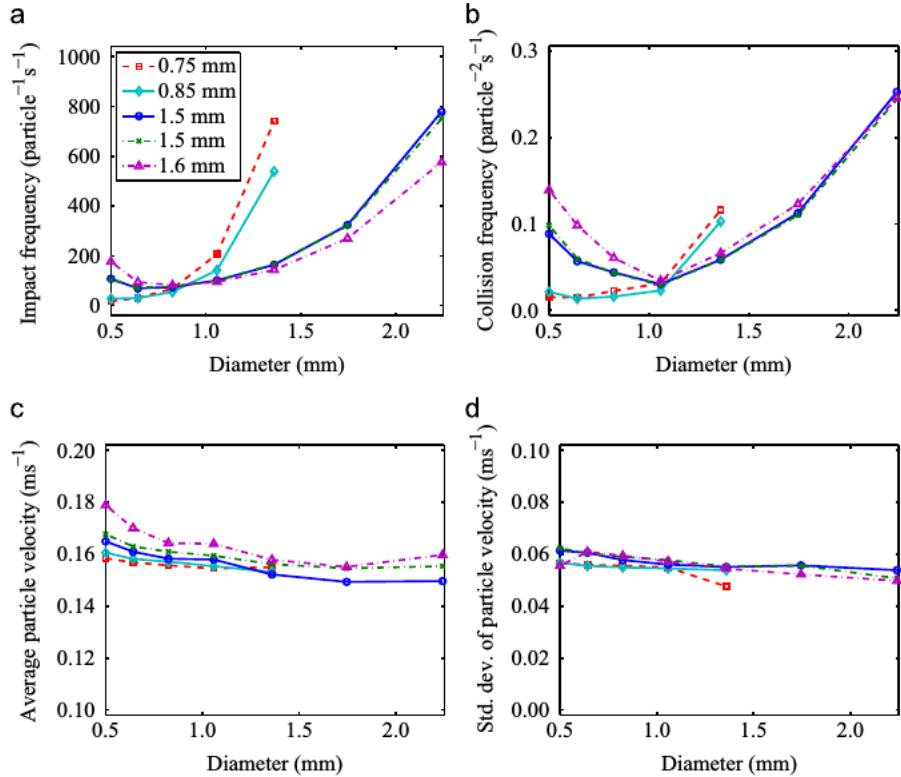


Fig. 4. DEM results showing the effects of size distribution on (a) impact frequency, (b) collision frequency with 1-mm particles, (c) average particle velocity, and (d) standard deviation of particle velocity for each size class. Median diameters are listed in the legend. The standard deviation of the diameter is fixed at 0.2 mm for the smallest two simulations and 0.5 mm for the larger simulations.

