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# CFD-DEM modeling of fluidized beds with heat production: Influence of the particle size distribution and heat source

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[DPI Project # 751 Predictive Modeling of Polyolefin Reactors]

# CFD-DEM modeling of fluidized beds with heat production: influence of the particle size distribution and heat source

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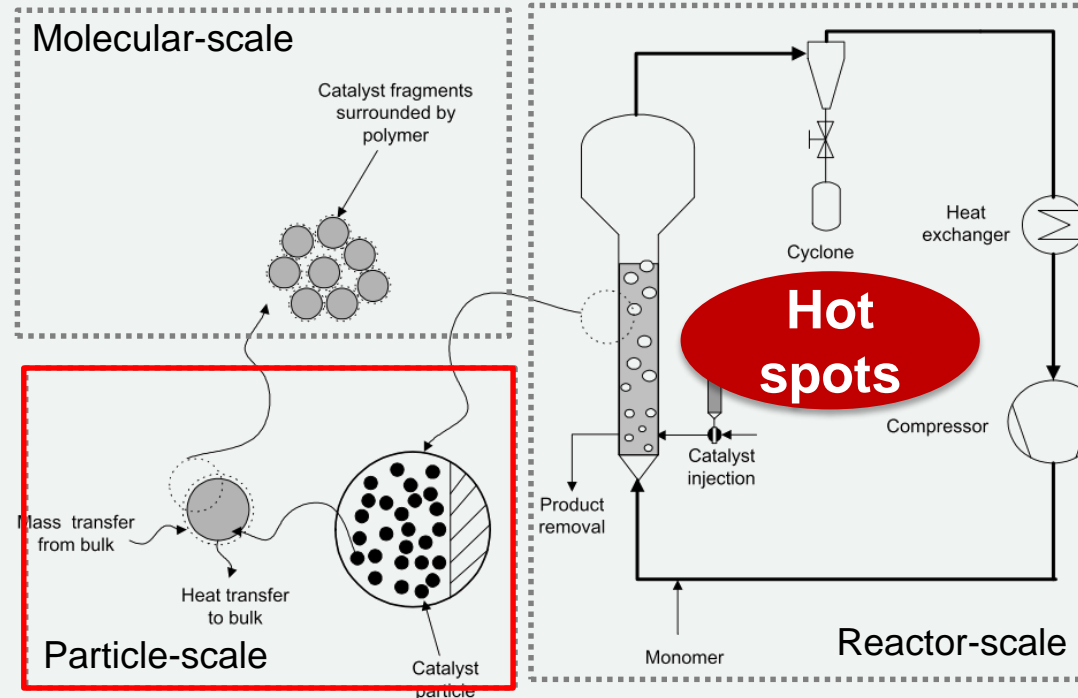
May 22-27, 2016  
Fairmont Le Chateau Montebello  
Quebec, Canada



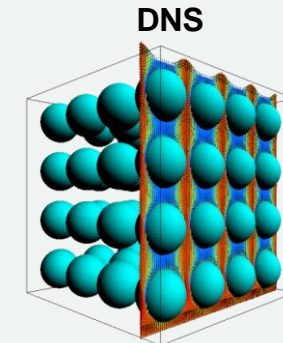
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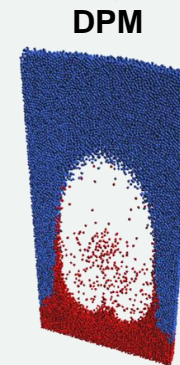
# Project background Polymerization process



Several characteristic length scales in a fluid bed reactor for catalytic olefin polymerization.

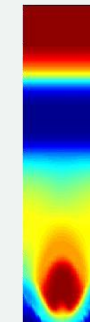


Particle number  $\sim 10^3$



Particle number  $10^3 \sim 10^5$

TFM



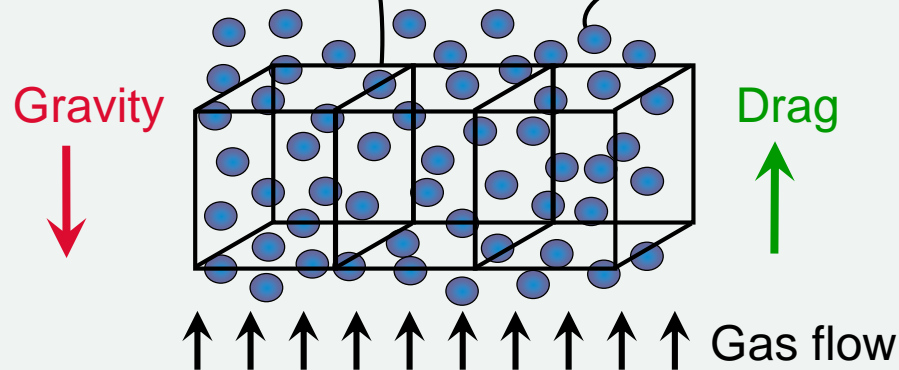
Particle/gas  
continuous phases

## Model introduction

### Discrete Particle Model (DPM)

Navier-Stokes equations solved in Eulerian cells

Element movement follows from external and contact forces:



$$m_a \frac{d\mathbf{v}_a}{dt} = \mathbf{F}_d + \mathbf{F}_p + \mathbf{F}_g + \mathbf{F}_c$$

