

A new predictive tool for design and operational optimisation of spray dryers

Advanced Process Modelling Forum
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On behalf of team:

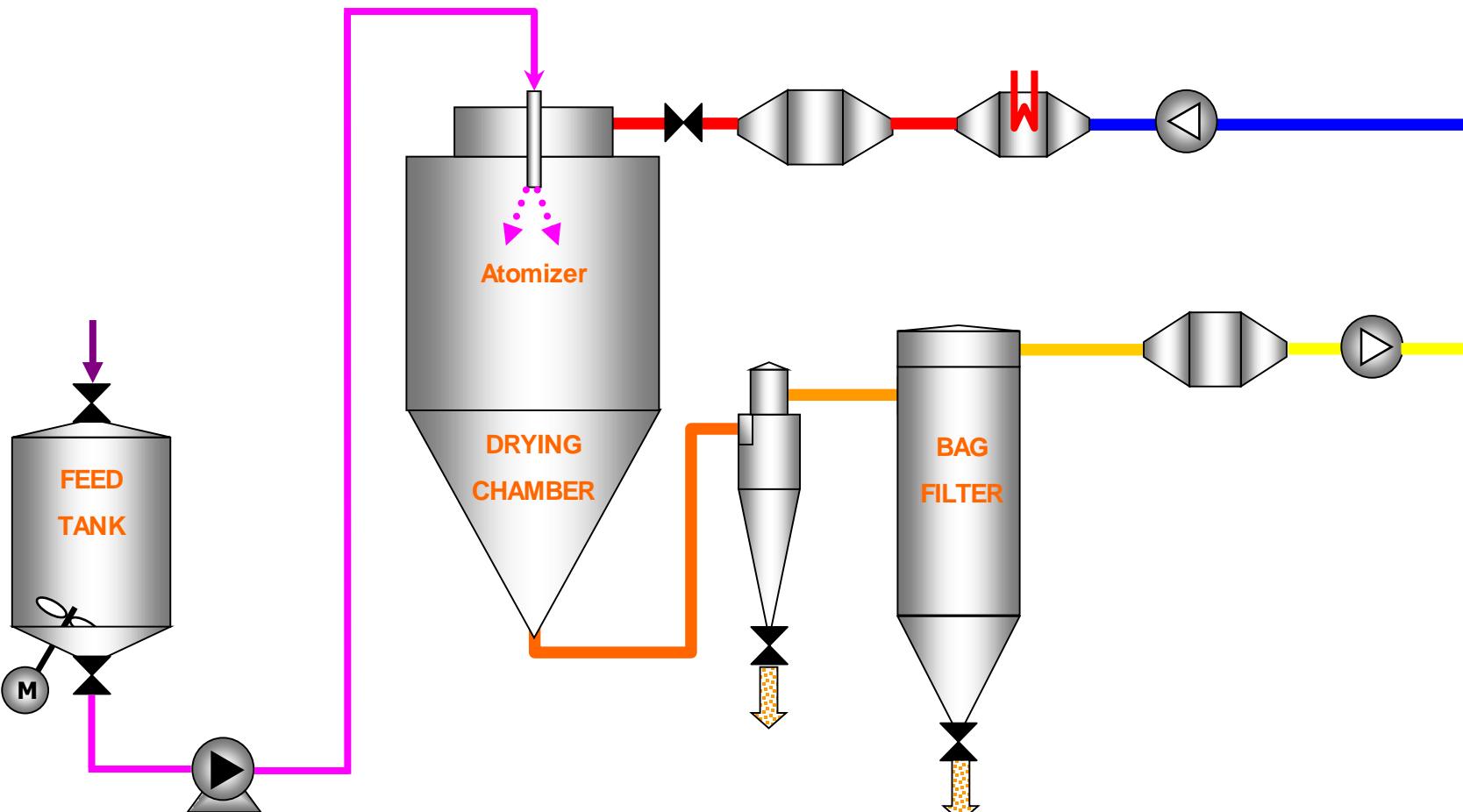
Sean Bermingham (PSE)

Poul Bach (Novozymes)

Luis Martindejuan (P&G)

Mazaher Molaei, Muzammil Ali, Peter Heggs, Tariq Mahmud & Mojtaba Ghadiri (University of Leeds)

Typical Co-current Spray Drying Process



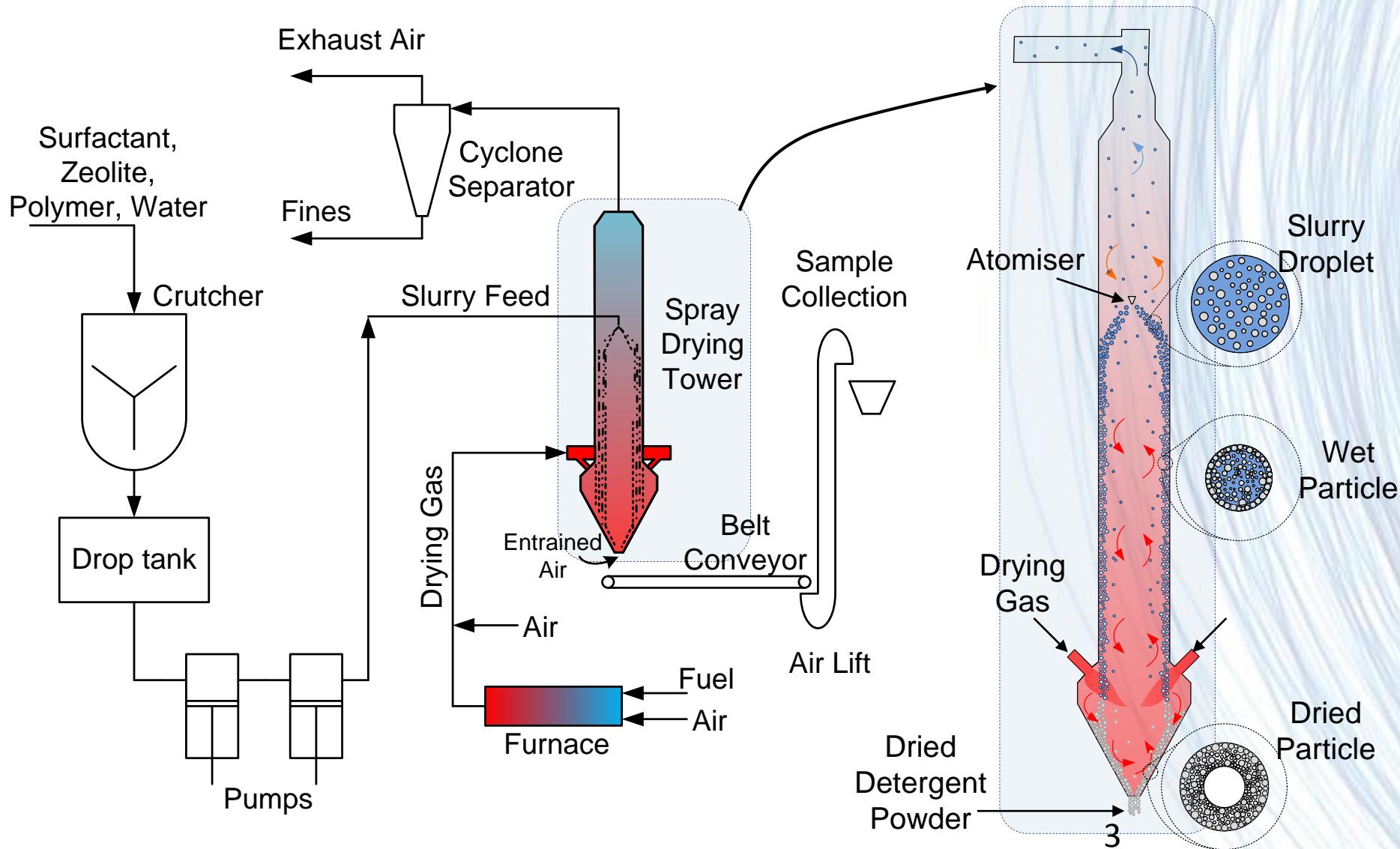
Co-current tower

Product particle size range: 5-200 microns

Spray Drying Process Flow Diagram for Detergent Powder Manufacture



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Introduction

- **Spray drying is commonly used in many different industries**
 - pharmaceuticals, foods, detergents, enzymes
- **Complex interacting phenomena determine critical quality attributes of product**
- **Desire to understand process to optimise and control**
 - product quality i.e. particle properties
 - production rate
 - production reliability, e.g build-up
- **Important to understand droplet drying history in a spray dryer particularly for thermally sensitive ingredients**
- **Current modelling mainly concentrated at two extremes**
 - **Mass and energy balance models**
 - **Computationally demanding and inefficient CFD calculations**

A high fidelity, efficient and user-friendly modelling tool that can be used to increase understanding, optimise existing processes and explore operation space

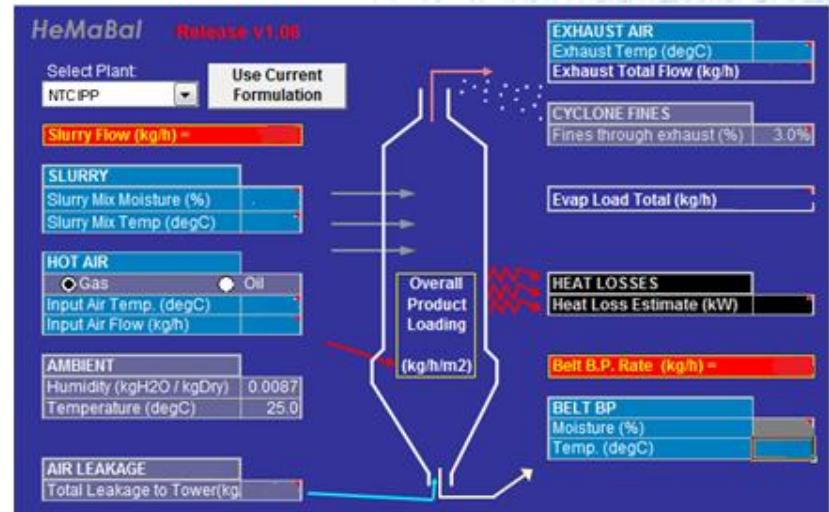
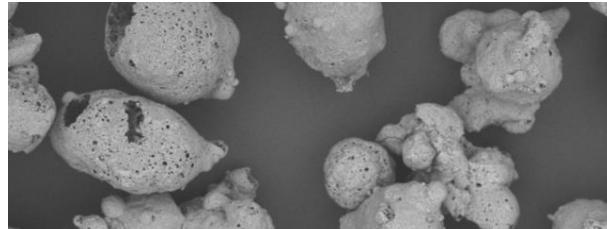
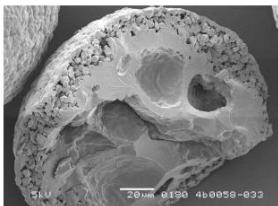
The Overall Challenge

Predictability: Process results and product properties:

- Currently can predict rate or moisture content (overall)
- Cannot predict PSD and moisture, porosity and chemistry per size range.
- Cannot be used to scale-up from mini -> macro -> manufacture or across scales.

Innovation: influencing the cycle:

- How do cut innovation cycle?
- Can we use the model as a source of innovation? Design novel morphologies.
- Understand product-process interplay!



Simplicity: Not CFD:

- Available to typical process engineer without training/expertise on using complex tools such as CFD.
- Ensure we do not need to re-run a CFD model for each scenario.
- Need to solve population balance equations efficiently.

Innovate UK (formerly TSB) funded consortium

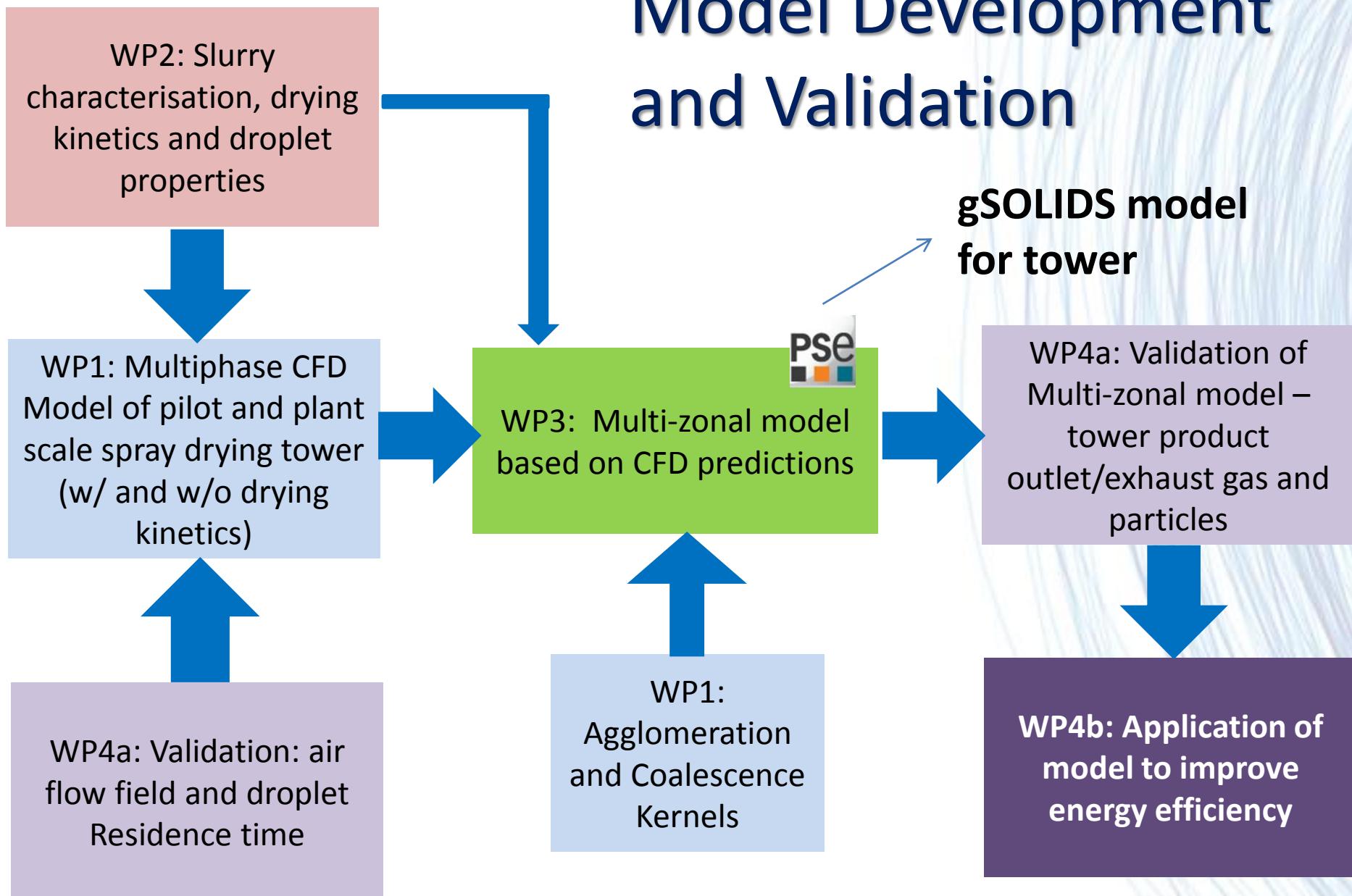


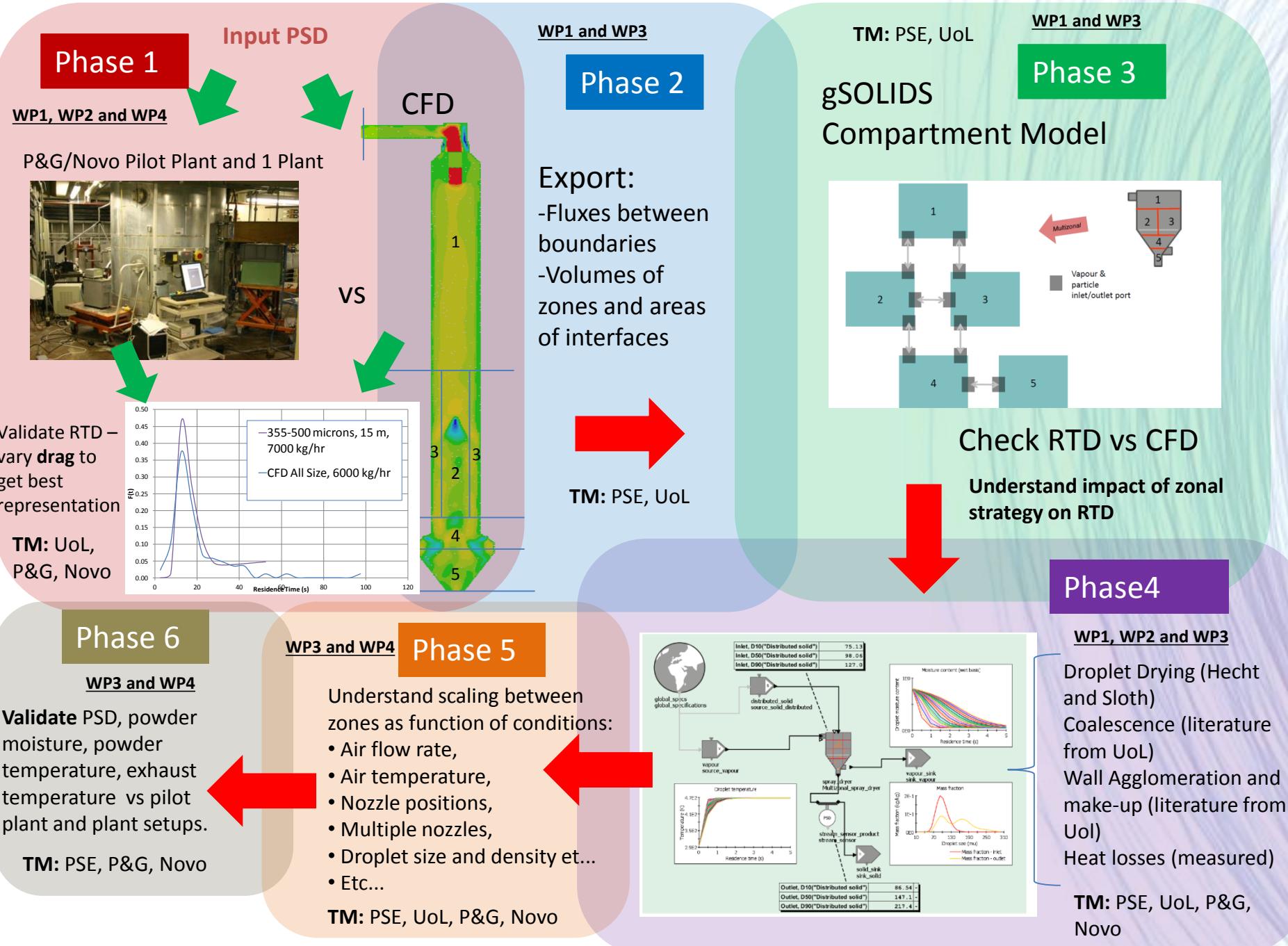
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Technology Strategy Board
Driving Innovation



Model Development and Validation





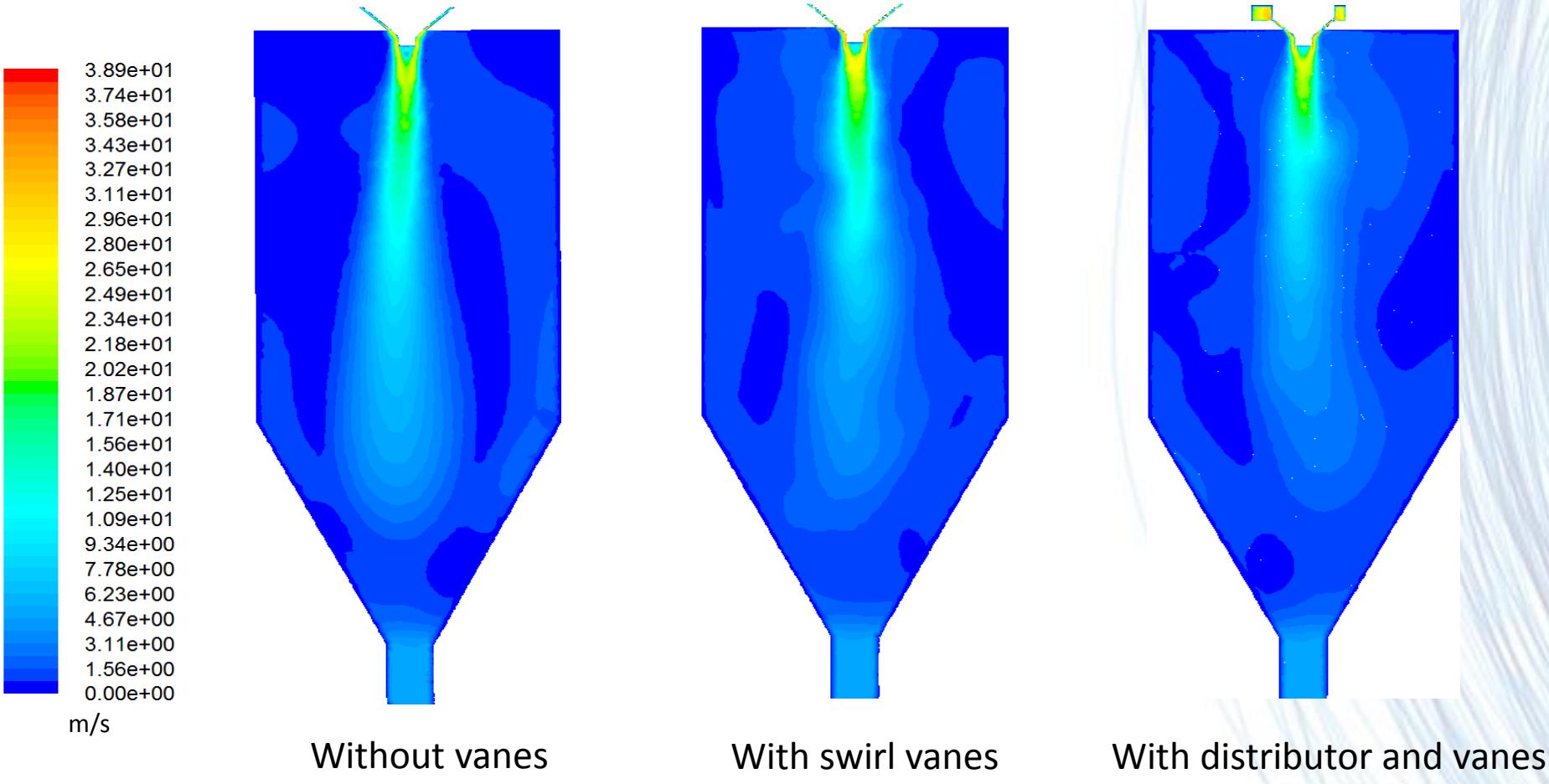
What do we need from CFD?