Figure 11: fig from dana 2015 mechanistic bi-directional

291 4.2.2. DEM Performance

292 show that performance is mostly unaffected by RP
293 1. fig scaling

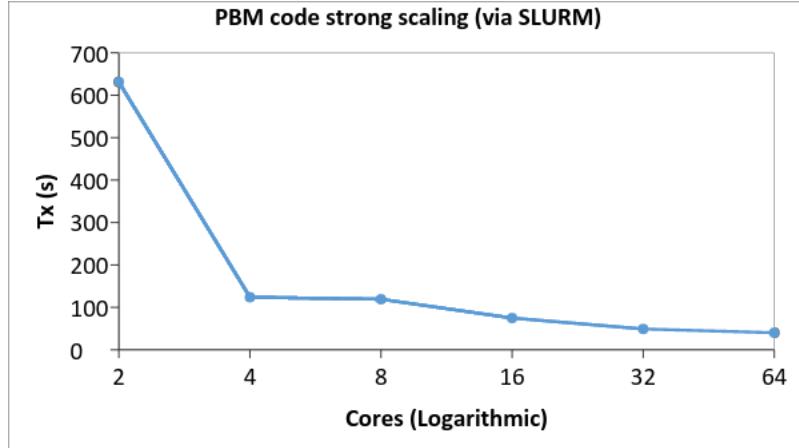


Figure 12: DEM scale just slurm

294 2. fig scaling w/ RP

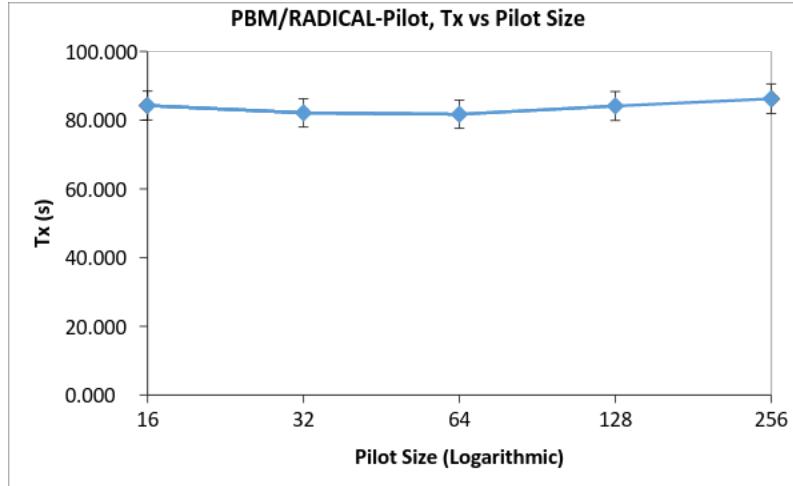


Figure 13: DEM scale with RP

295 4.3. PBM+DEM - RP

296 4.3.1. PBM+DEM Validation/Accuracy?

297 4.3.2. PBM+DEM Performance

298 strong scaling

fig PBM + DEM RP strong scaling

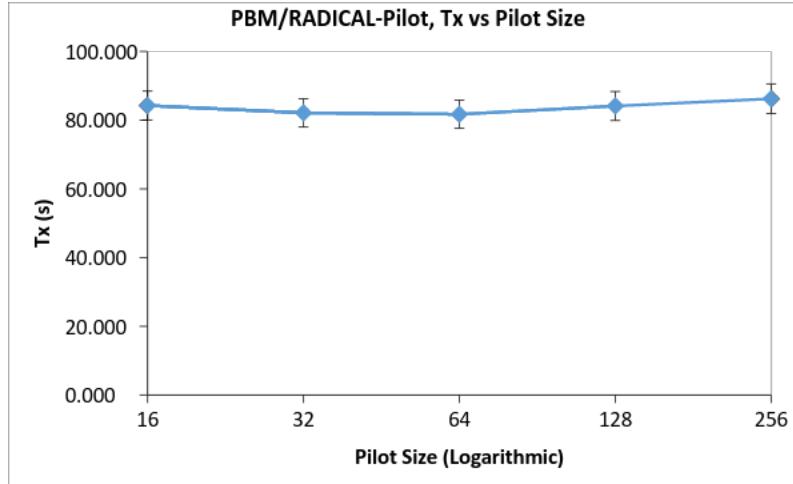


Figure 14: PBM+DEM scale with RP

299

300 4.3.3. PBM+DEM Parameter studies

301 show how PBM+DEM captures multi-physics as parameters changed. helps validate and support model development. show we have made a useful tool for future work.

303 fig

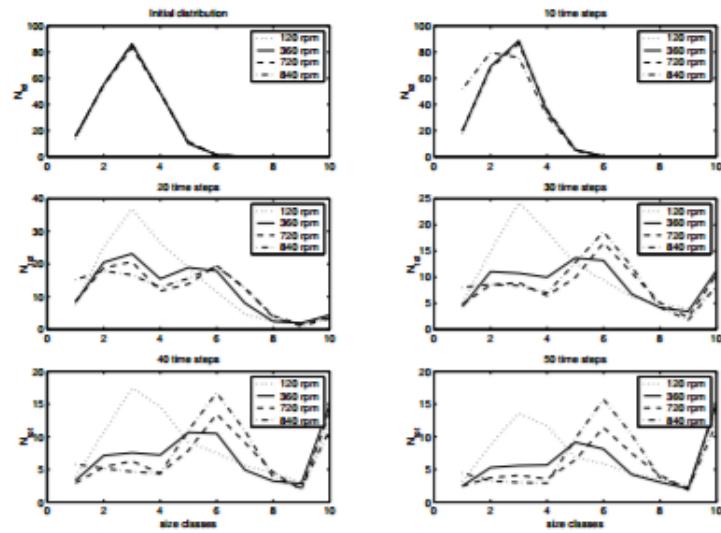


Figure 8: PSD evolution for simulations run at 120 rpm, 360 rpm, 720 and 840 rpm.

Figure 15: PBM+DEM scale with RP

304 PSD over time for different impeller RPM

305 **5. Conclusions**

306 **References**