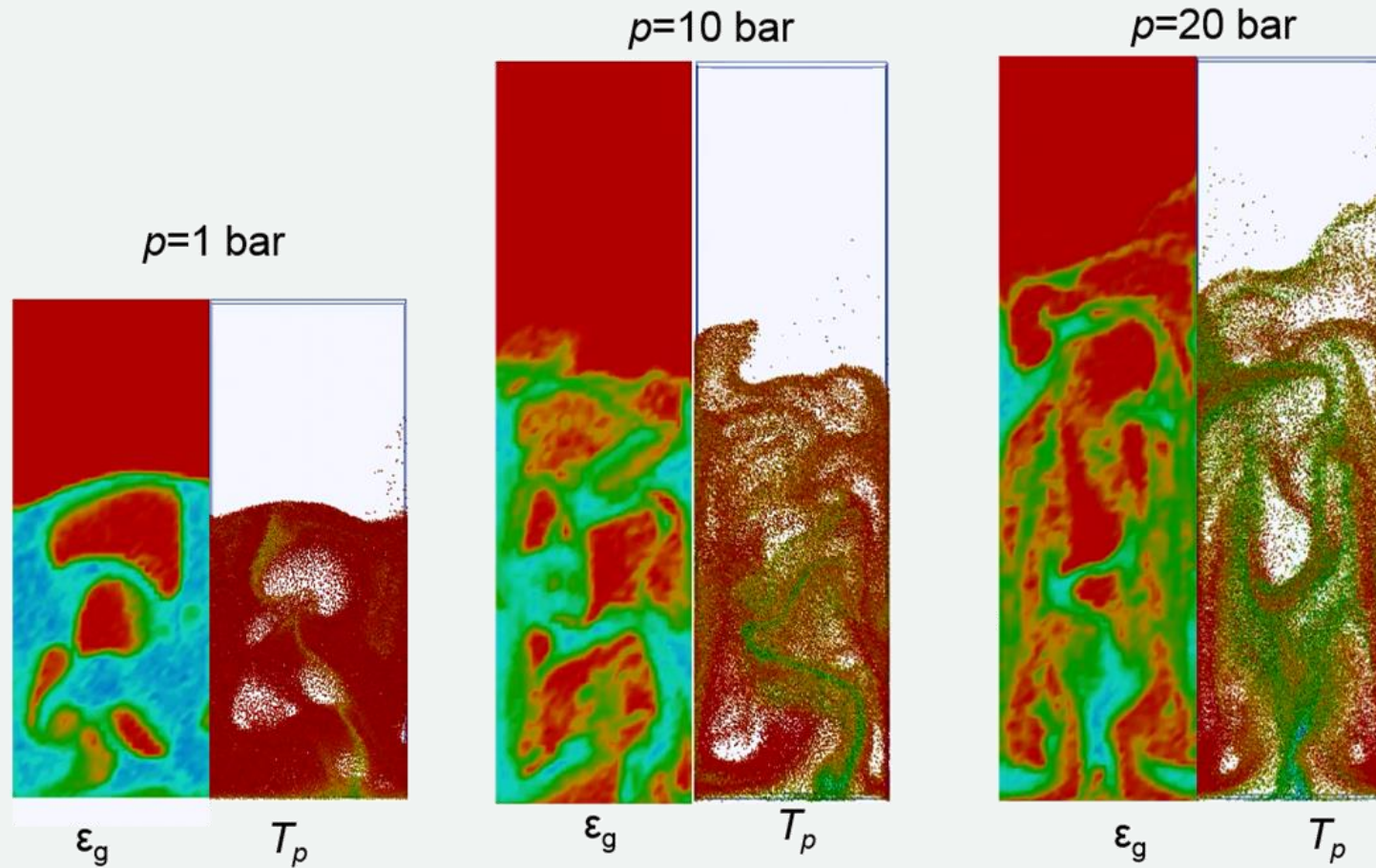
$$\rho_p V_p C_{p,p} \frac{dT_p}{dt} = -hA_p (T_{p,a} - T_g) + q_v V_p$$

$$\frac{\partial}{\partial t} \varepsilon \rho_g \mathbf{u} + \nabla \cdot \varepsilon \rho_g \mathbf{u} \mathbf{u} = -\varepsilon \nabla p - \nabla \cdot \varepsilon \boldsymbol{\tau}_g - S_p + \varepsilon \rho_g \mathbf{g}$$

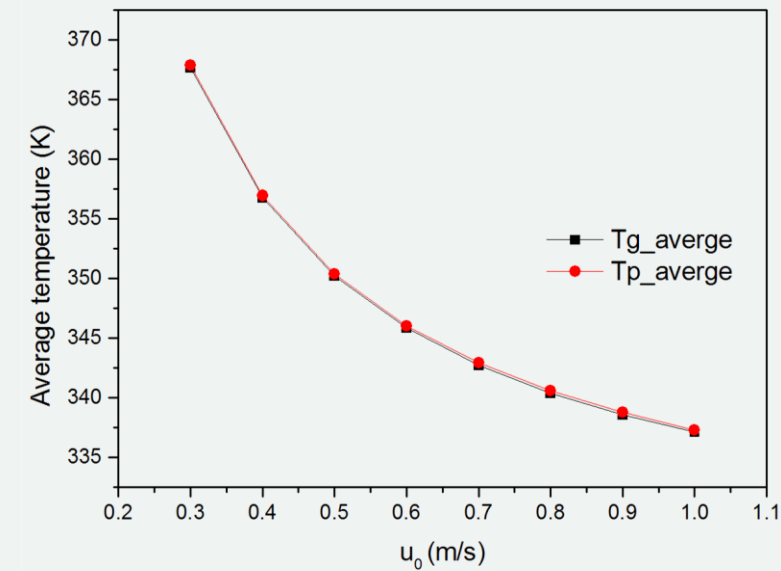
$$C_{p,g} \left[ \frac{\partial(\varepsilon_g \rho_g T_g)}{\partial t} + (\nabla \cdot \varepsilon_g \rho_g \mathbf{u}_g T_g) \right] = -(\nabla \cdot \varepsilon_g \mathbf{q}) + Q_p$$