- How good are multi-phase CFD models at predicting the tower performance?
 - Issues input data, quality validation data
- What do the air and particle flow patterns tell us about how to create zones?
- Understand if it possible to ‘scale’ air and particle flows.

Air velocities in co-current tower



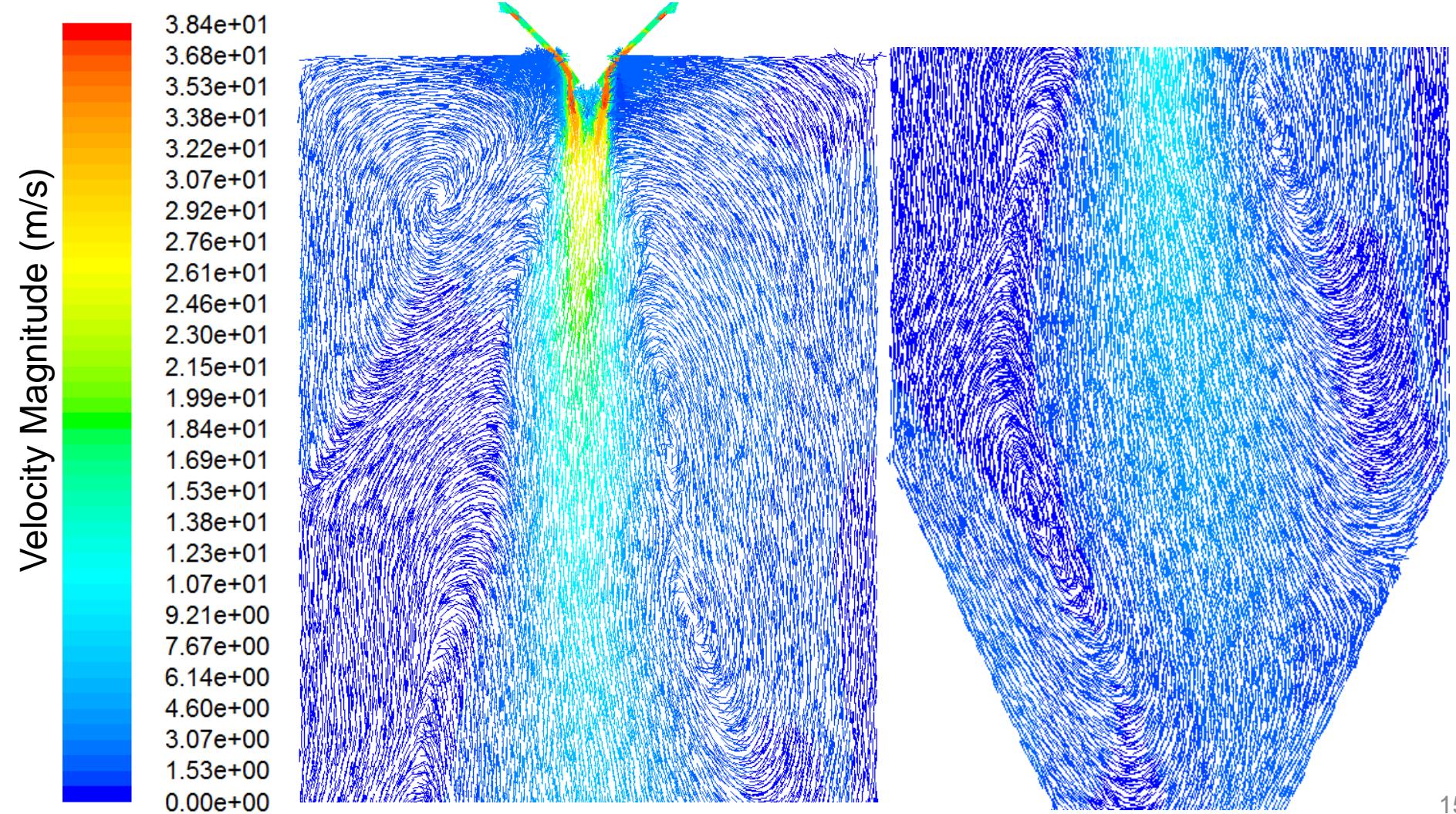
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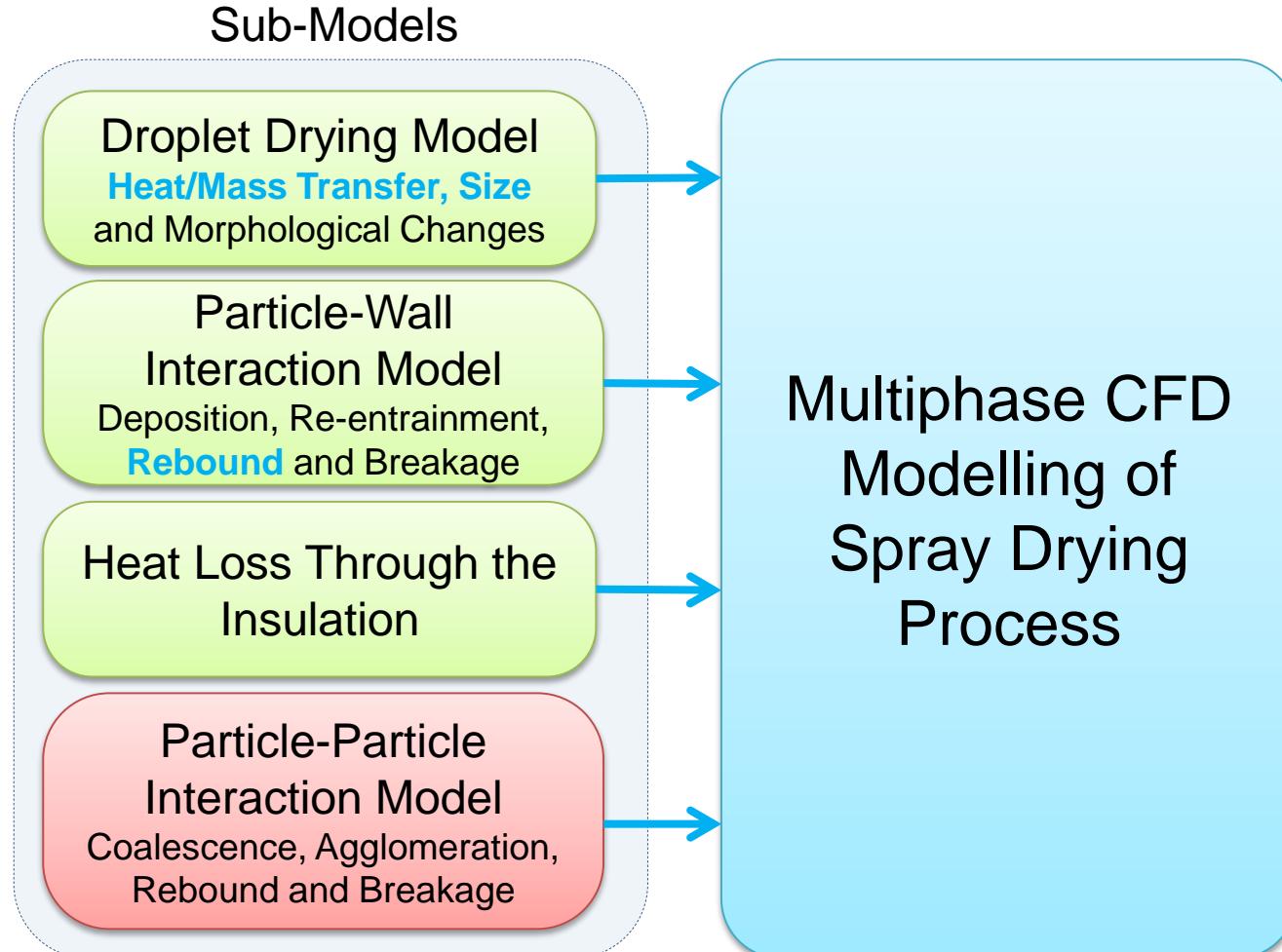
Single Phase Simulations Velocity Magnitude Contours

CFD Modelling Results (cont.)

- Vector plot coloured by velocity magnitude:



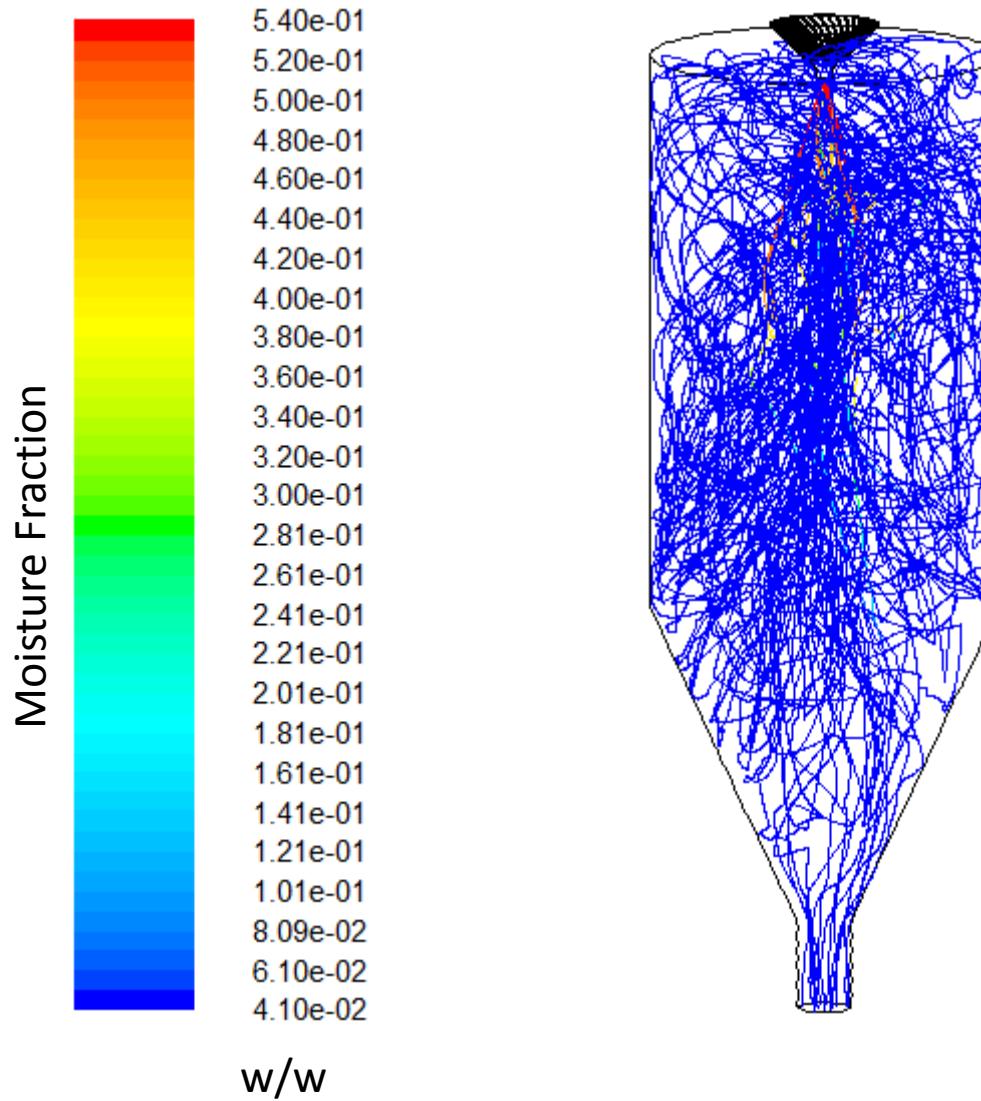
Modelling of Spray Drying Process



Trajectories coloured by Moisture Fraction



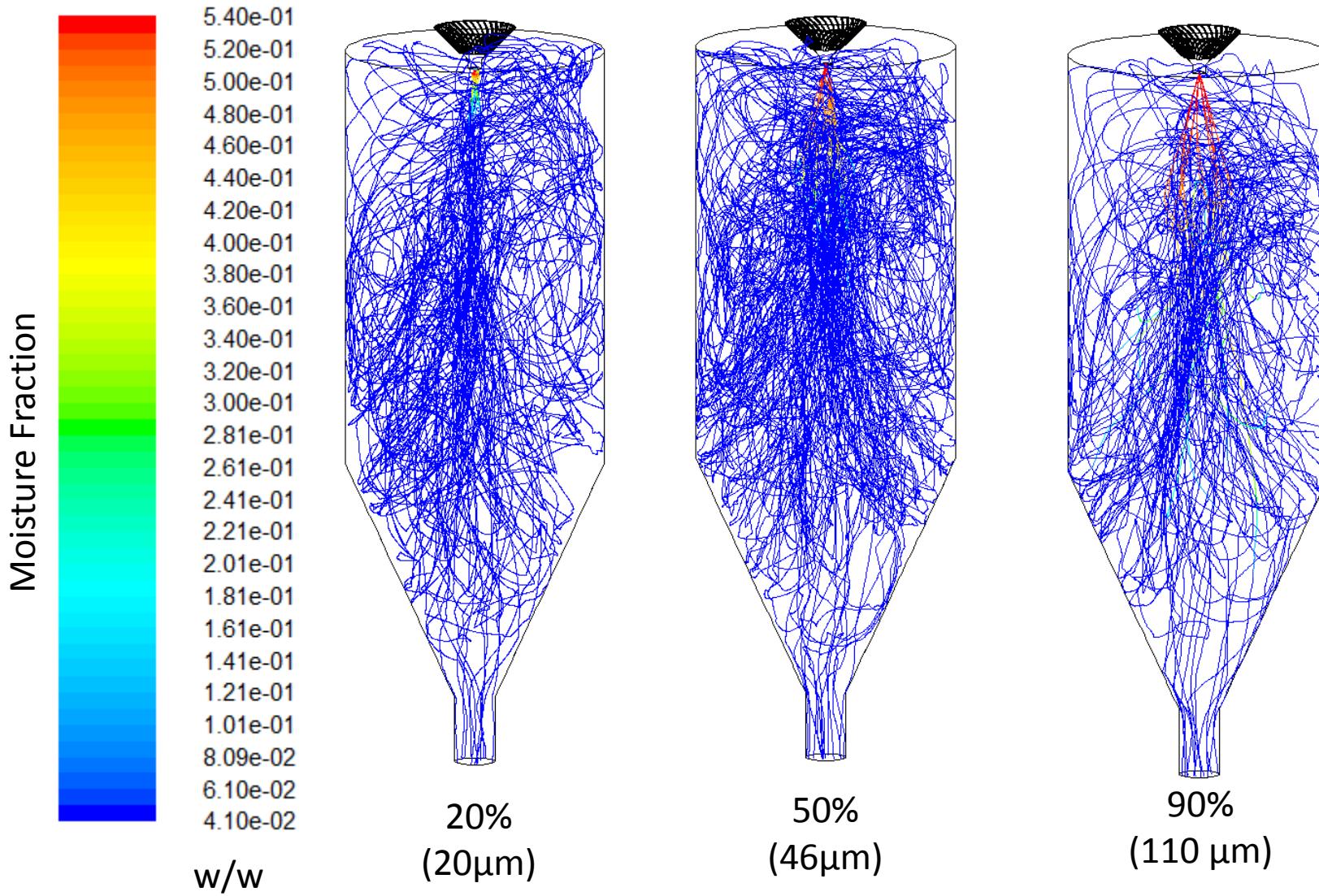
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Trajectories coloured by Moisture Fraction



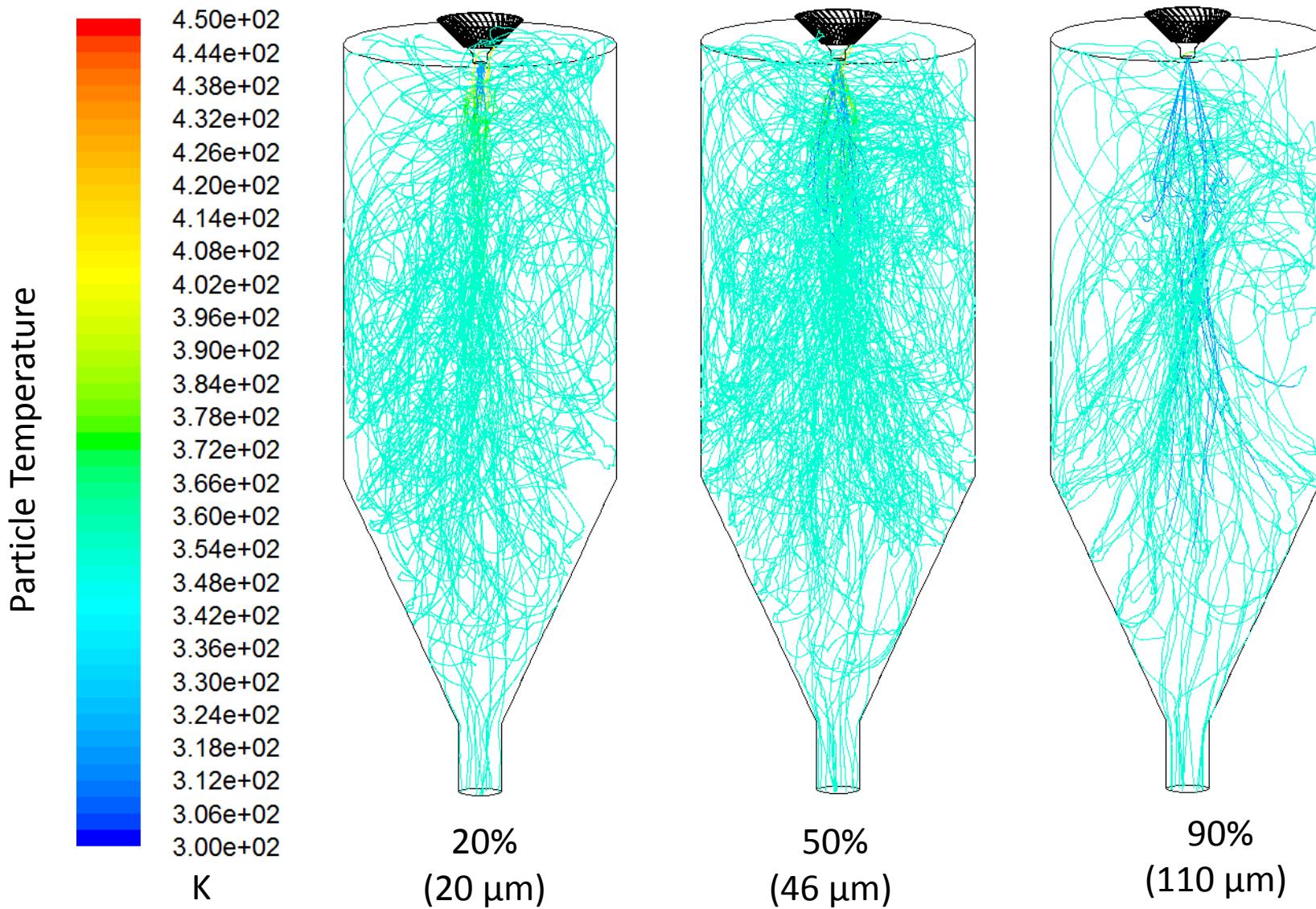
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Trajectories coloured by Particle Temperature