## Simulations with mono-dispersed particles



- **General understanding of fluidization and energy balance: with mono-dispersed particles**

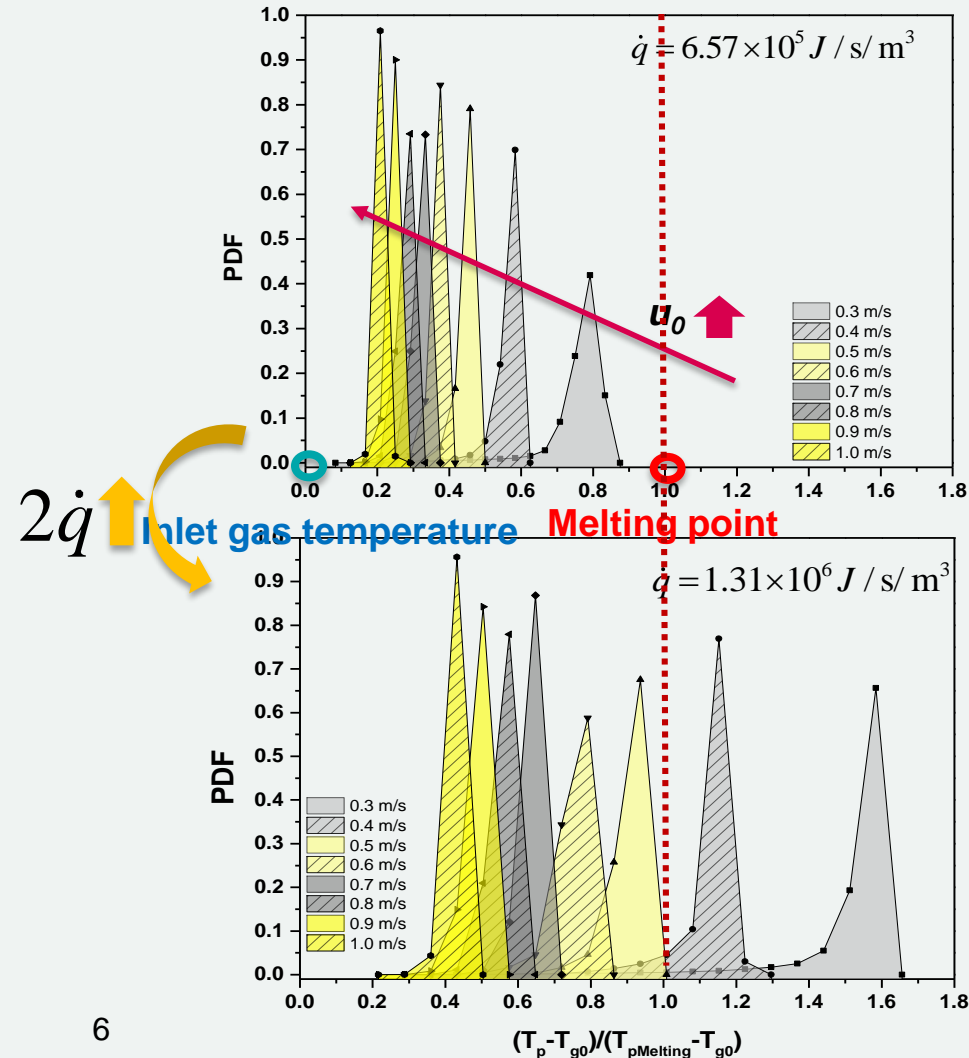


## Simulations with mono-dispersed particles

### Particle temperature distribution

- Probability distribution function (PDF) of the **dimensionless particle temperature**.
- Definition:

$$T_0 = (T_p - T_{g,0}) / (T_{p,melting} - T_{g,0})$$



# Simulations with poly-dispersed particles

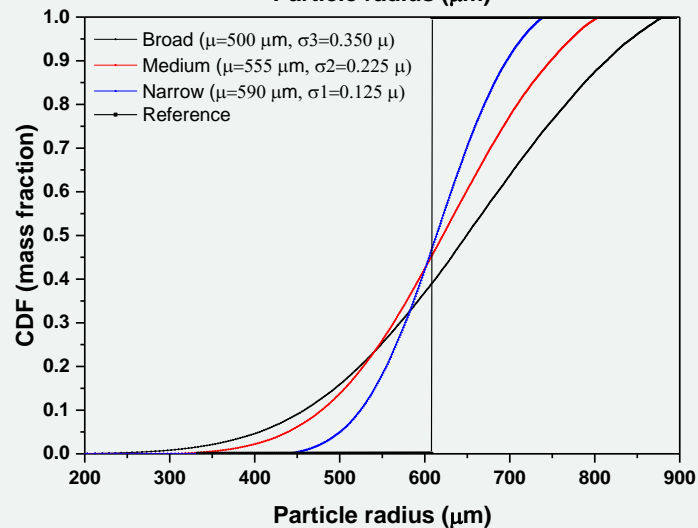
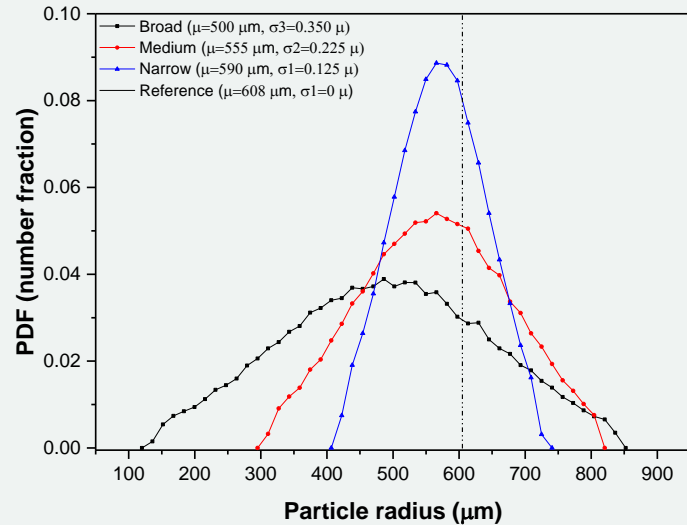
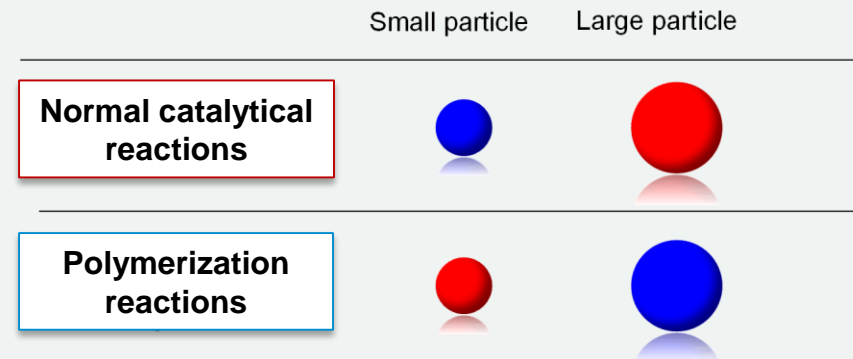


Table. Particle properties

	Mean radius ( $\mu\text{m}$ )	Standard deviation ( $\mu\text{m}$ )	Sauter mean radius ( $\mu\text{m}$ )	Mass of the bed (g)	Particle number
Reference	608	0	608	35.6	56,601
$\sigma_1$ (narrow)	590	75	608	35.6	59,908
$\sigma_2$ (medium)	555	125	608	35.6	66,807
$\sigma_3$ (broad)	500	175	608	35.6	80,000