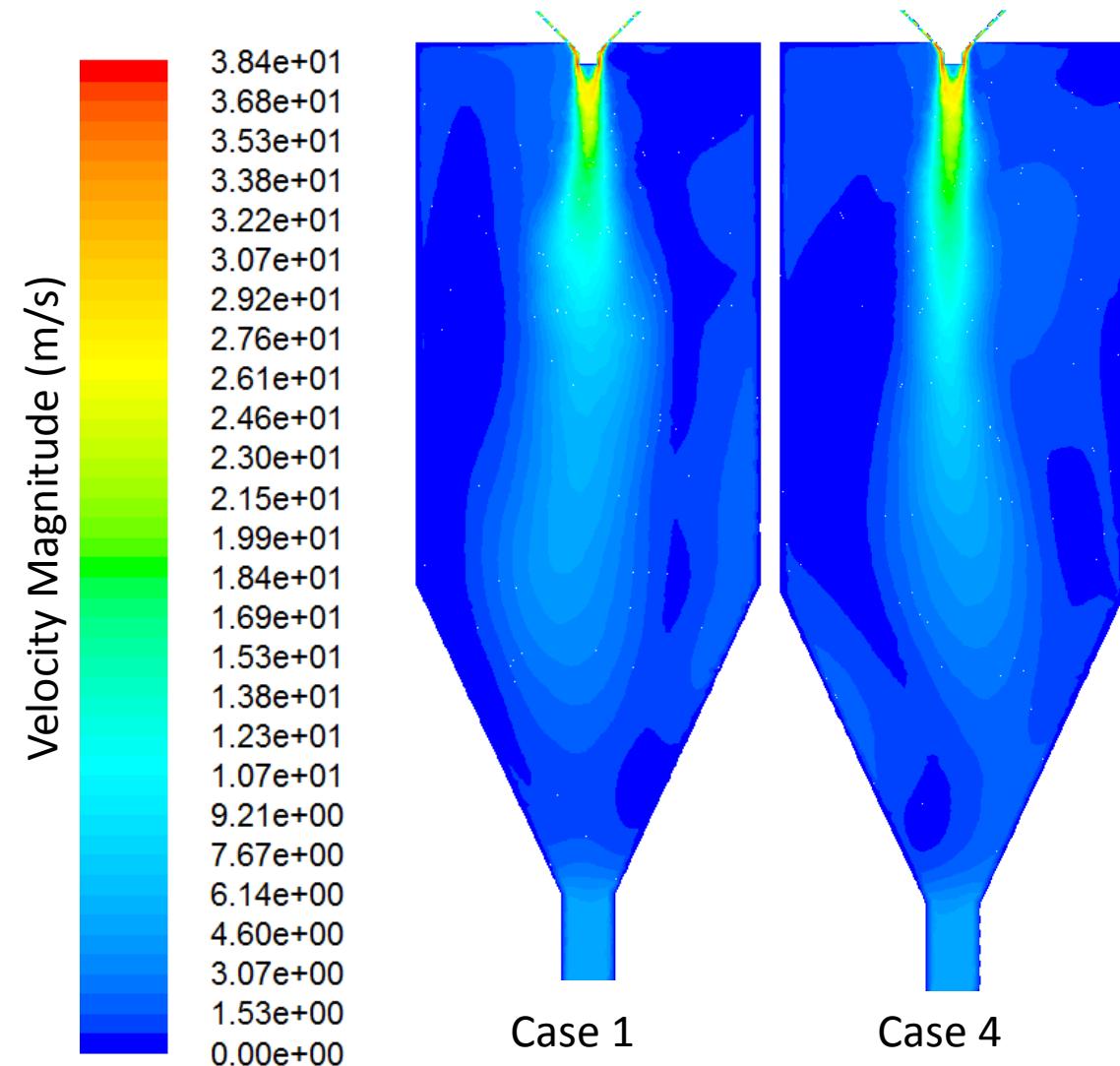
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Air Velocities with Particles



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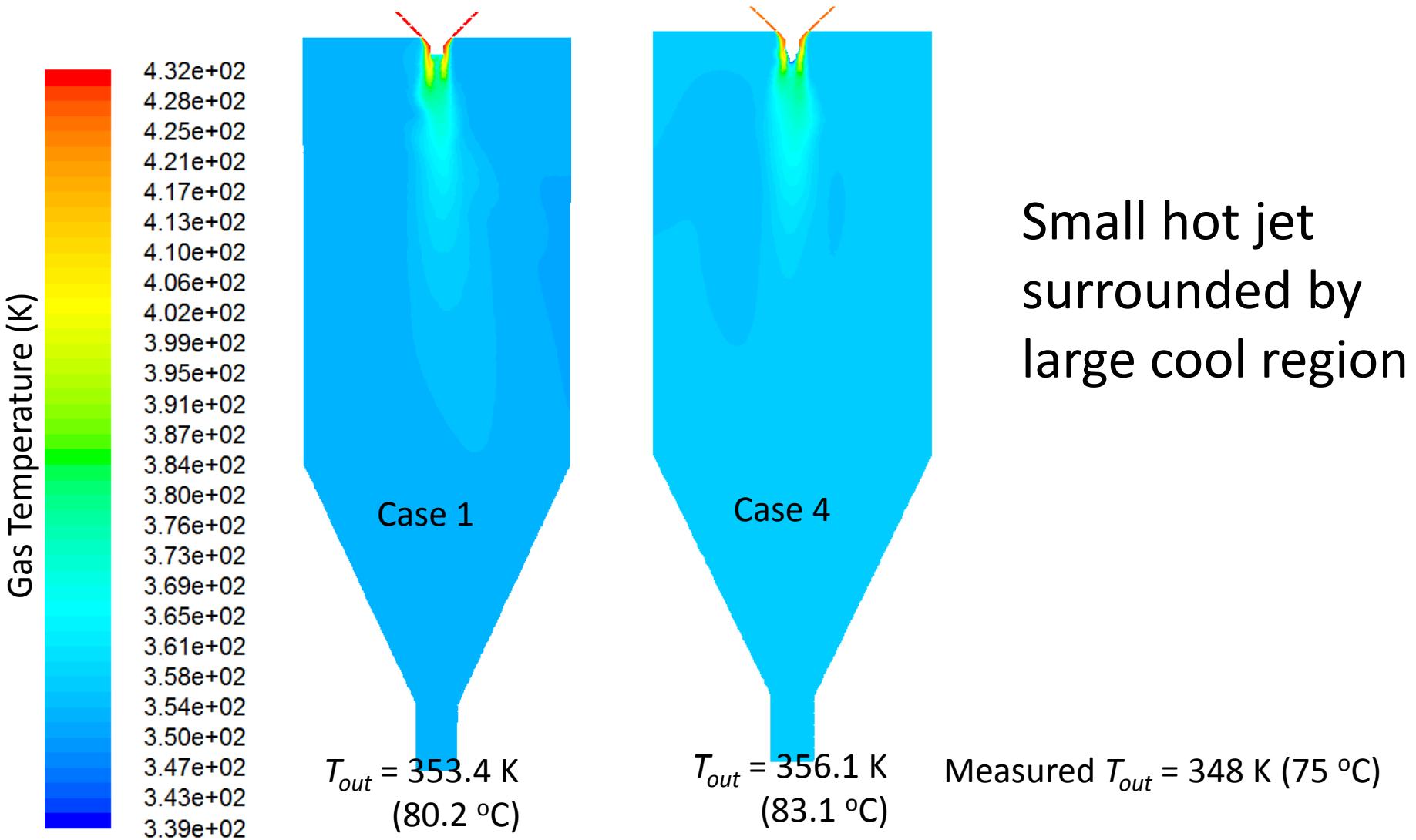


No significant
change versus
simulation without
particles

Air Temperature



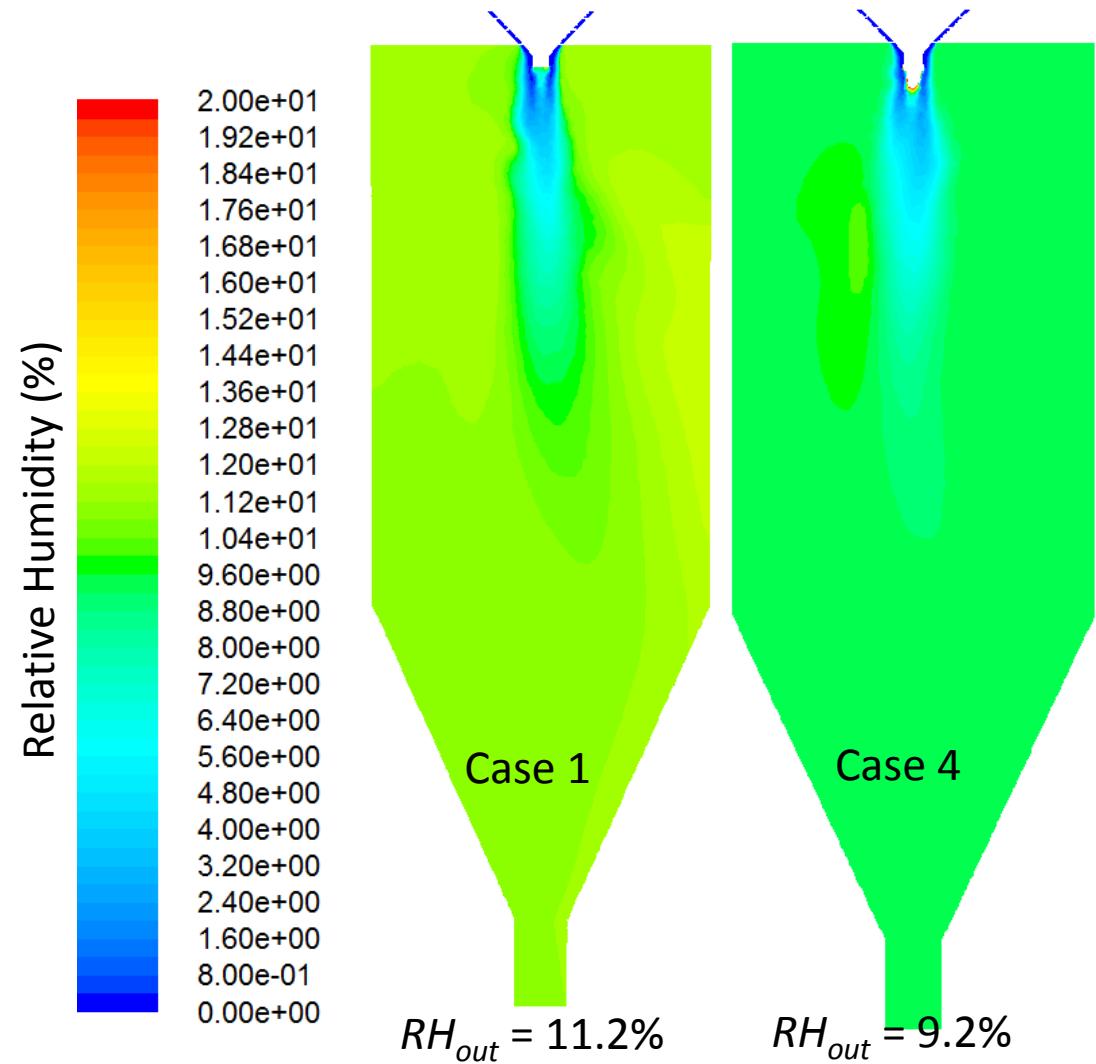
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Air Moisture



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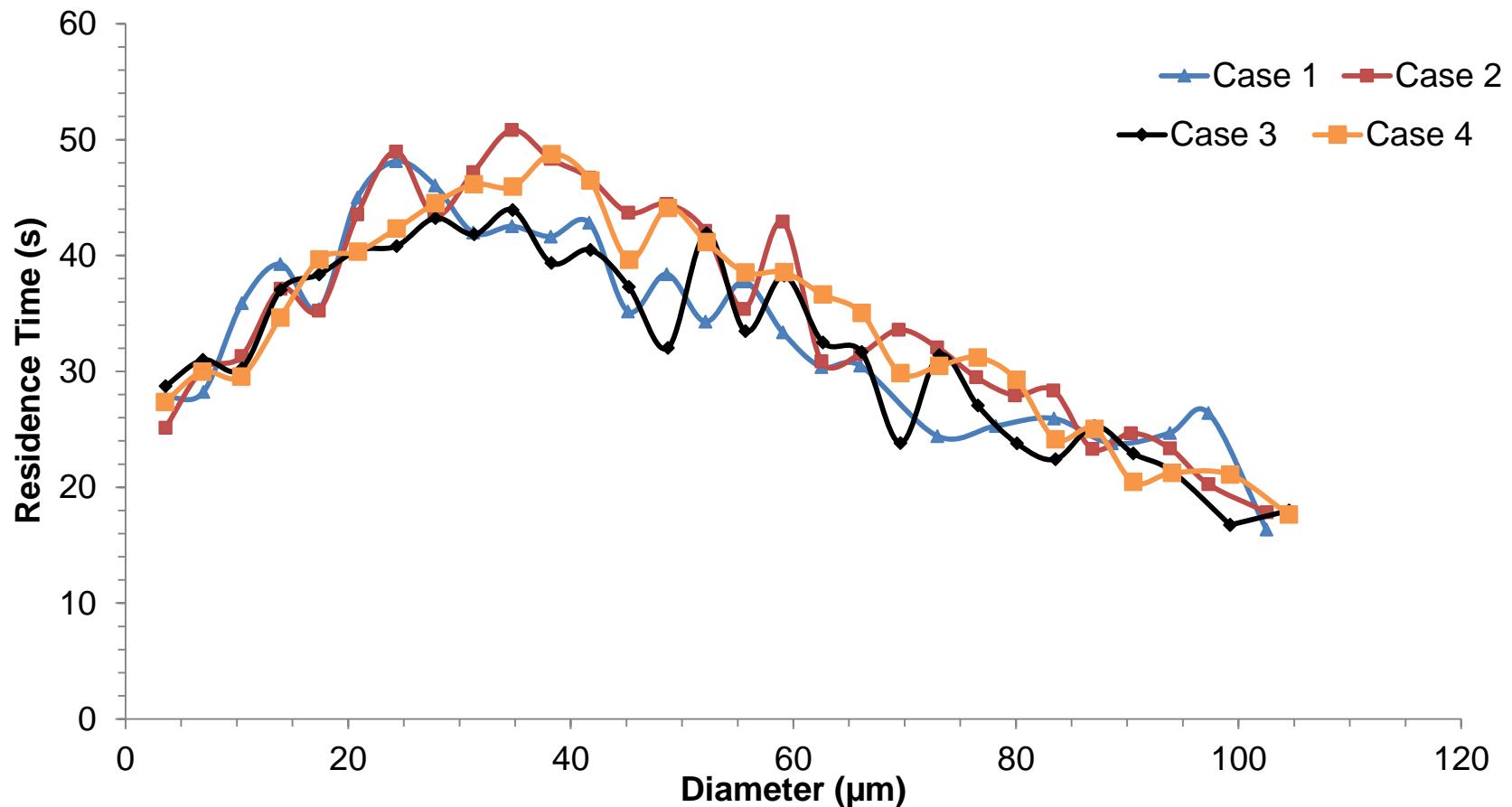
Small dry jet
surrounded by large
humid region

CFD Modelling Results (cont.)



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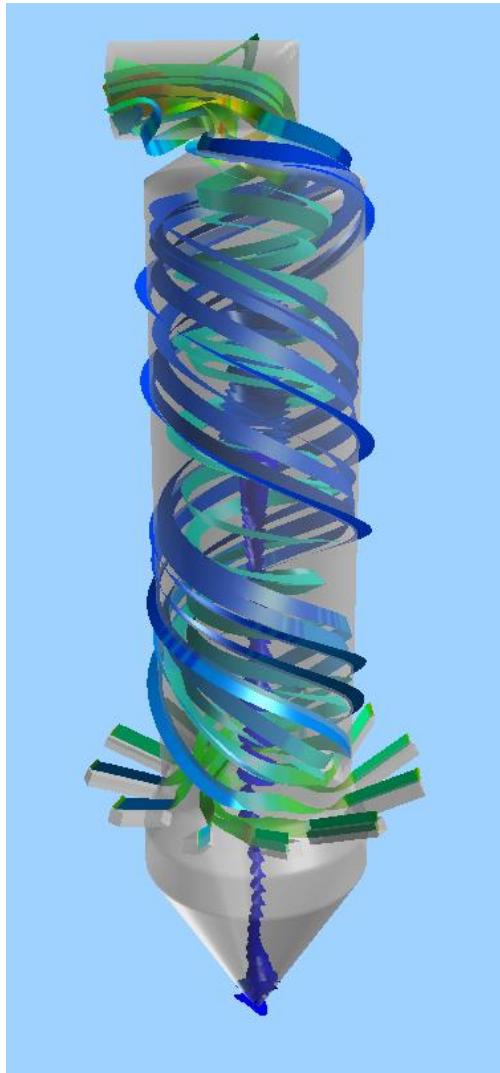
Average residence times of particles of various sizes.