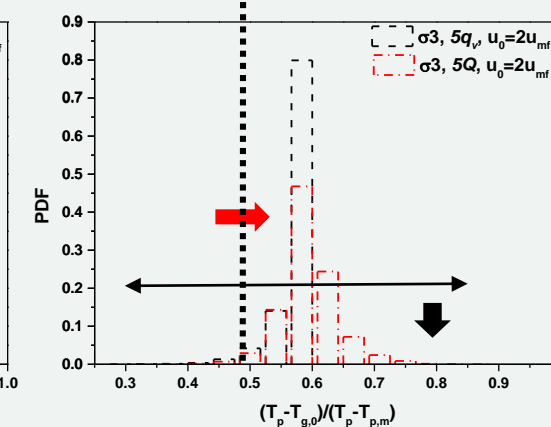
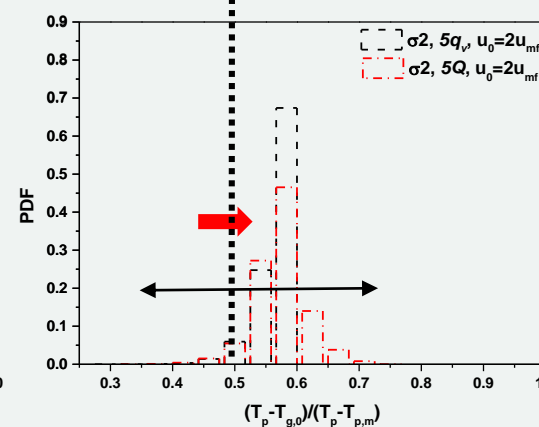
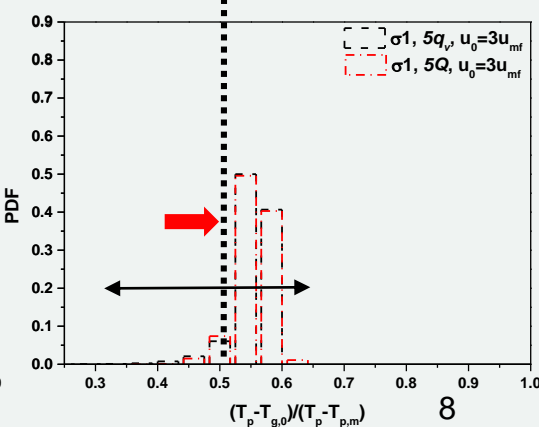
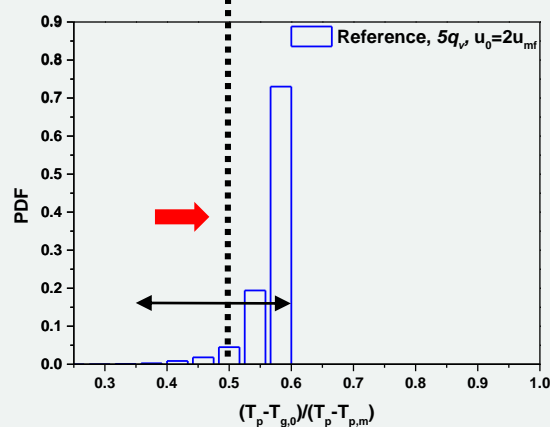
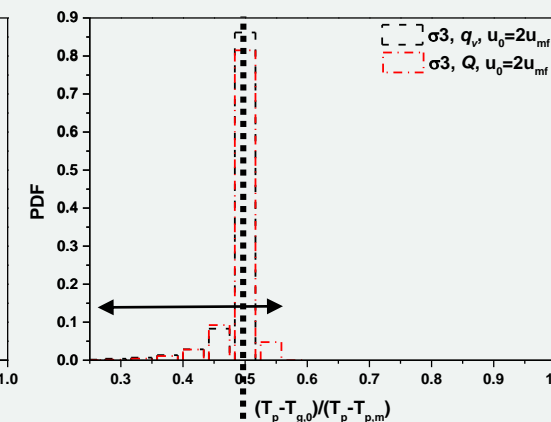
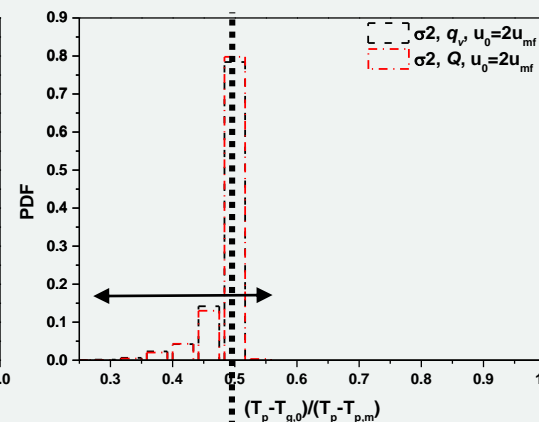
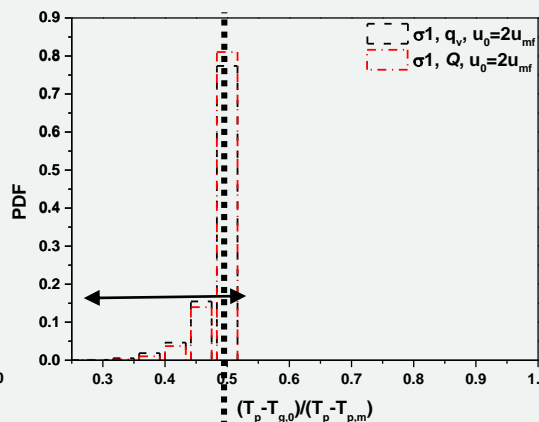
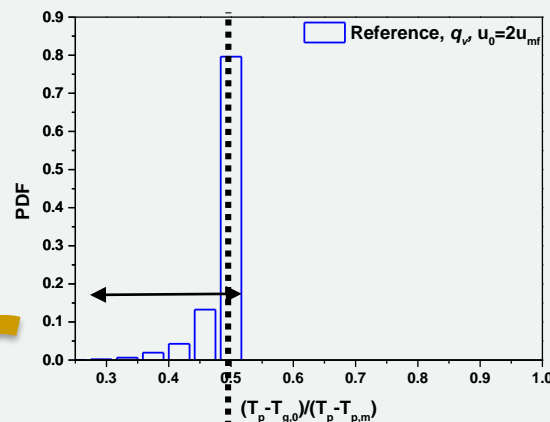
# Simulations with poly-dispersed particles - Particle temperature PDF

mono

narrow

medium

broad



Small heat production

5

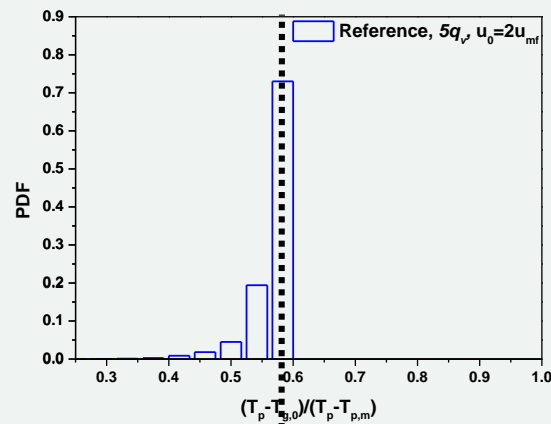
Large heat production



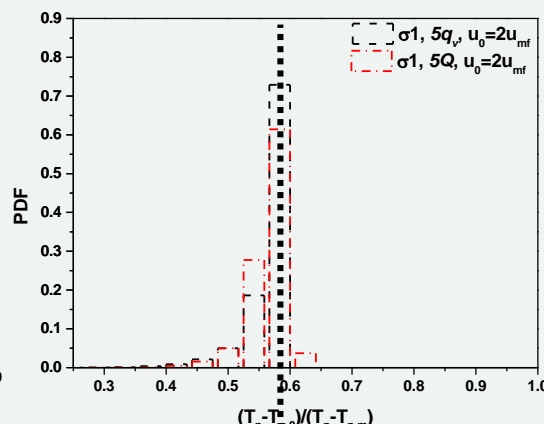
# Simulations with poly-dispersed particles - Particle temperature PDF