Co-current Summary

- Drying all occurring near nozzle
 - > Particle moisture in equilibrium with exhaust air
- You don't need CFD to predict moisture (in this case), however to model deactivation of enzyme you need particle histories
- A given particle size's residence time is independent of the overall initial particle size

Counter-Current Tower



Counter-current

- Inlet Temp. 300C
- Swirling component to inlet air

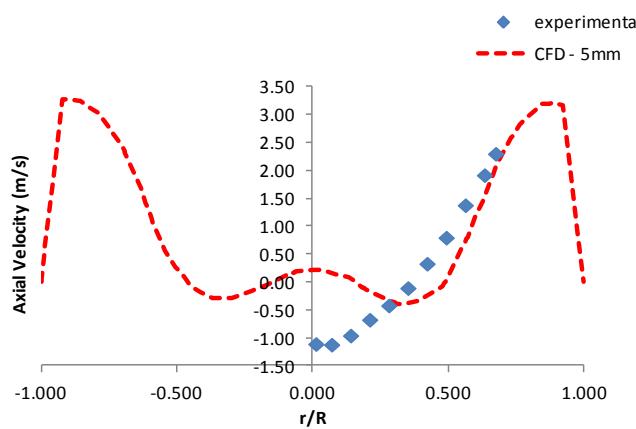
Multiple nozzles and nozzle levels

Some granules collide and stick together – agglomeration

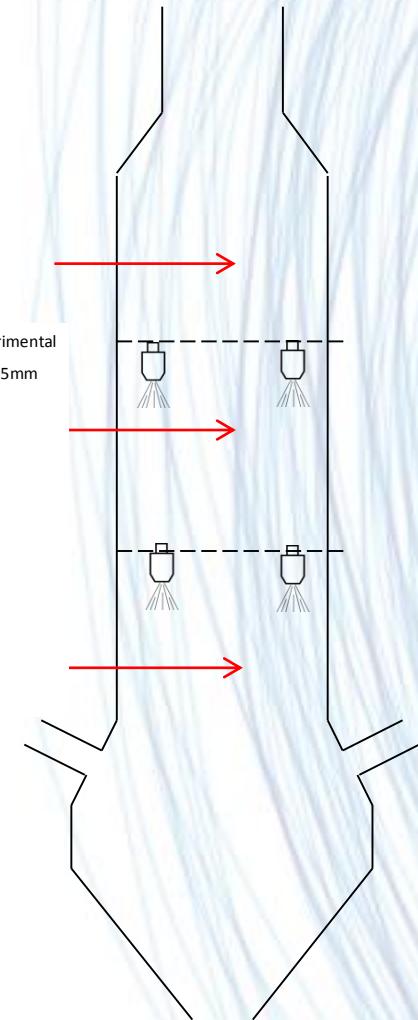
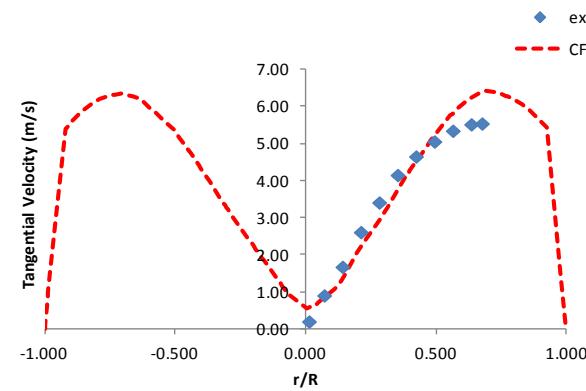
Puffing occurs creating internal porosity

Experimental Air Flows vs CFD

Axial



Tangential



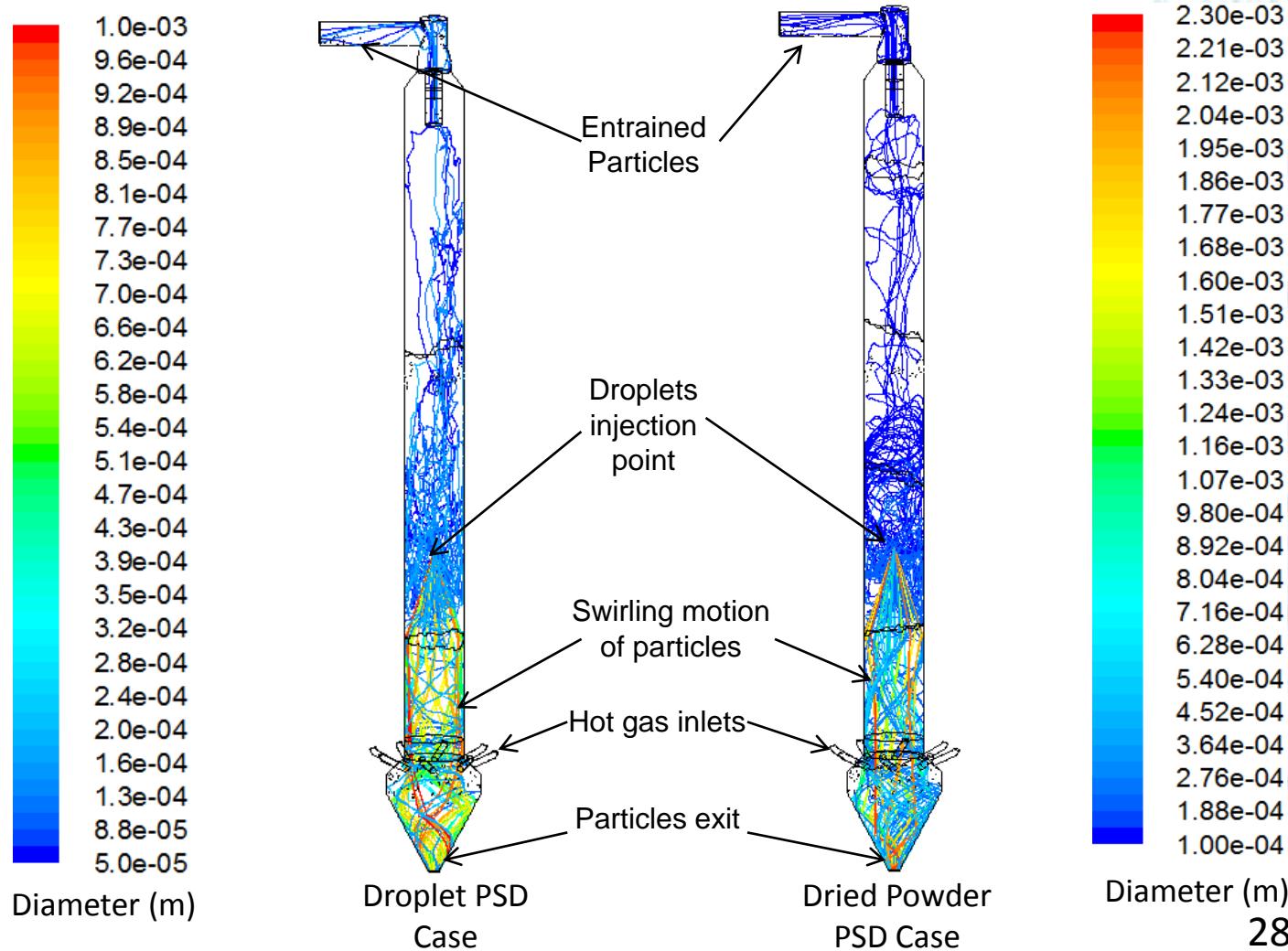
Critical to calibrate the level of wall friction in CFD to give correct tangential velocity

CFD Modelling Results - Trajectories



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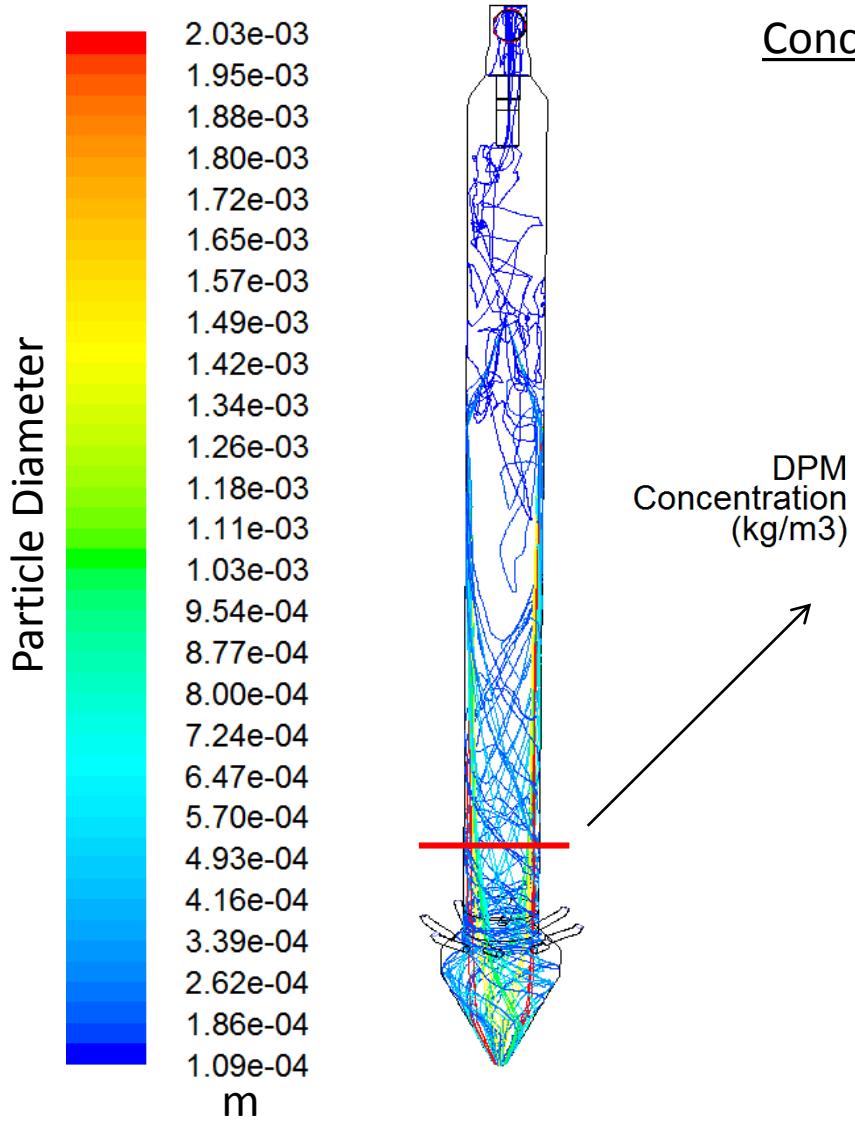
Predicted Droplets/Particle Trajectories



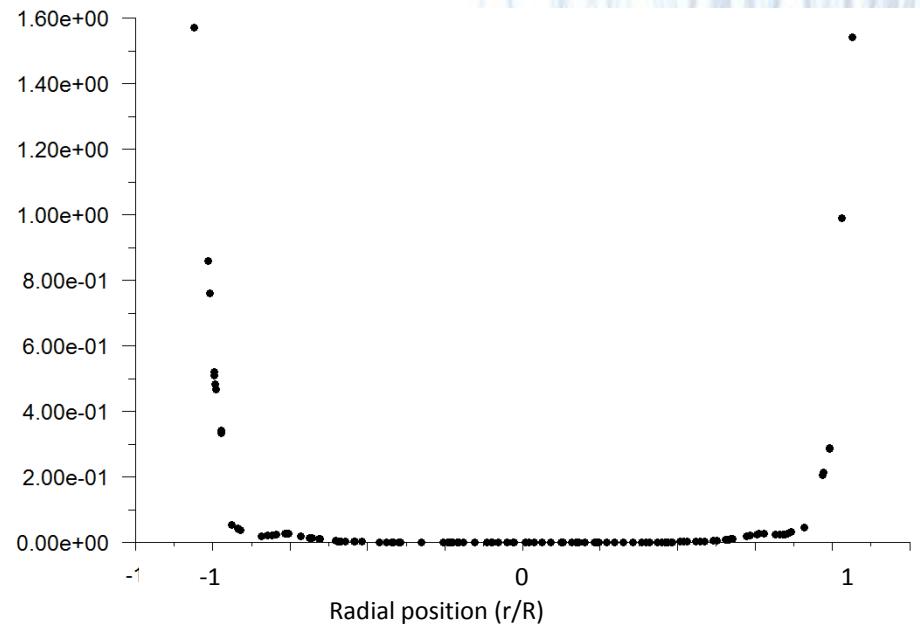
Trajectories and concentration



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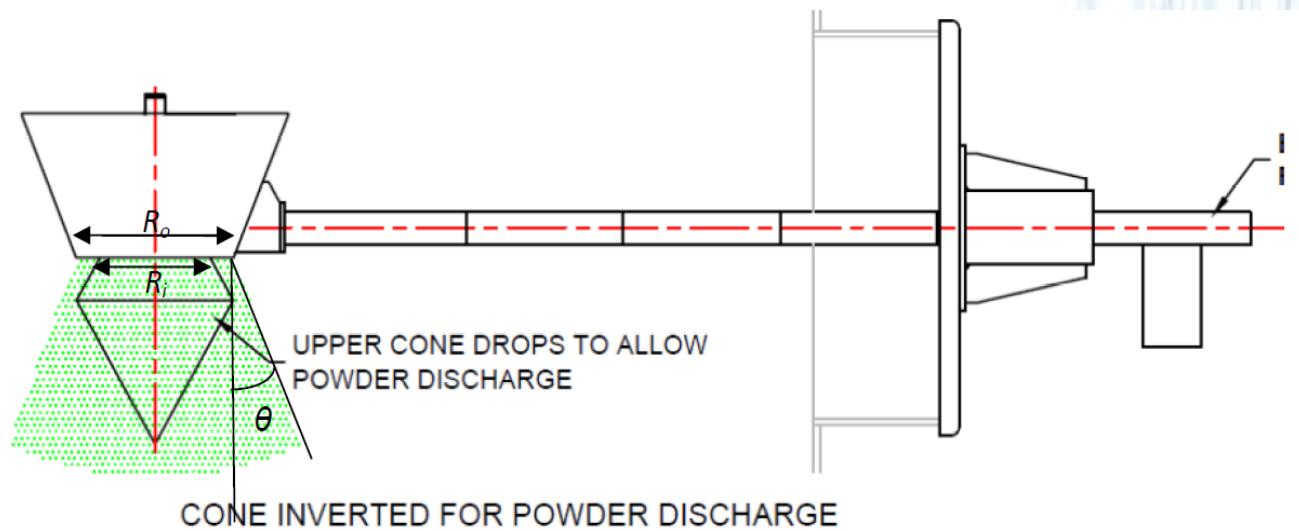
Concentration of particles along the radius in the cylindrical region ($z/Z=0.2$)



RTD measurements glass beads discharge



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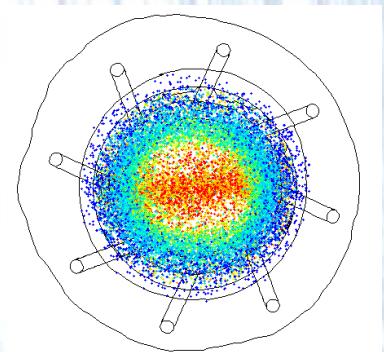
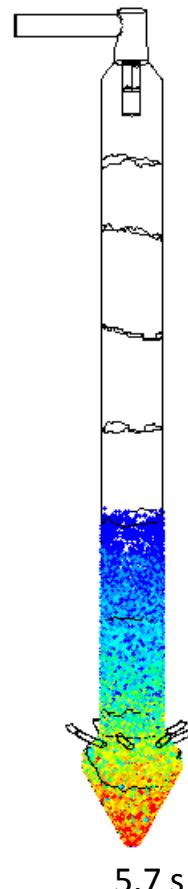
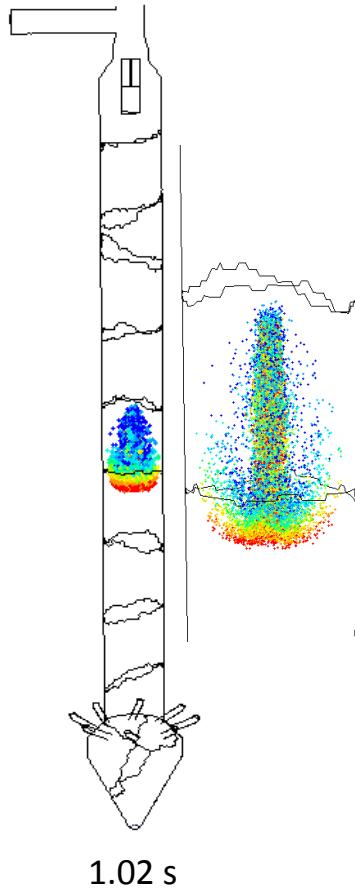
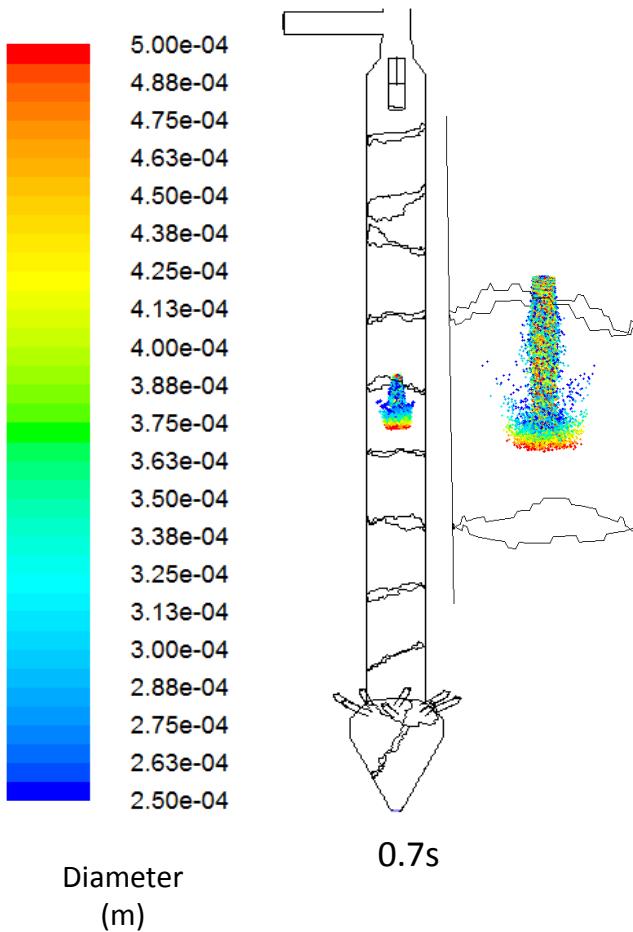


Pulse of glass beads added, time to exit measured

Glass Beads



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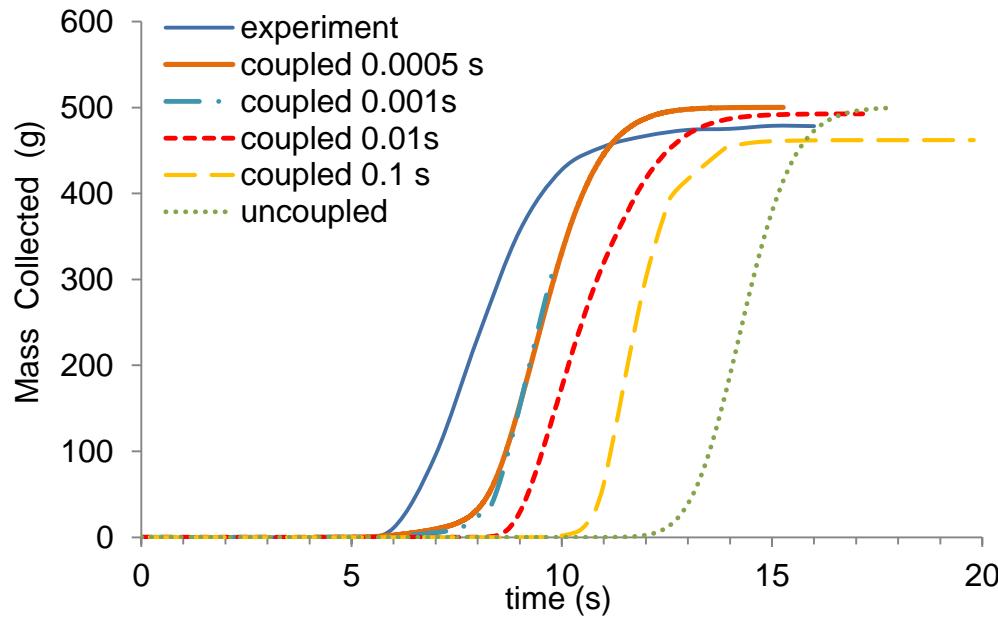


Top view

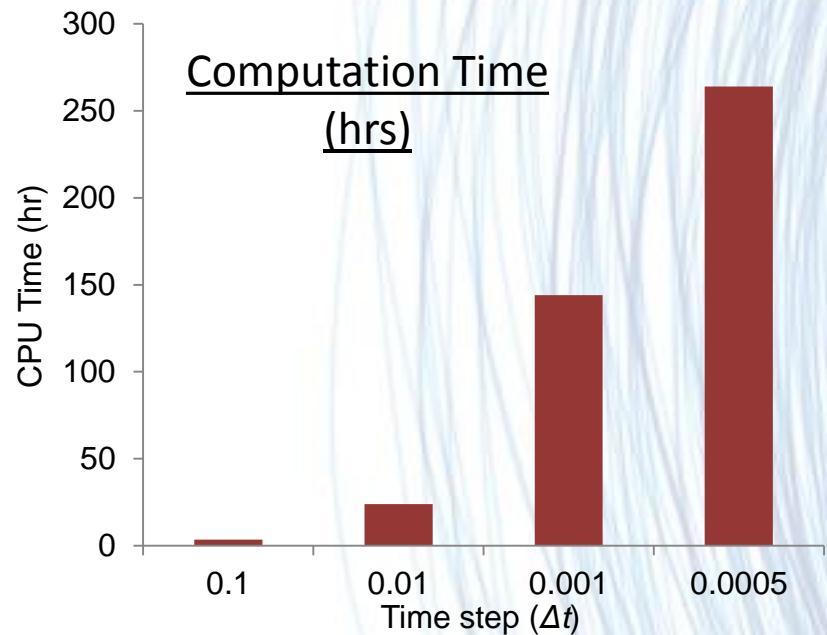
Predicting Residence Time



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Effect of time step on predicted residence times