$u_0 = 2u_{mf}$

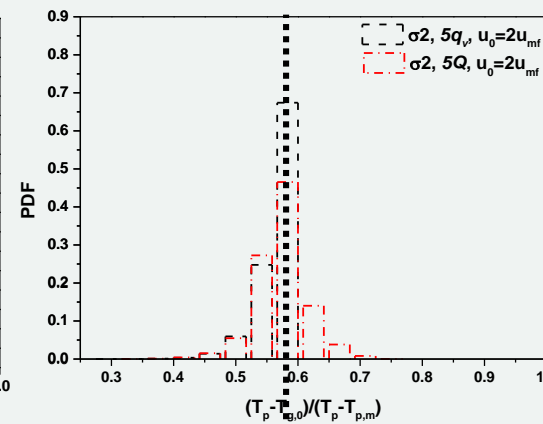
mono



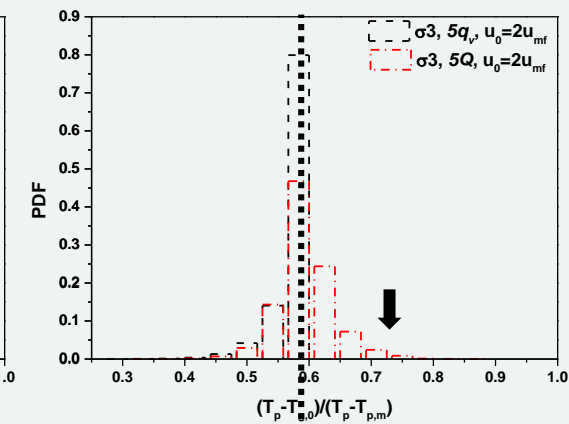
narrow



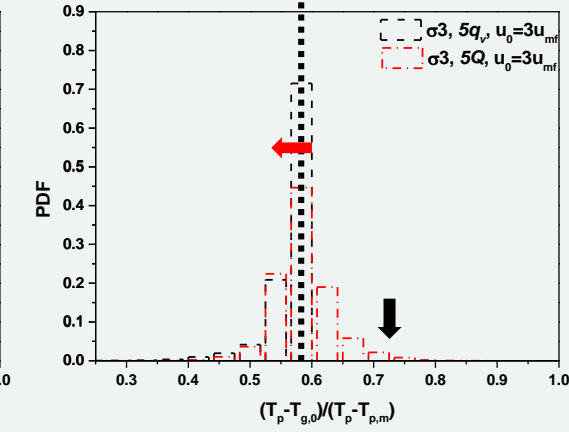
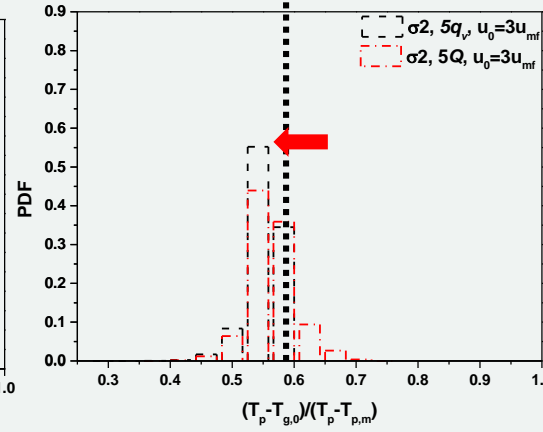
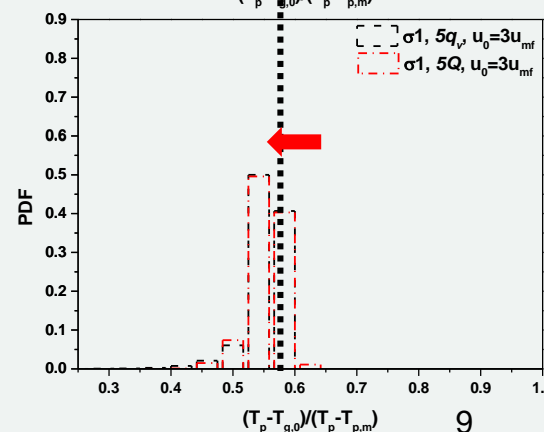
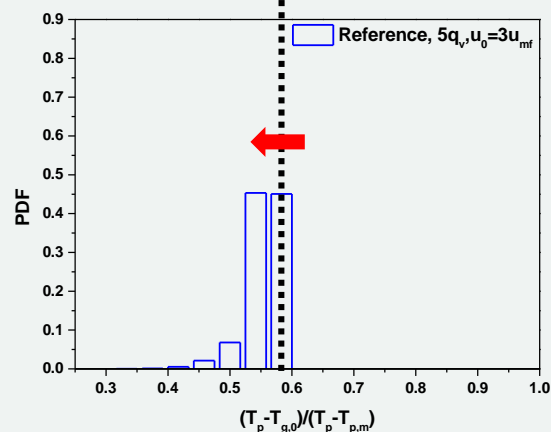
medium



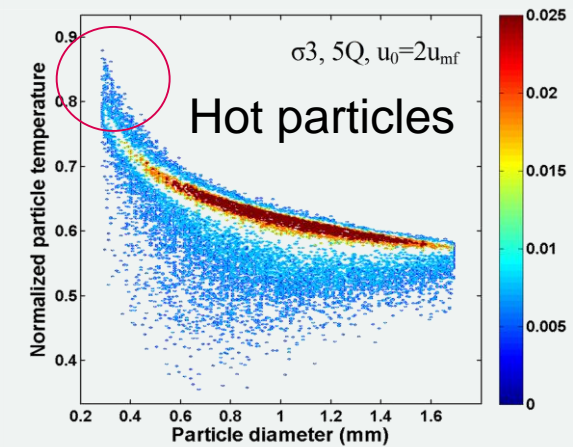
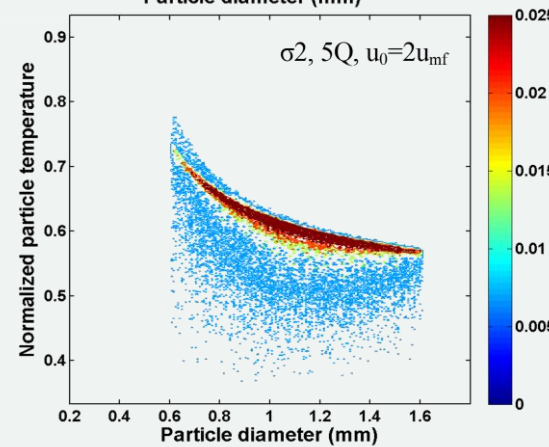
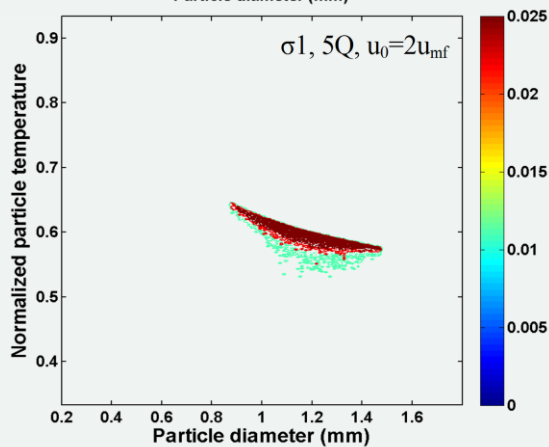
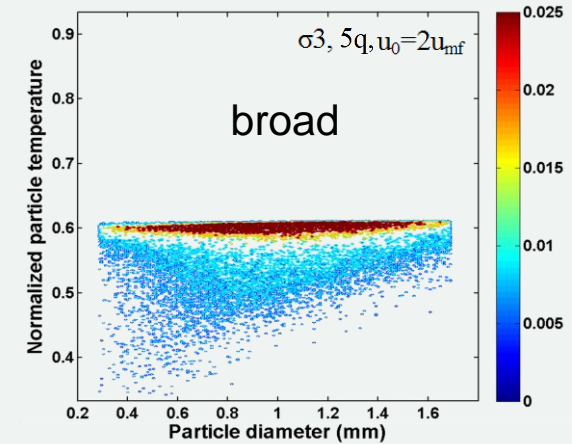
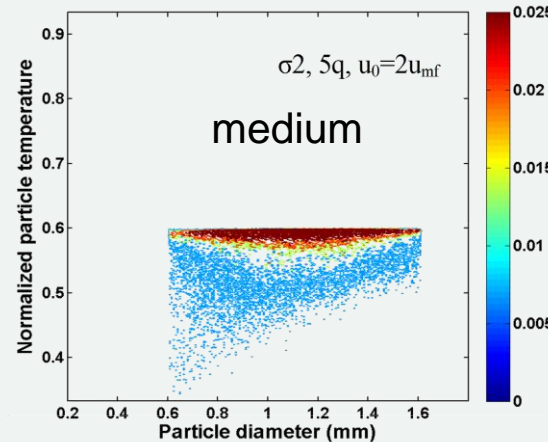
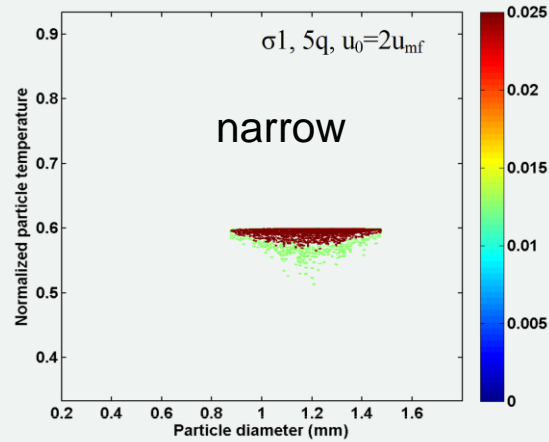
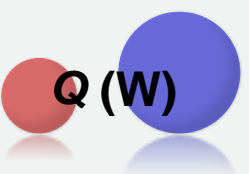
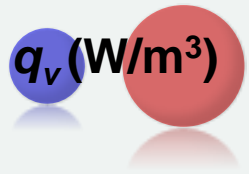
broad