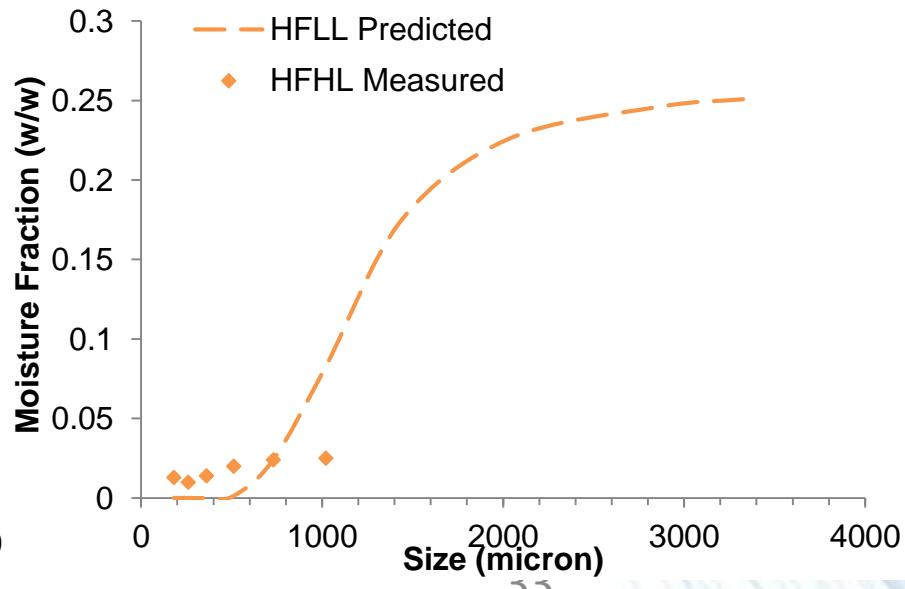
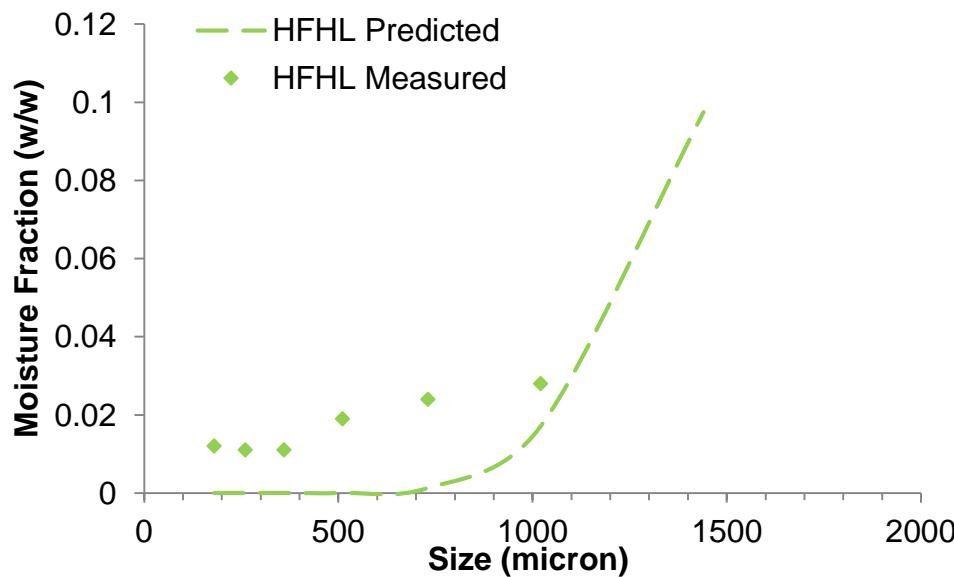
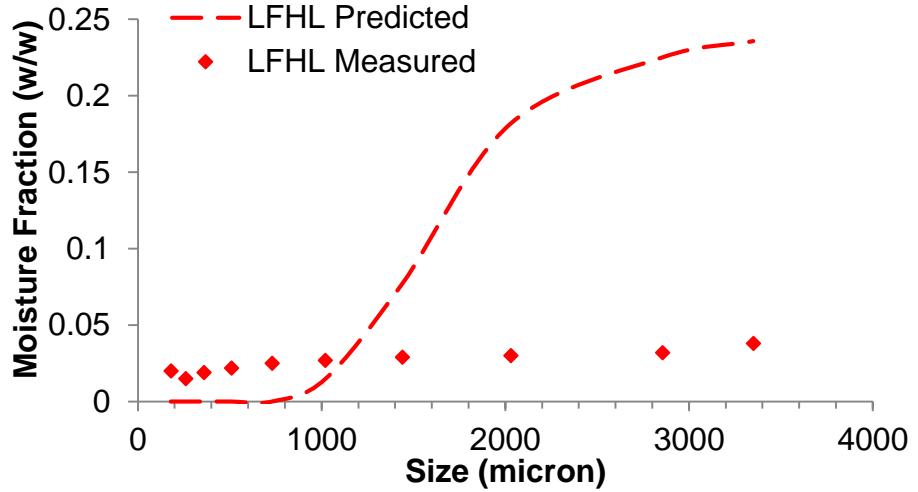
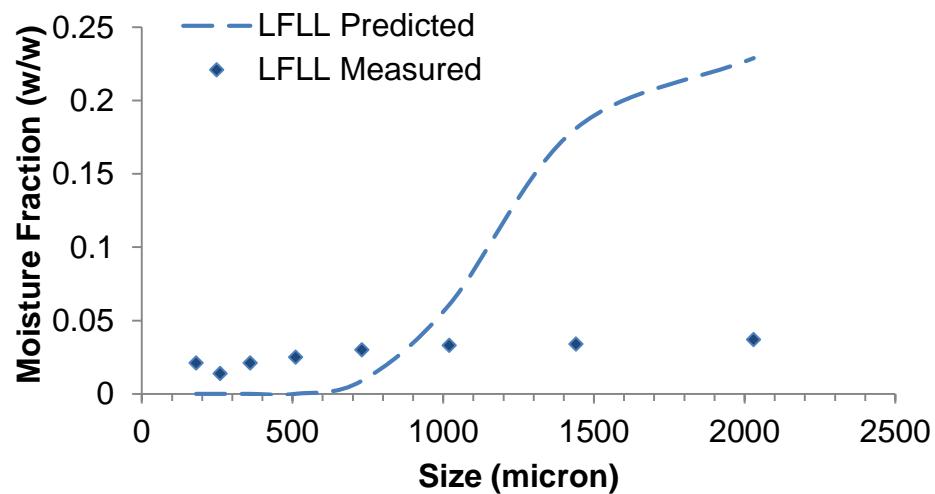
- Unsteady simulation
- Momentum coupling is important and must be included
- Wall collision model important

CFD Modelling Results

Comparison of Exit Moisture



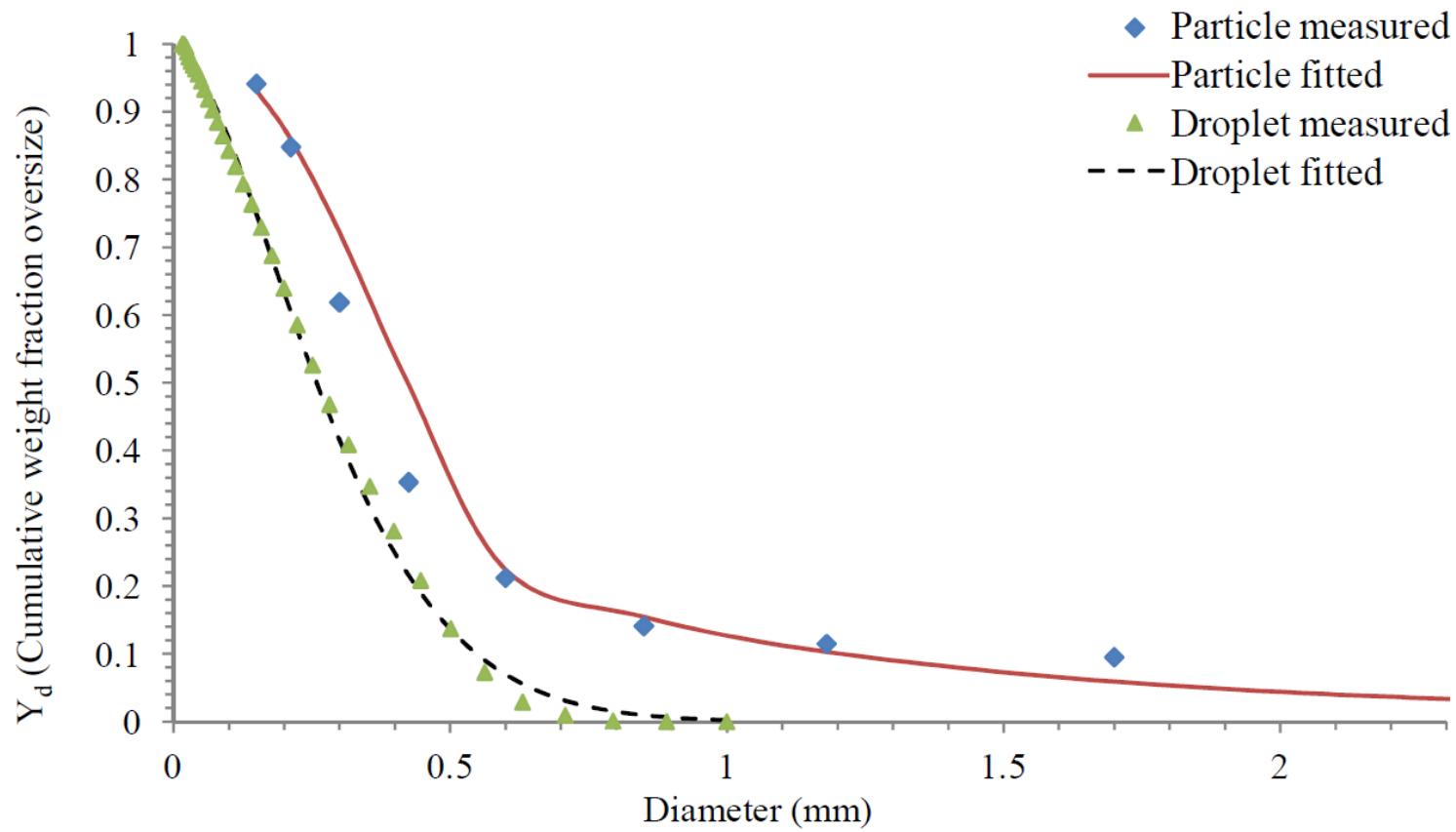
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Size Distributions – Droplet and Product



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Measured data and Rossin-Ramler fits

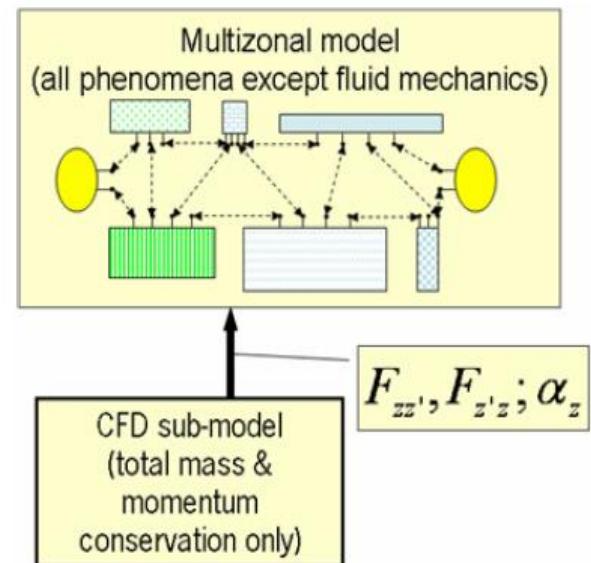
Counter Current Summary

- Complex air flow dominated by swirl.
- Residence time agrees (in some cases)
- Agglomeration
- We definitely do need compartment model, however wall collisions are likely to be key

What do we need from CFD?

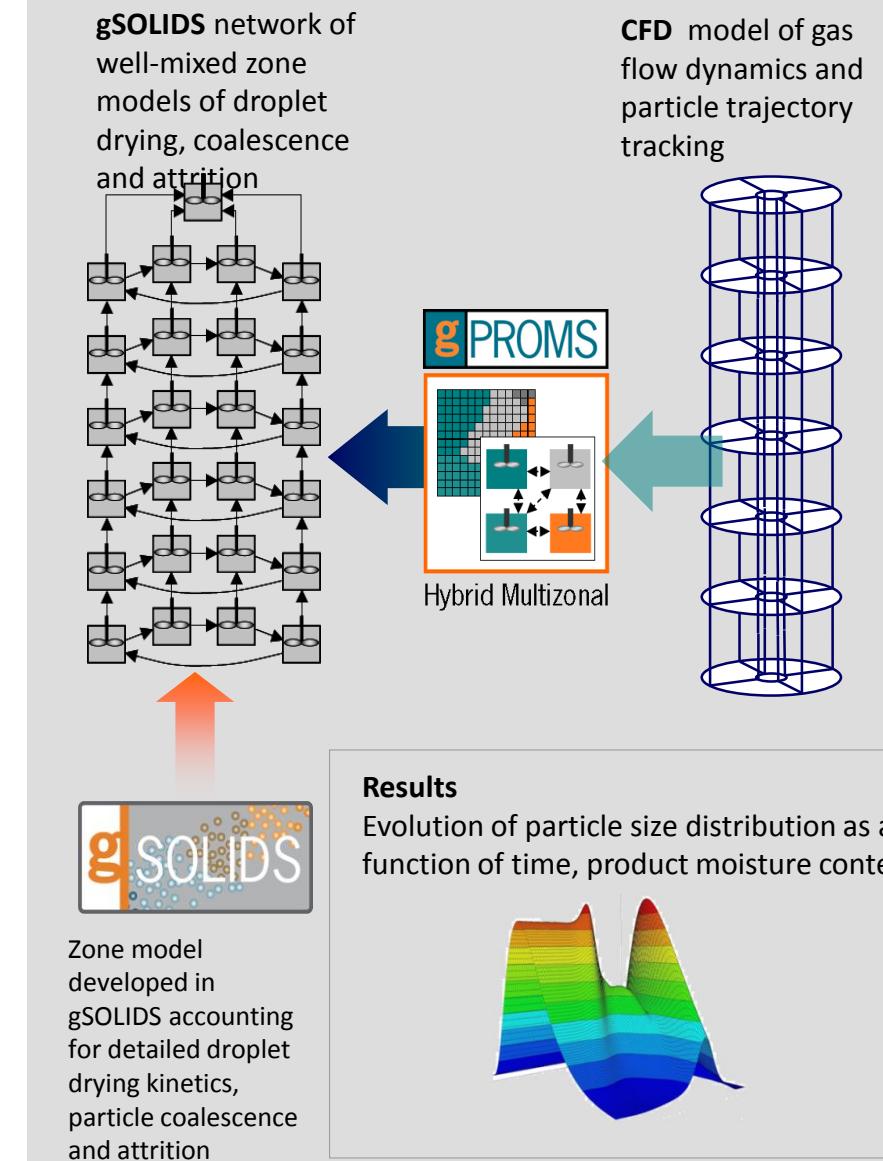
- How good are multi-phase CFD models at predicting the tower performance?
 - OK, need agglomeration, drying models, accurate BCs
- What do the air and particle flow patterns tell us about how to simplify?
 - Insights gained, especially for the co-current tower.
- Is it possible to scale the behaviour so we don't have to run a CFD model for every condition
 - work in progress, some simplifications possible

- Well-established concept
 - separation of intrinsic phenomena (e.g. drying kinetics, agglomeration modelled in gPROMS) and macroscopic hydrodynamics (from CFD)
 - also referred to as **compartmental modelling**
- Divide the CFD solution domain into a network of zones
 - Each of these ‘internal’ zones represents a subset of cells in the CFD model
- The Multizonal model comprises a network of internal and environment zone models
 - Environment zones represent boundary conditions from CFD (e.g. inlet of hot air, outlet of particles)
 - Flow between zones defined by CFD data



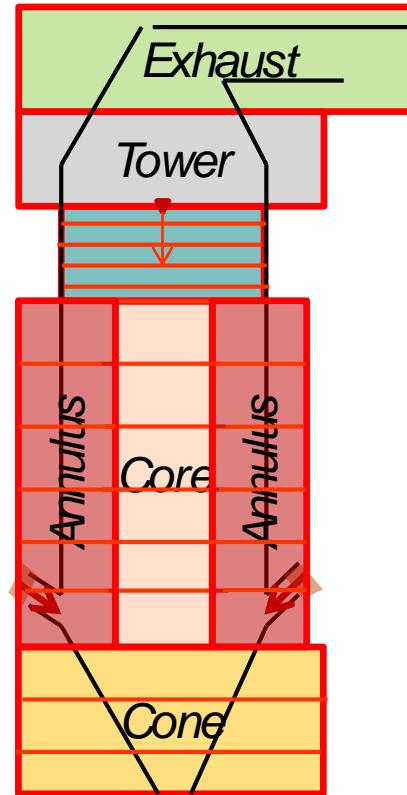
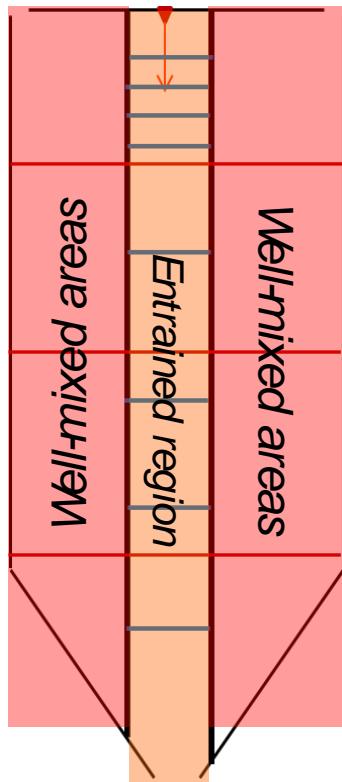
Extension to Eulerian-Lagrangian simulations

- Multizonal concept previously for continuous phase only
- CFD
 - Fluid dynamics (Eulerian)
 - Particle dynamics (Lagrangian)
- gSOLIDS
 - Well-mixed zone model
 - Detailed droplet drying model
 - Population balance model to account for droplet coalescence, agglomeration and heat losses
- Flow between Multizonal internal zones extracted from CFD for both particles and vapour



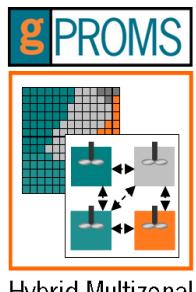
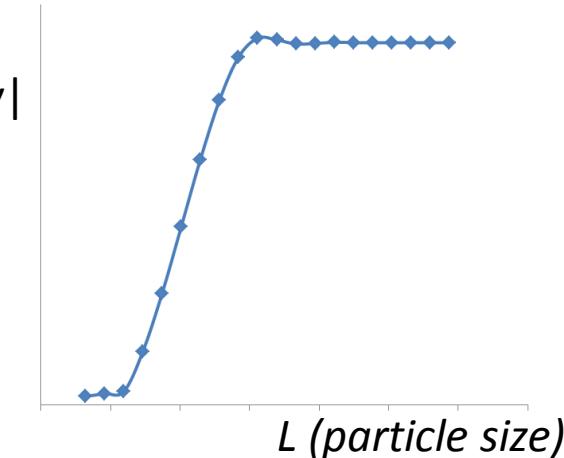
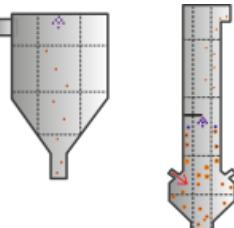
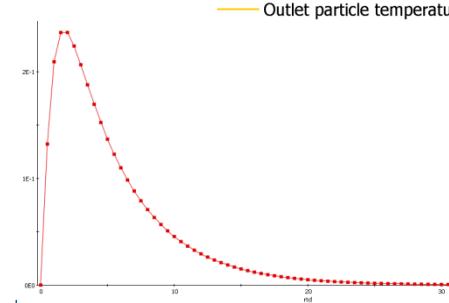
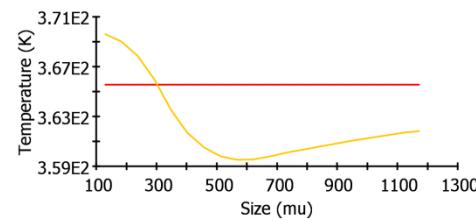
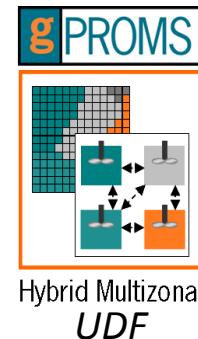
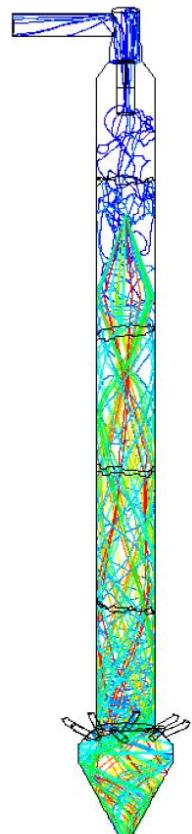
Zoning strategy

- The zoning strategy is key to extracting informative and appropriate data to configure the particle and vapour flow between zones
 - Use previous studies and knowledge, as well as CFD results, to compartmentalise areas of similar characteristics such as concentration, temperature and flow pattern.