$u_0 = 3u_{mf}$

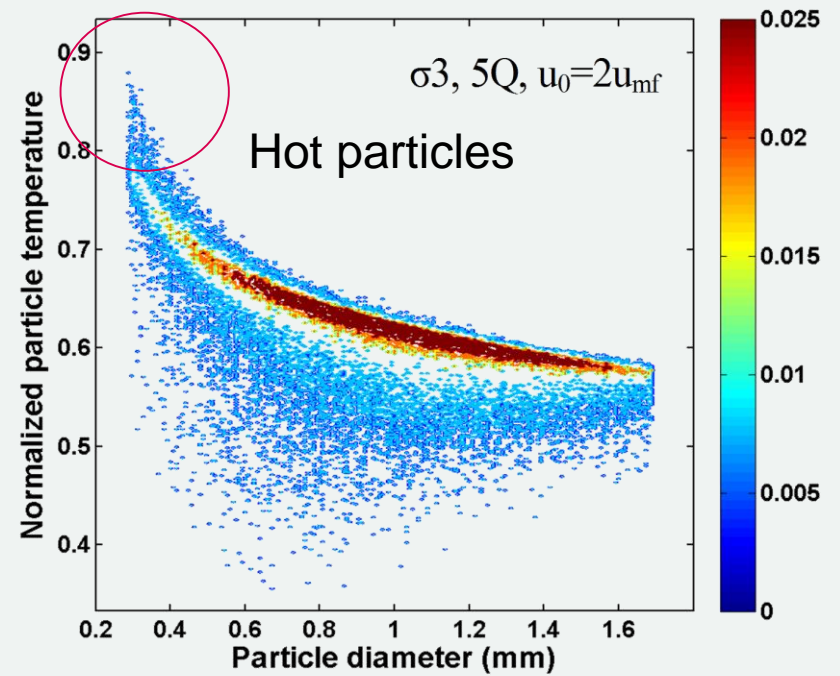
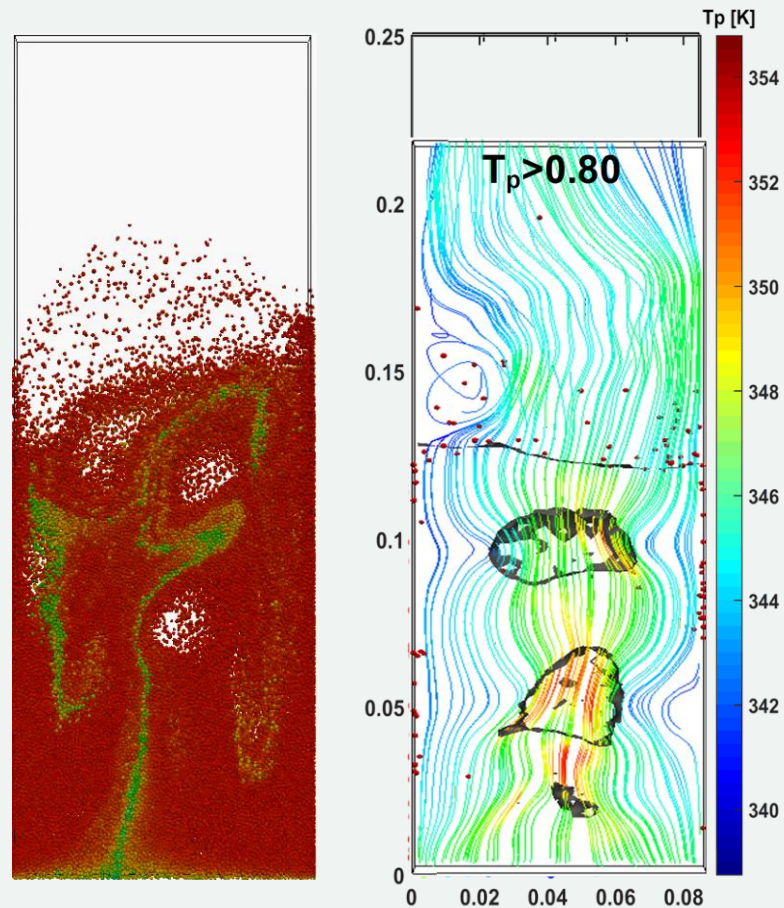


# Simulations with poly-dispersed particles - Temperature contour





## Mechanism of hot spots formation





## Conclusions

- With the same total heat generation and same cooling capacity in the bed, particles with a constant  **$Q$**  show a **broader temperature distribution** compared to those with a constant volumetric heat production  $q_v$ .
- The spread in temperature distribution increases as the heat generation is increased.
- The largest difference between the highest and lowest particle temperature in the bed occurs in the case with the broadest PSD and constant heat production per particle (i.e. polymerization).  
The hot particles that are close to the melting point are those **small particles with high catalyst activity**.
- They are mostly found in the free board and near the side walls.



### **Acknowledgment**

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**Thanks  
for your attention!**