Coupling CFD and gSOLIDS

- Particle velocities sampled at each zone interface
 - Multizonal UDF extracts and writes data
 - Multizonal FO processes data to create velocity distribution at each interface of an internal zone to pass to compartmental model

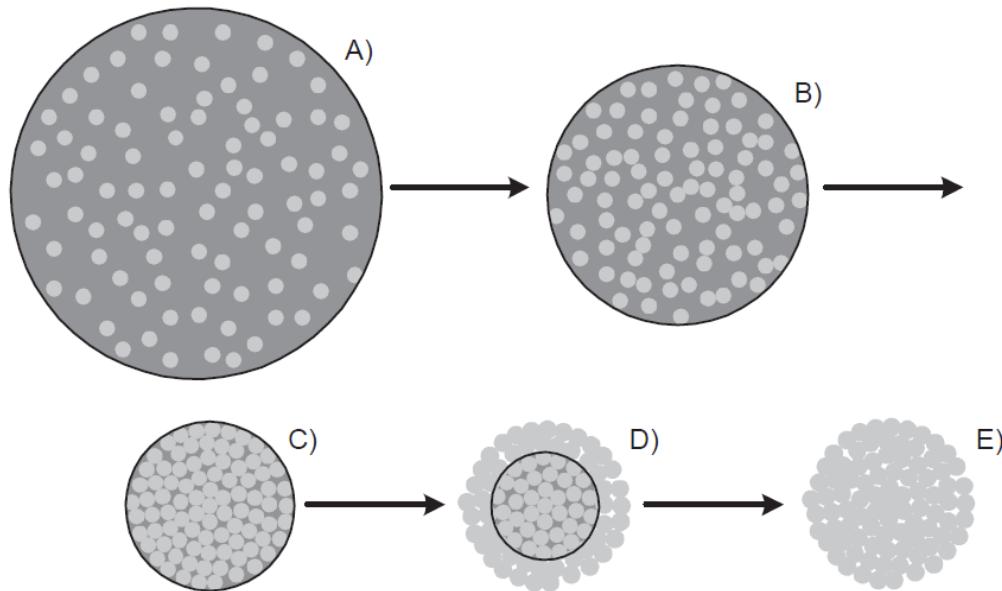




Modelling of key phenomena

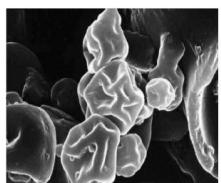
In the Multizonal model

Droplet drying model

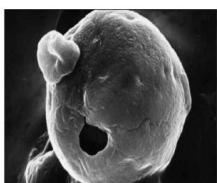


Constant rate drying: Heat transfer to surface from bulk and diffusion into vapour are rate limiting

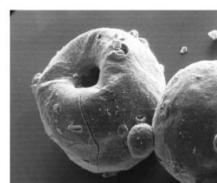
Falling rate drying: Moisture transport to particle surface is rate limiting



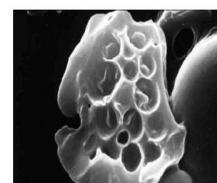
(a) Collapse.



(b) Blow hole.



(c) Crater.



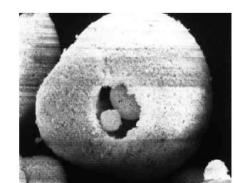
(d) Cavities.



(e) Fractures.



(f) Mushroom-head.

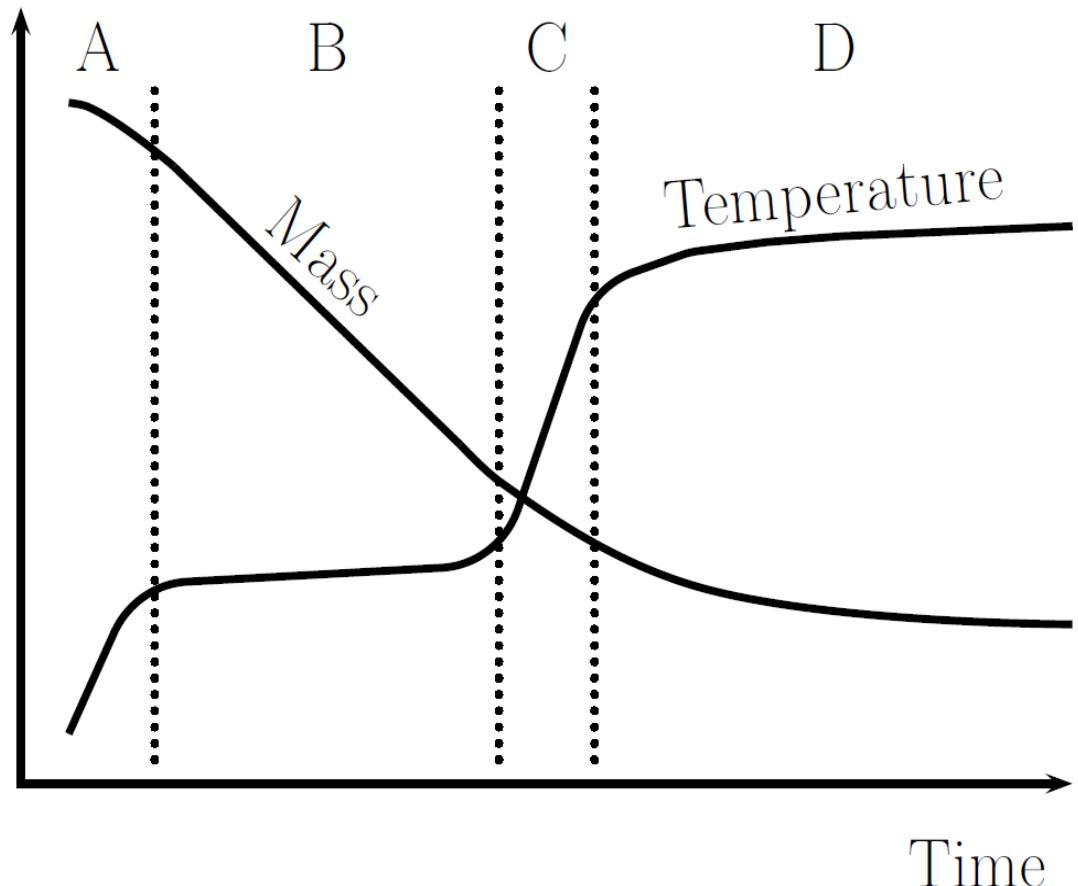


(g) Small particles inside larger.

[1] J. Sloth (2007) Formation of enzyme containing particles by spray drying. Ph.D. thesis, Technical University of Denmark and Novozymes A/S

[2] Jakob Sloth, Poul Bach, Anker D. Jensen, Søren Kiil, Evaluation method for the drying performance of enzyme containing formulations, Biochemical Engineering Journal, Volume 40, Issue 1, 15 May 2008, Pages 121-129

Droplet drying model: four stages of drying

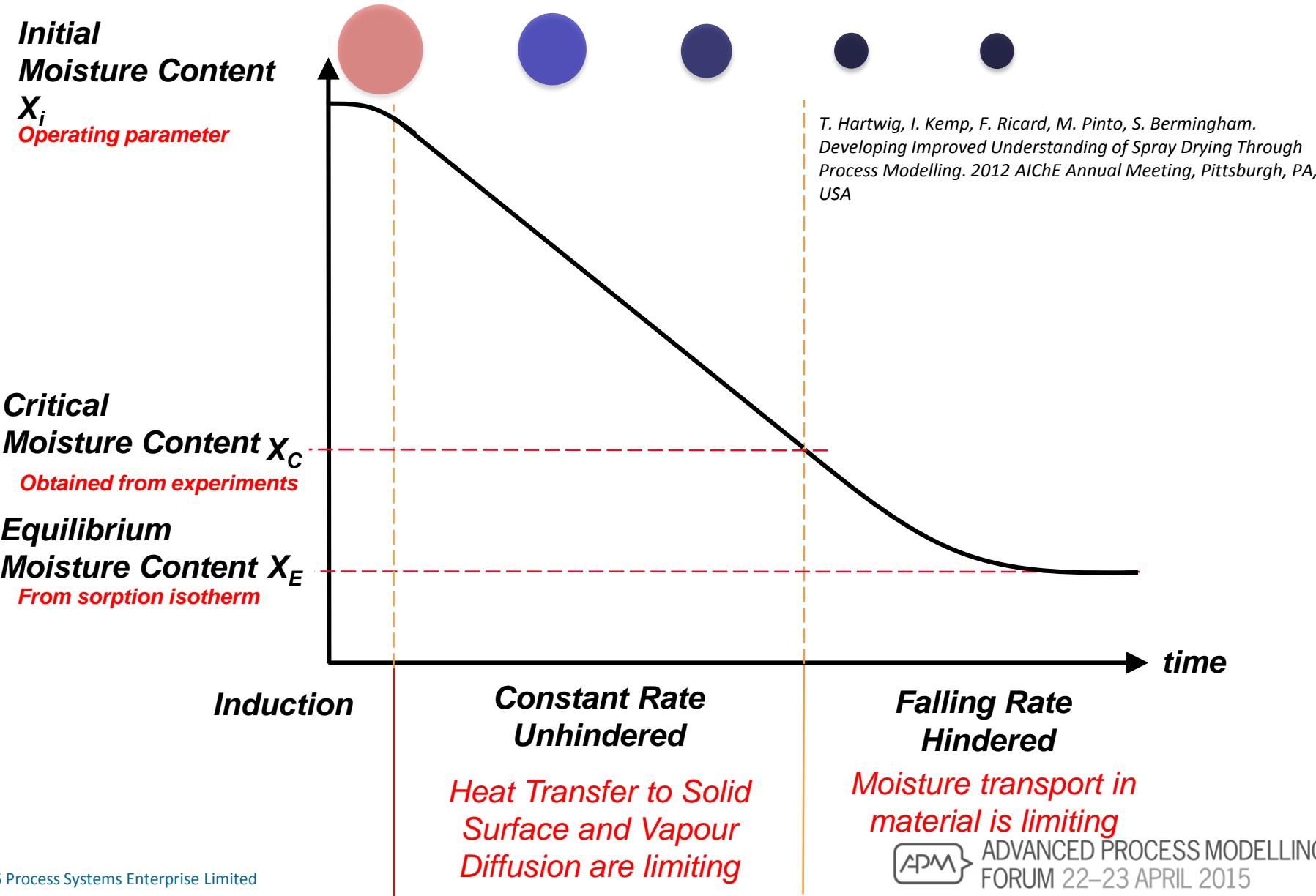


- A. *Induction: Heating droplet to wet bulb temperature*
- B. *Constant rate drying period*
- C. *Falling rate drying period*
- D. *Further heating of dry particle*

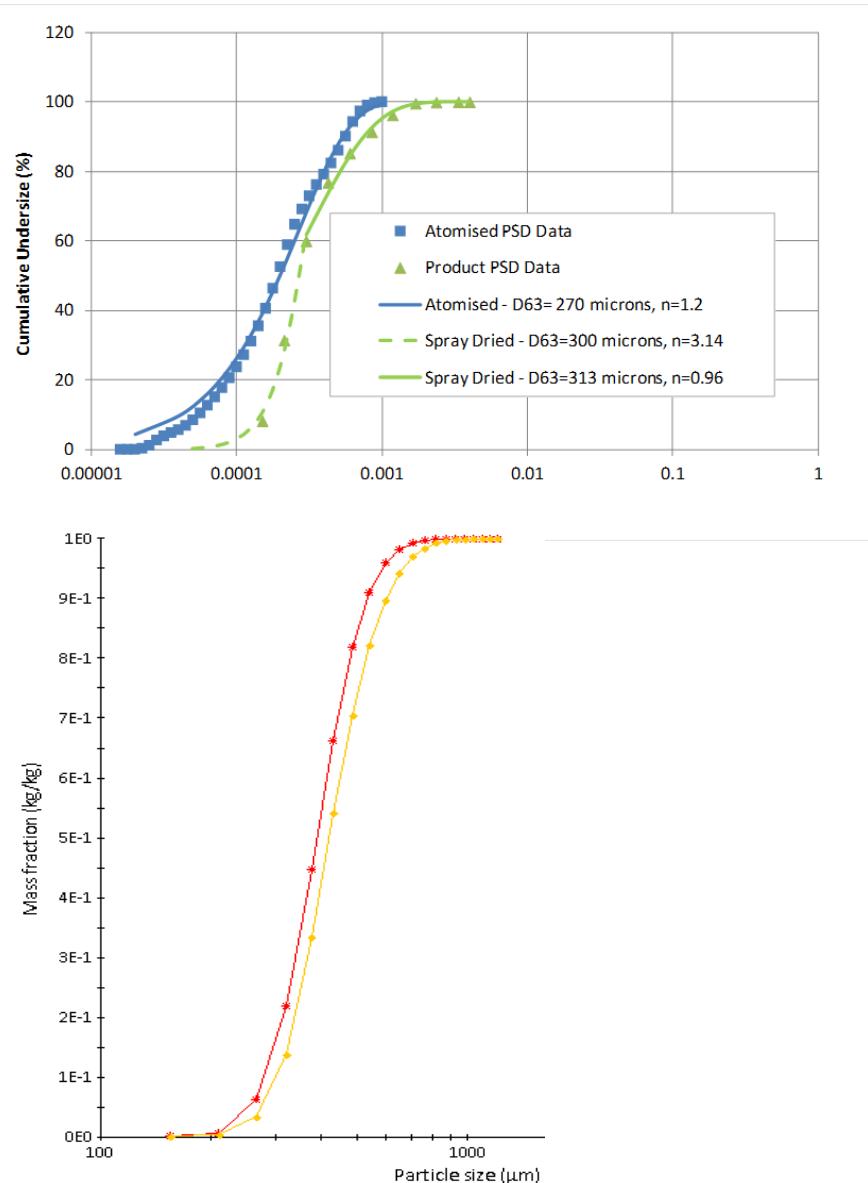
[1] J. Sloth (2007) Formation of enzyme containing particles by spray drying. Ph.D. thesis, Technical University of Denmark and Novozymes A/S

[2] Jakob Sloth, Poul Bach, Anker D. Jensen, Soren Kiil, Evaluation method for the drying performance of enzyme containing formulations, Biochemical Engineering Journal, Volume 40, Issue 1, 15 May 2008, Pages 121-129

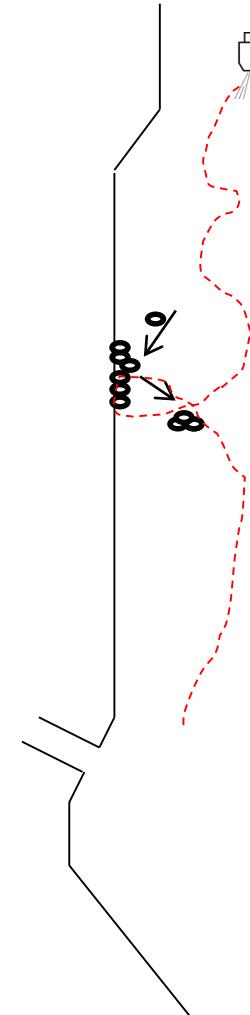
Droplet drying model: size change



Agglomeration & coalescence



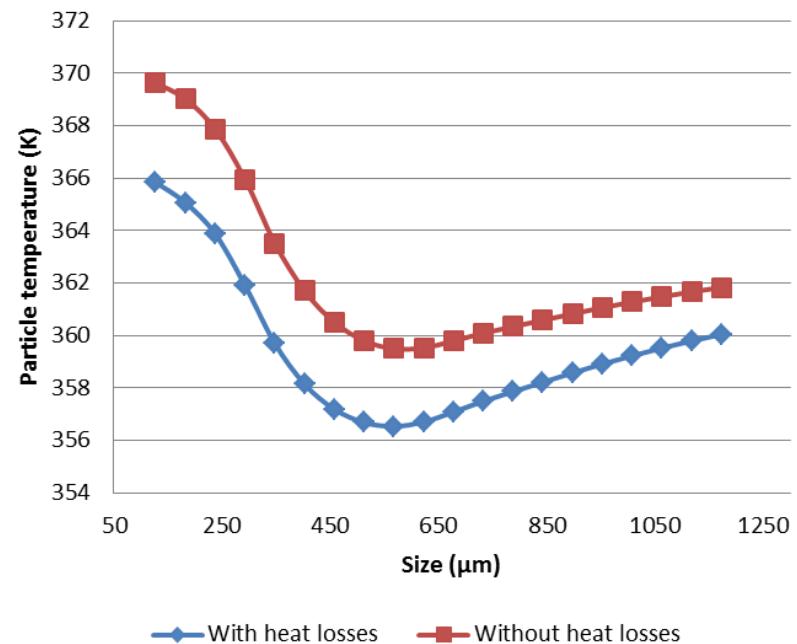
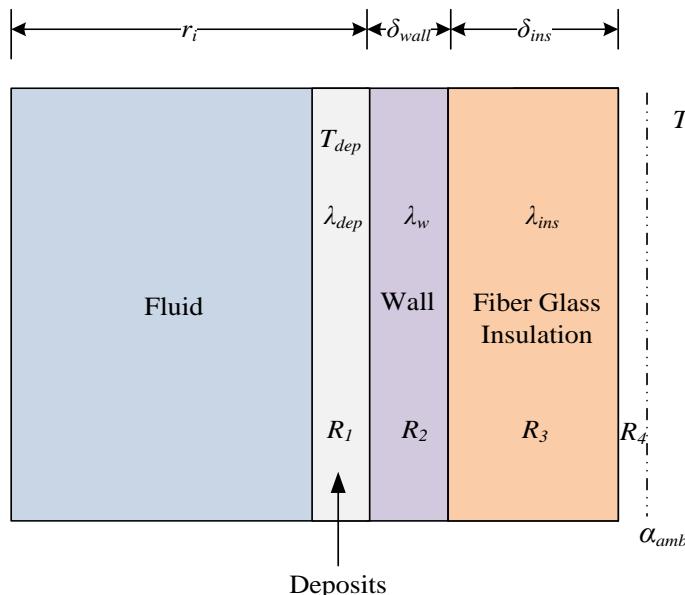
- Coalescence of droplets is incorporated where appropriate and prevalent
- Wall agglomeration and drying to be implemented to capture wet particles sticking to chamber walls
- Ability to capture shift in PSD from atomised droplet size



Heat losses

- Heat losses in tower can impact heavily the drying rate and temperature in the tower

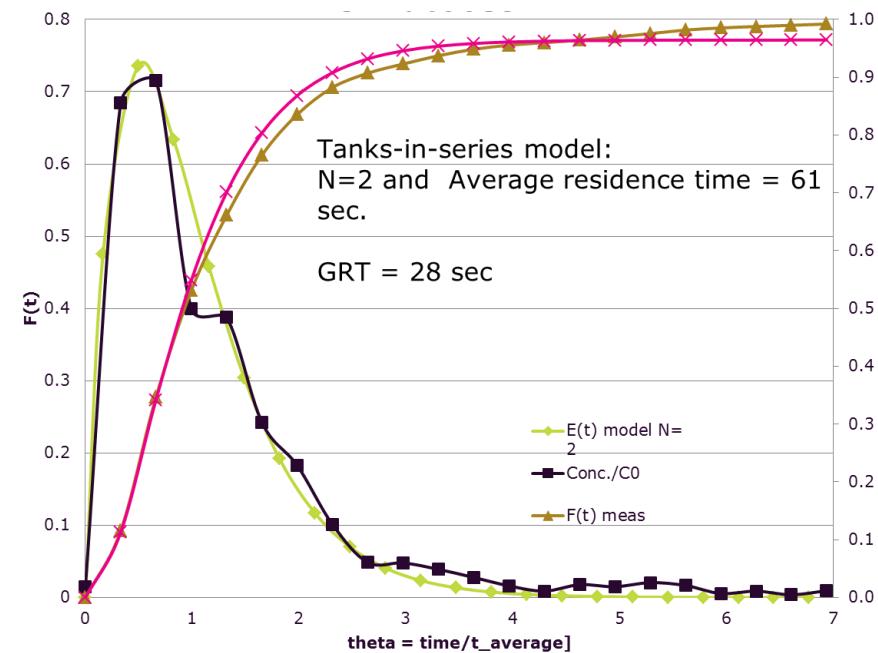
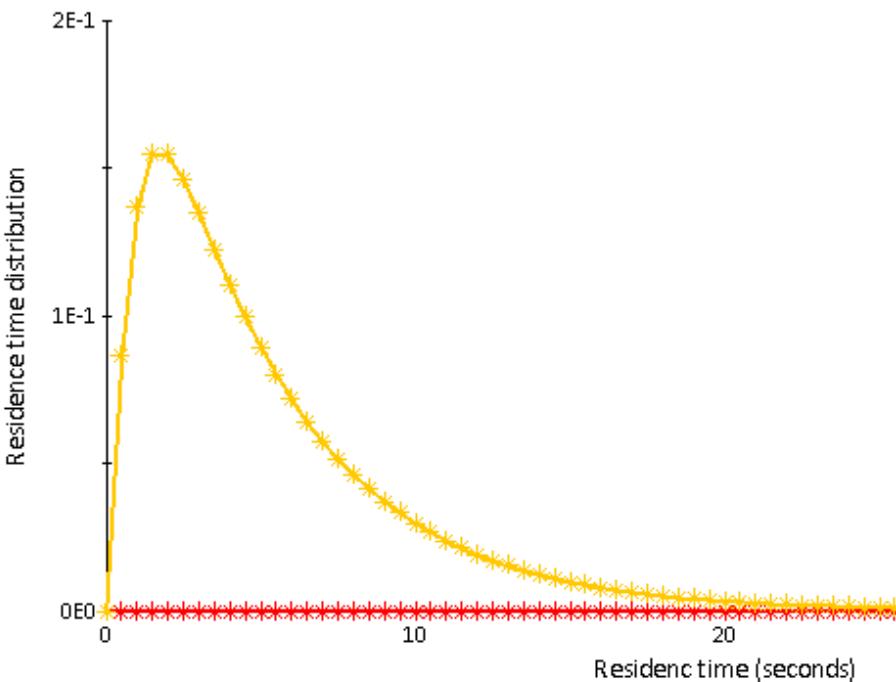
$$\frac{1}{U} = \frac{r_i \ln\left(\frac{r_i}{r_i - \delta_d}\right)}{\lambda_{dep}} + \frac{r_i \ln\left(\frac{r_i + \delta_w}{r_i}\right)}{\lambda_w} + \frac{r_i \ln\left(\frac{r_i + \delta_w + \delta_{ins}}{r_i + \delta_w}\right)}{\lambda_{ins}} + \frac{r_i}{\alpha_{amb}(r_i + \delta_w + \delta_{ins})}$$



Residence time distribution

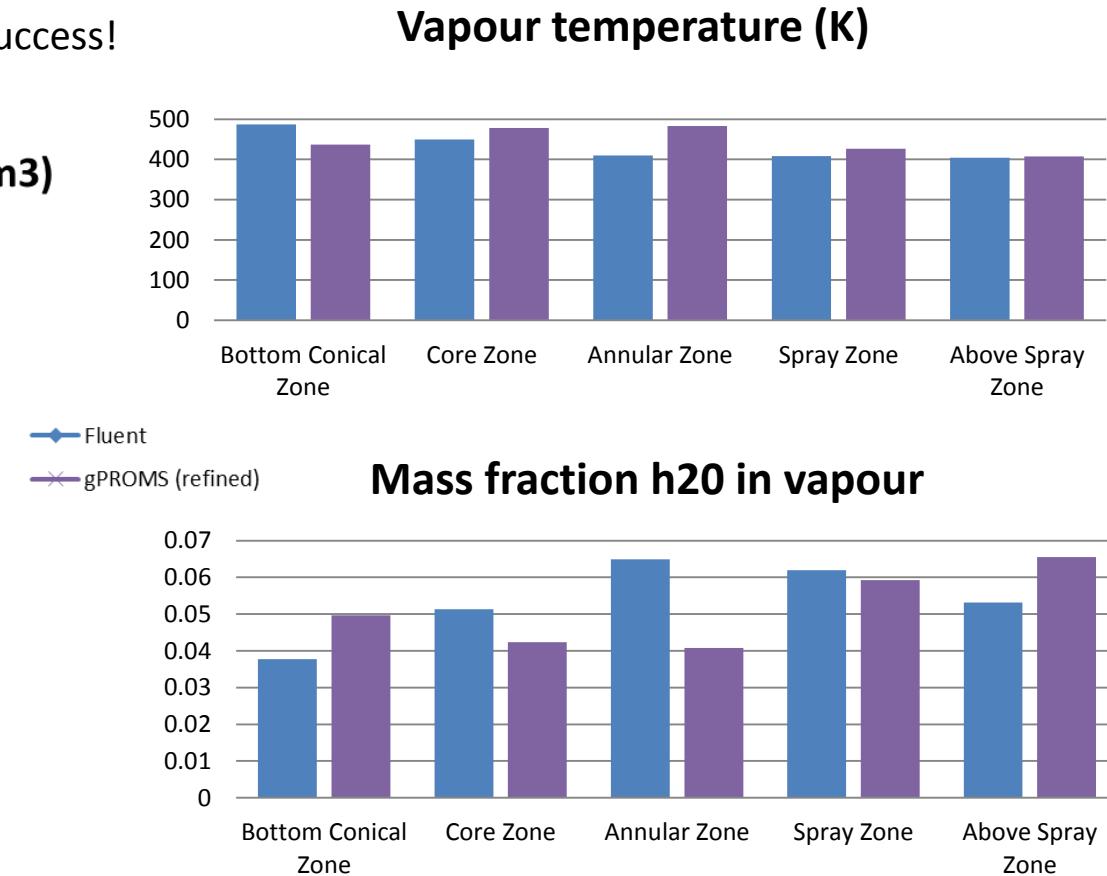
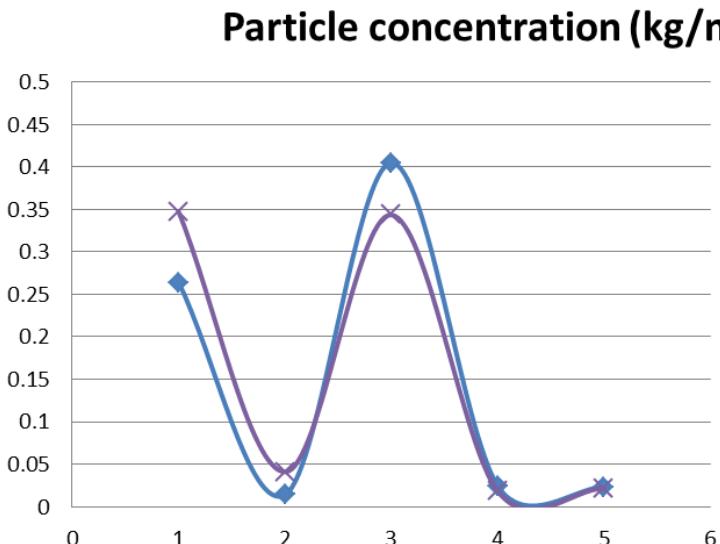
- Residence time is determined by the fluxes extracted from CFD
 - Informs mass flow between the zones of the particles

- Important to develop understanding of input process parameters on fluxes between compartments
 - Develop scaling relationships based on process conditions -> reduces number of CFD simulations



Comparison to CFD

- Capturing the dynamics and gradients within the spray dryer from CFD is vital to successfully creating compartmental model
 - Key variables include concentration of particles, temperature and vapour humidity as well as residence time
 - Zoning strategy is key to success!





Implementation in gSOLIDs

User interface and reports

- Key requirement of the compartmental model is to be user-friendly and not expert dependent like CFD

Model dialogs

Preview dialog: Multizonal_spray_dryer_countercurrent

Specify

- Drying calculations: On
- Drying model: Oakley (2004)
- Heat and mass transfer correlation: Ranz and Marshall, 1952
- Size change model: Shrinkage until critical moisture content
- Drying calculation approach: User specified single particle drying curve
- Drying curve source: Global specifications

Critical moisture content: kg/kg

Critical moisture content (dry basis) Uniform for entire array Per element

Results for Multizonal_spray_dryer

This unit is described by library model **Multizonal spray dryer** in gSOLIDS Unit Op - Drying. A description of this model can be found [here](#).

This report contains the following information:

- Inlet and outlet vapour properties (table).
- Inlet and outlet distributed phase properties (table).
- Mass fraction - inlet and outlet (graph).
- Particle temperature (graph).
- Wet basis moisture content (graph).

For further results, please see the trajectories in the case.

Model report summaries

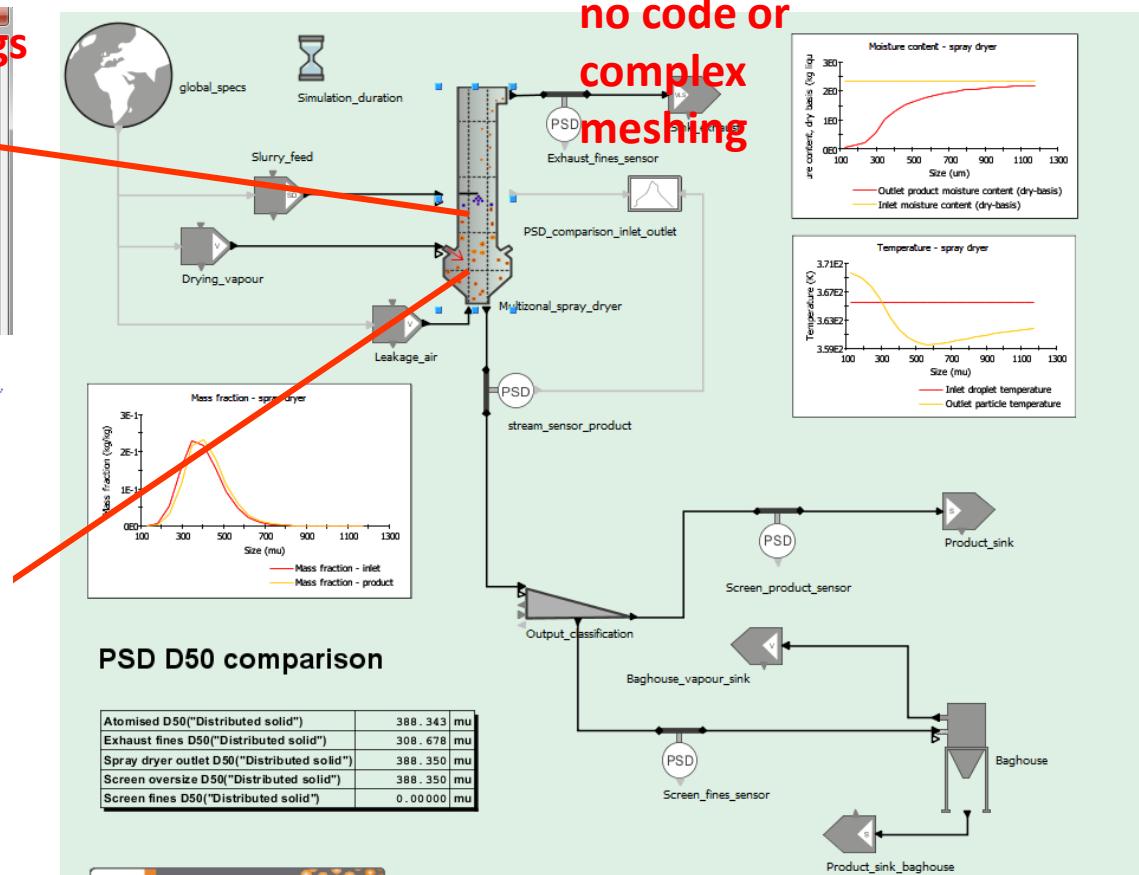
1. Inlet and outlet vapour properties

Property	Value at time 360.000	Units
Drying gas temperature	559.800	K
Exhaust vapour temperature(1)	357.574	K
Humidity drying gas (wet basis) ("Water")	0.000429002	kg/kg
Humidity exhaust gas (wet basis)(1,"Water")	0.0452575	kg/kg

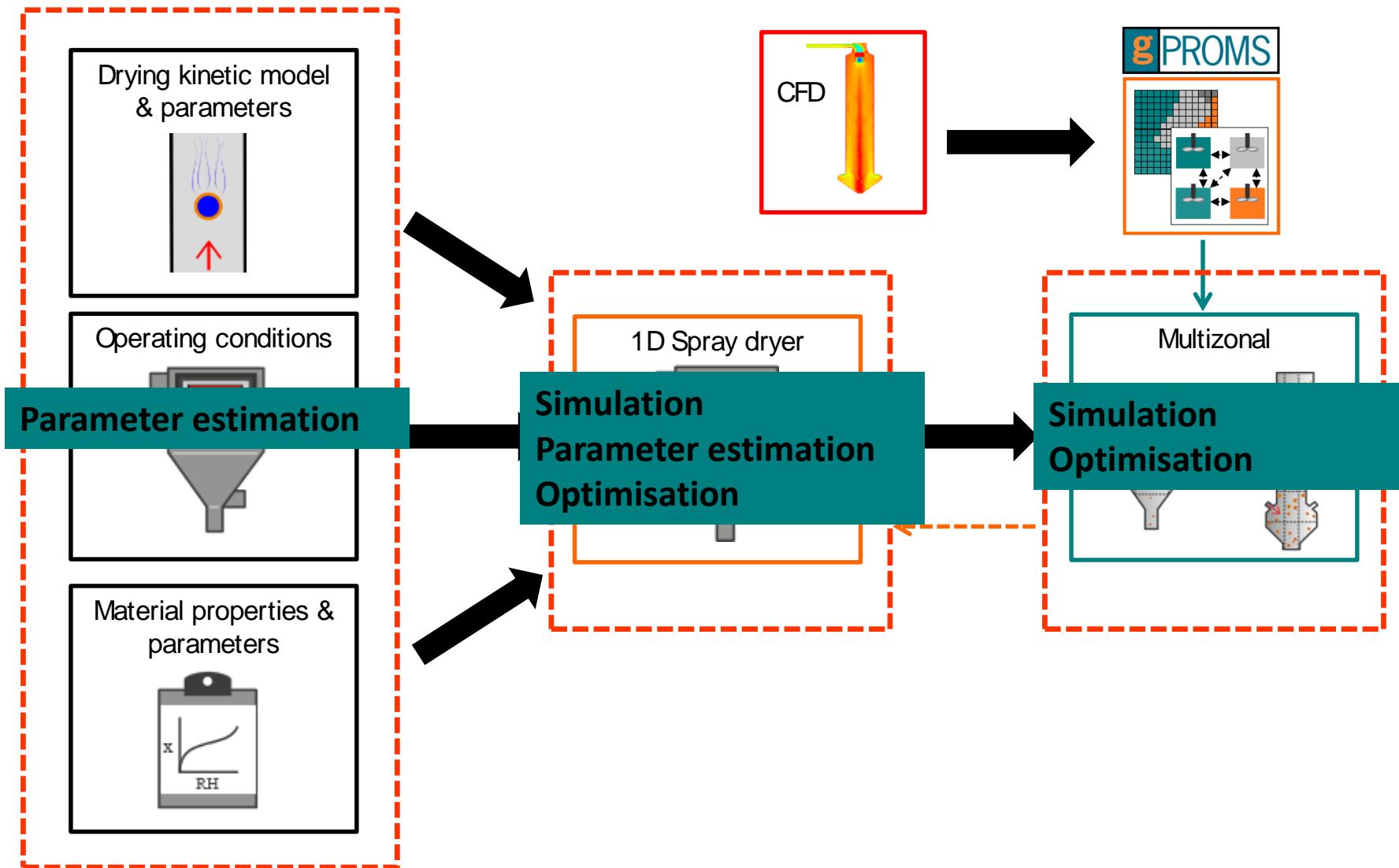
2. Inlet and outlet distributed phase properties

Property	Value at time 360.000	Units
Inlet solid mass flowrate("Distributed solid")	0.400000	kg/s
Fines mass flowrate(1,"Distributed solid")	2.49179E-05	kg/s
Product mass flowrate("Distributed solid")	0.315174	kg/s
Inlet solid temperature("Distributed solid")	365.550	K
Fines temperature(1,"Distributed solid")	360.795	K
Product temperature("Distributed solid")	420.621	K
Average moisture content at inlet (wet basis) ("Distributed solid","Water")	0.300000	kg/kg
Average moisture content of fines (wet basis)(1,"Distributed solid","Water")	0.225712	kg/kg
Average moisture content of product (wet basis) ("Distributed solid","Water")	0.111247	kg/kg

3. Mass fraction - atomised droplet, product and fines



Workflow of modelling spray drying process



Summary and conclusions

- Multizonal concept extended to Eulerian-Lagrangian CFD simulations
 - Compartmental model captures key phenomena of spray drying
 - Coupled to CFD for flow of particles and vapour between compartments (for co- and counter-current towers)
- A new predictive spray drying tool has been developed, it can be incorporated into an easy to use, flowsheeting setting which can be rolled out to non-expert modellers
 - Optimise process and explore design space
- Multizonal approach can be easily adopted for other unit operations
 - For example: fluid bed dryers and granulators

Acknowledgements & contributions



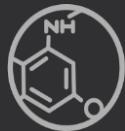
■ Project partners

- P&G: Luis Martin de Juan, Zayeed Alam, Mark Crosby, Hossein Ahmadian
- University of Leeds: Muzammil Ali, Mojtaba Ghadiri, Tariq Mahmud, Peter Heggs, Mazaher Molaei
- PSE: Sean Bermingham
- Novozymes: Poul Bach

■ Innovate UK funded project

- Spray Drying Process Efficiency Step Change - 101332

Thank you



Tower Modelling Capability Development – C+D Projects



UNIVERSITY OF LEEDS

Spray Drying gPROMS Model

TSB: 2013-2015

Atomisation



The University
Of
Sheffield.

Post-doc: 2012-2013

CFD RTD

UNIVERSITY OF LEEDS

PhD: 2011-2014

Agglomeration



EngD: 2010-2013

Droplet Coalescence

Experimentation
Imperial College
London

Post-doc: 2013-2016

Droplet Coalescence PBM

University of
Strathclyde
Glasgow

Experimental in Air

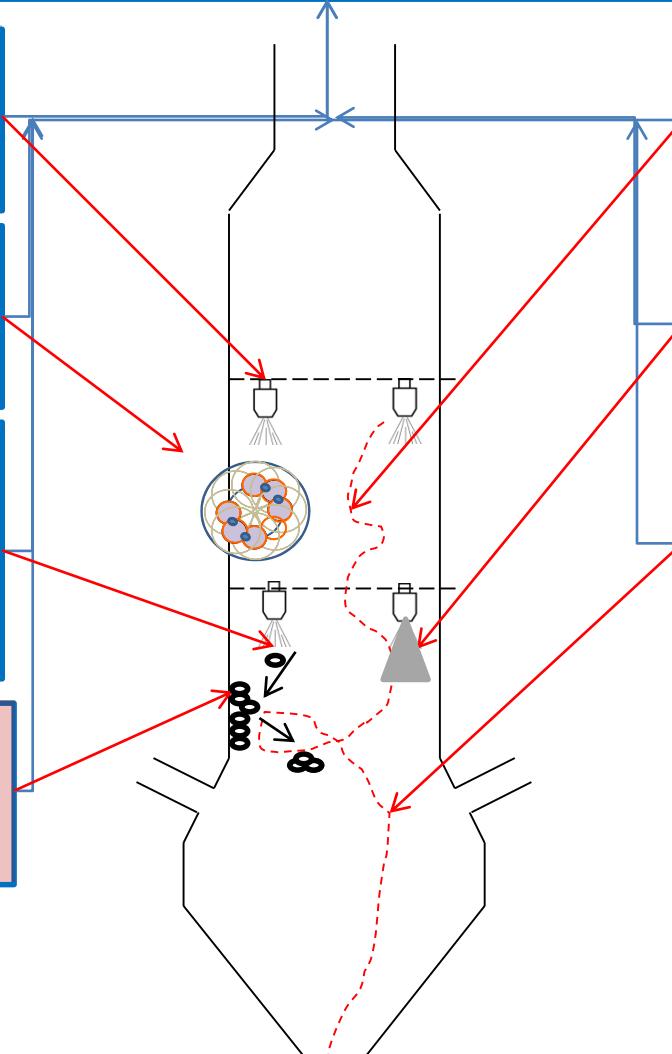
Imperial College
London

PhD: 2014-2017

Wall Make-up Mechanisms

Imperial College
London

Post-doc: 2014-2016

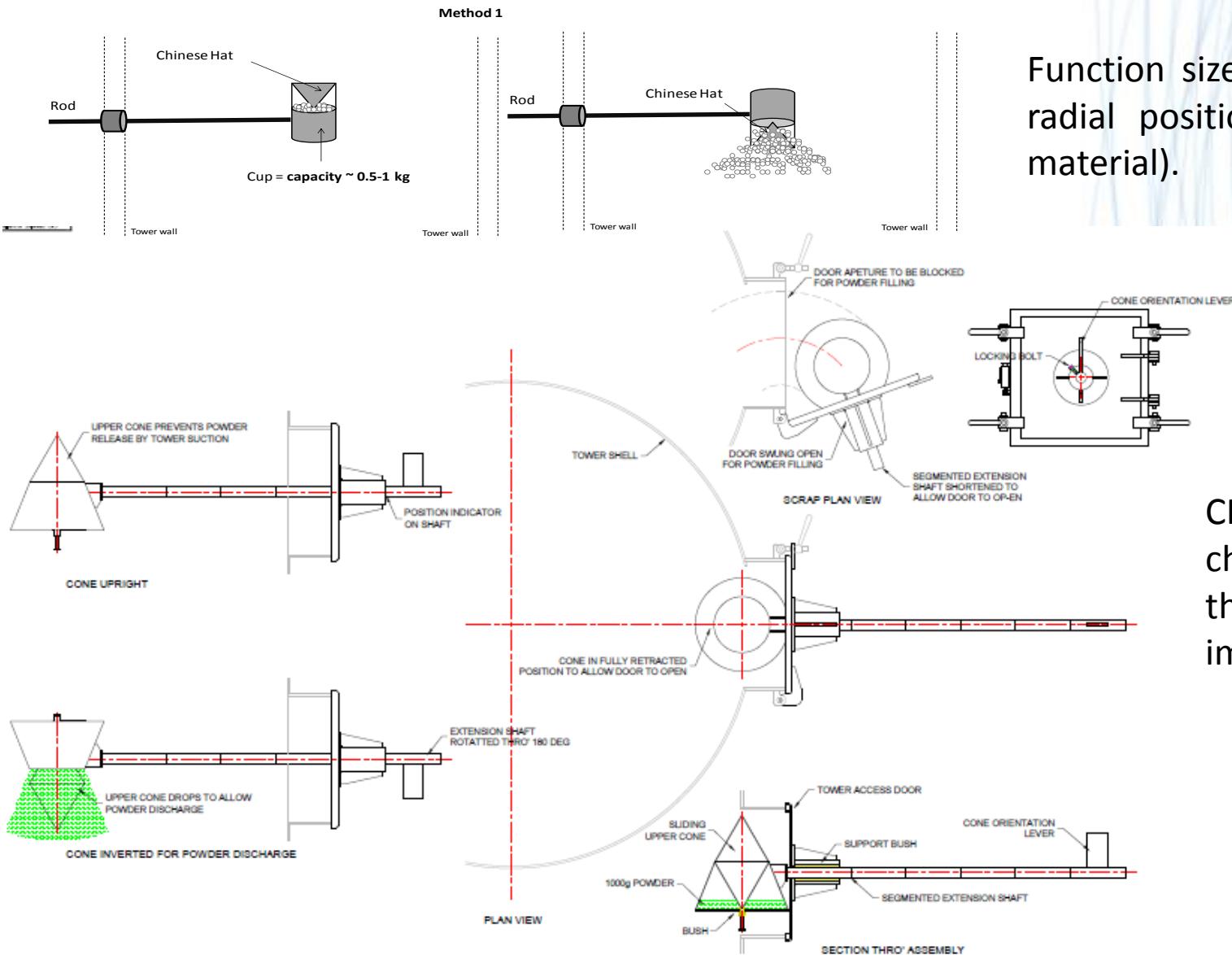


Long term capability projects in key areas leading to better understanding and predictability.

Work Packages

Work Package	Leader	Description	Team members
WP1	University of Leeds	<p>Developmental of compartmental modelling approach using CFD simulations for various tower systems:</p> <ul style="list-style-type: none"> • Model the range of operational scenarios in P&G/Novozymes 1 pilot plant and 1 manufacturing plant using CFD simulations. • Validate the CFD model using pilot plant data/measurements. • Construct approach to compartmentalise towers (both co-current and counter-current). 	Mazaher Molaei, Mojtaba Ghadiri Peter Heggs, Andrew Bayly and Tariq Mahmud (Poul Bach and Hossein Ahmadian,
WP2	Novozymes A/S (as sub-contractor)	<p>Characterisation of slurries and single droplet drying. Analysis of slurry thermo-physical properties, atomisation and selection of correct drying model:</p> <ul style="list-style-type: none"> • P&G slurry characterisation done in NIC. • Novozymes slurry characterisation done in Bargsvaerd, Denmark. 	Poul Bach (and Hossein Ahmadian/Luis Martin De Juan). Possibly other members of MSUC and Process Design.
WP3	Process Systems Enterprise	<p>Development of robust spray drying unit operation model based on air flow and droplet motion:</p> <ul style="list-style-type: none"> • Develop first compartment model block with selection of single droplet drying models (Hecht and Sloth). • Develop multi-compartment model to represent spray drying unit operation. • Implement a selection of models for population balancing (agglomeration) and heat losses. • Integrate model into a flowsheet. 	David Slade, Sean Birmingham and Mark Pinto (Mazaher Molaei)
WP4	P&G	<p>a) Verification and validation of model on various spray drying tower scales.</p> <ul style="list-style-type: none"> • Check fidelity of drying model as well as parameter estimate coalescence and agglomeration in towers. • Validate model on plant scale. <p>b) Application of validated model for energy minimisation per unit product.</p> <ul style="list-style-type: none"> • Demonstrate usage of model (for energy saving) by changing nozzle configuration, air flowrates and temperature, loading, reduction in coarse material and changes in ancillary equipment. 	David Slade, Hossein Ahmadian, Poul Bach, Luis Martin De Juan (others in M&S/MSUC)

WP4: Tower in process measurement (Particles)



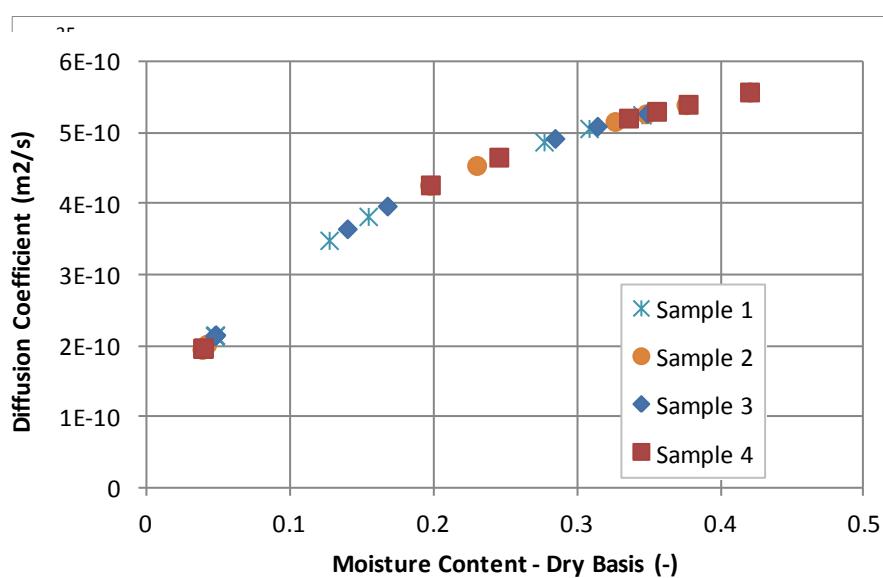
Function size, axial and radial position (1kg of material).

CFD underway to check how badly the assembly impact air flow

WP2: Diffusion Coefficient – P4

Diffusion coefficients is measured using the drying slab method. The procedure involves:

- using slurry or granules which have been mixed with water back to the target slurry moisture.
- placing them in petri dish (8.5 cm in diameter) with different heights (8 and 12 mm). This equates to around 60-100g of slurry depending on size.
- drying them mix in an above (top of petri dish open) at 75 °C whilst monitoring the weight of the sample for 3-4 days.

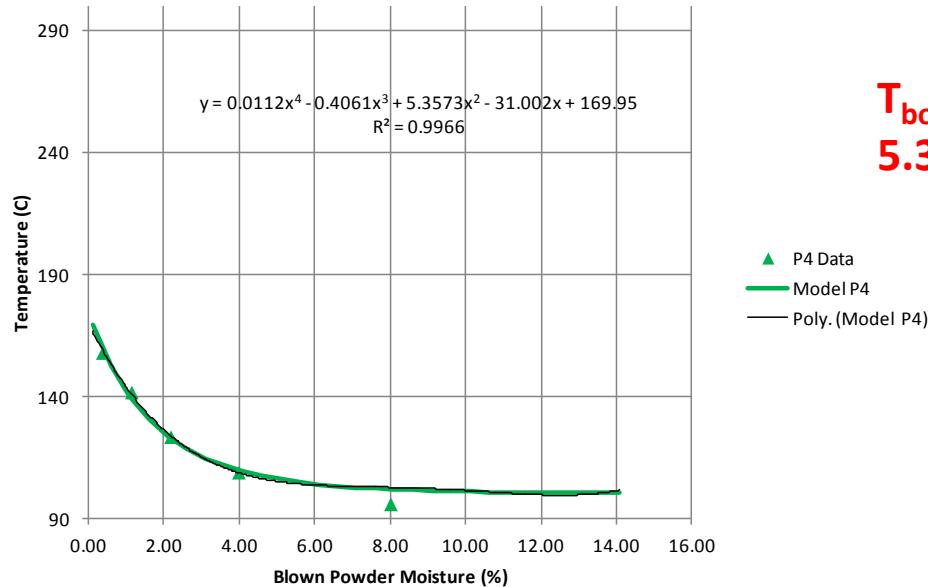


- This plot is then fitted to find a diffusion coefficient as a function of moisture content for a slab (using gPROMS).
- The coefficients for diffusion, density, specific heat capacity etc.. are then used to run the full Hecht and King (2002) drying model in gPROMS to extract coefficients A, B and C.
- For this formulation, these are A = 40, B=0.29 and C=16.5.

WP2: Boiling Point – P4

Boiling point rig involves placing around 10-13g of pre-sieved powder (300-425 microns) in vials and pre-conditioning the samples to various moistures (e.g. 8%, 4%, 2%, 1%).

The vial is then place in the boiling point rig (pressure vessel) where the temperature is set at 100 °C then increased every 2 hrs to 115, 130, 140 and finally 150 °C. The vapour pressure inside the vial is monitored allowing to calculate the boiling point – this is then plotted for all case as shown below:



$$T_{boil} = 0.0112 w_i^4 - 0.4061w_i^3 + 5.3573w_i^2 - 31.002w_i + 169.95$$

Particle motion only

- Motion (transfer between zones) and accumulation of particles in a zone under well mixed assumption – mass flux in calculated in adjacent zones:

$$\frac{dM(z)}{dt} = \sum_{j=1}^{NI} (\phi_{in}^j(z) - \phi_{out}^j(z))$$

At $t = 0$, $M(z) = m_0$

$$M(z) = V C(z)$$

$$\phi_{out}^j(z) = SA(j) v_j(z) C(z)$$

$$C(z) = N(z) \frac{\pi}{6} z^3 \rho(z)$$

$$\tau_{avg} = \frac{M(z)}{\sum_j \phi_{out}^j(z)}$$

$M(z)$: mass holdup of particles of diameter z (kg),

NI : number of interfaces with adjacent zones,

$\phi_{in}^j(z)$: mass flux in of particles of diameter z through interface j (kg / s),

$\phi_{out}^j(z)$: mass flux out of particles of diameter z through interface j (kg / s),

m_0 : initial mass of particles in zone (kg),

V : volume of zone (m^3),

$C(z)$: mass concentration of particles of diameter z (kg / m^3),

$SA(j)$: surface area of interface j (m^2),

$v_j(z)$: velocity of particles of diameter z at interface j (m / s),

$N(z)$: number concentration of particles of diameter z ($\# / m^3$),

$\tau_{avg}(z)$: average residence time of particles of diameter z (s).

- NB: Surface area, velocities, volume of zone are the quantities to be extracted from CFD simulation via Multizonal interface.

Drying Model

- Using Hecht drying model

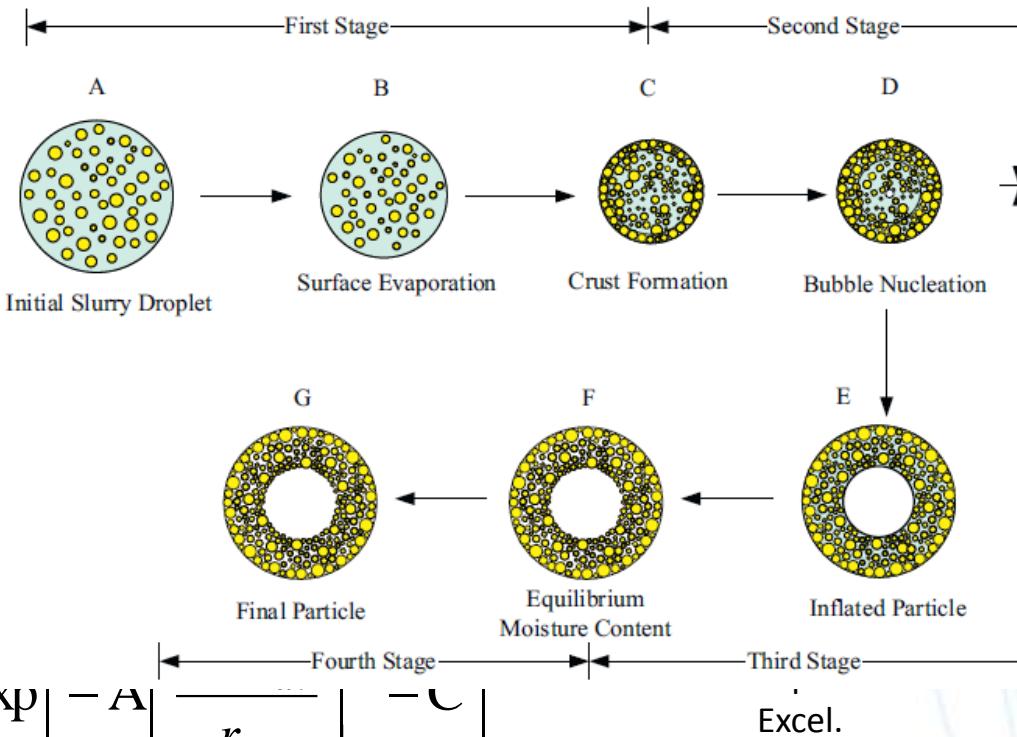
- 1st stage - Initial

$$D_R = 4 \cdot \pi$$

Heat and mass transfer

- 2nd stage - Part curve fit equation

$$D_R = r_p \times \exp \left[-A \left(\frac{r_p}{r_{p,i}} \right)^n \right]$$



- 3rd stage - Particle drying rate after the boiling point is given by an energy balance about the particle:

$$D_R = \frac{\alpha 4\pi \left(\frac{d_p}{2} \right)^2 (T_g - T_p)}{h_{fg} - (w_s c_{p,s} + w_l c_{p,l}) w_s \frac{dT_{boil}}{dw_l}}$$

$$T_{boil} = f(\text{moist})$$

an exponential

constants for the
ed in gPROMS or

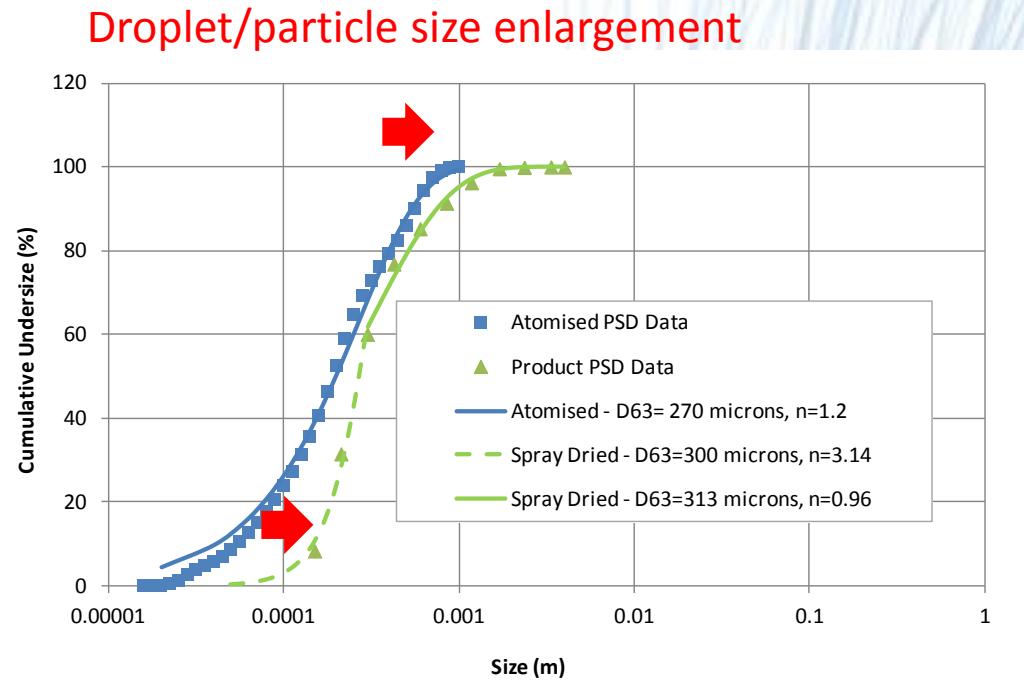
Coalescence/Agglomeration

Currently not accounted in CFD.

Population balances (e.g. Liu and Litster, 2002) already in gSOLIDs.

Multitude of models available for collisions kernels (6 in gSOLIDs) and plan to include 1-2 of:

- O'Rouke (parcels)
- Abrahamson



For collision efficiency, reapply work on Blei and Sommerfeld (2007) including different types of collisions based on Ohnesorge number:

ST-droplet	vs	ST – droplet
ST-droplet	vs	Dry/Viscous droplet
Viscous droplet	vs	Viscous/Dry particle
Dry particle	vs	Dry particle

$$Oh^2 = \frac{\mu_{droplet}^2}{d_{droplet} \rho_{droplet} \sigma_{Droplet}}$$

CFD vs Experiments (no agglomeration – full size)

Single nozzle tower

	Exp	CFD (spherical)	CFD (Rough)
Hot Air Inlet Temperature (°C)		268	
Hot Air Rate (kg/hr)		Confidential	
Slurry Rate (kg/hr)		Confidential	
Nozzle Position (m)		Confidential	
Exhaust temp (°C)	91.1	90.68	74.85
Powder Temperature (°C)*	71.6	168.5	170.59
Powder Rate (kg/hr)	1185	1181.1	1148
Yield (%)	~95%	94%	90%
Moisture content of particle (wt/wt%)	1.93	7.6	5

* Should be similar to boiling point ~125 °C

- Whilst for the smooth case, the exhaust gas temperature and rate can be predicted, the final product moisture is incorrect (due to lack of drying of larger particles).
- Lack of coalescence or agglomeration models in CFD may also cause issues given that atomised droplets are smaller and dry more prior to size enlargement.
- There is also significant heating of the dried droplets to much higher temperatures than boiling point (energy inefficient).

