5-24-2016

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]

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Fluidization XV
ECI Conference Series

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

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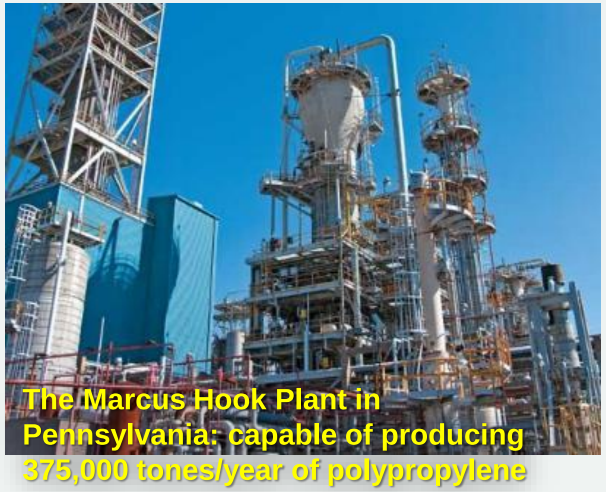
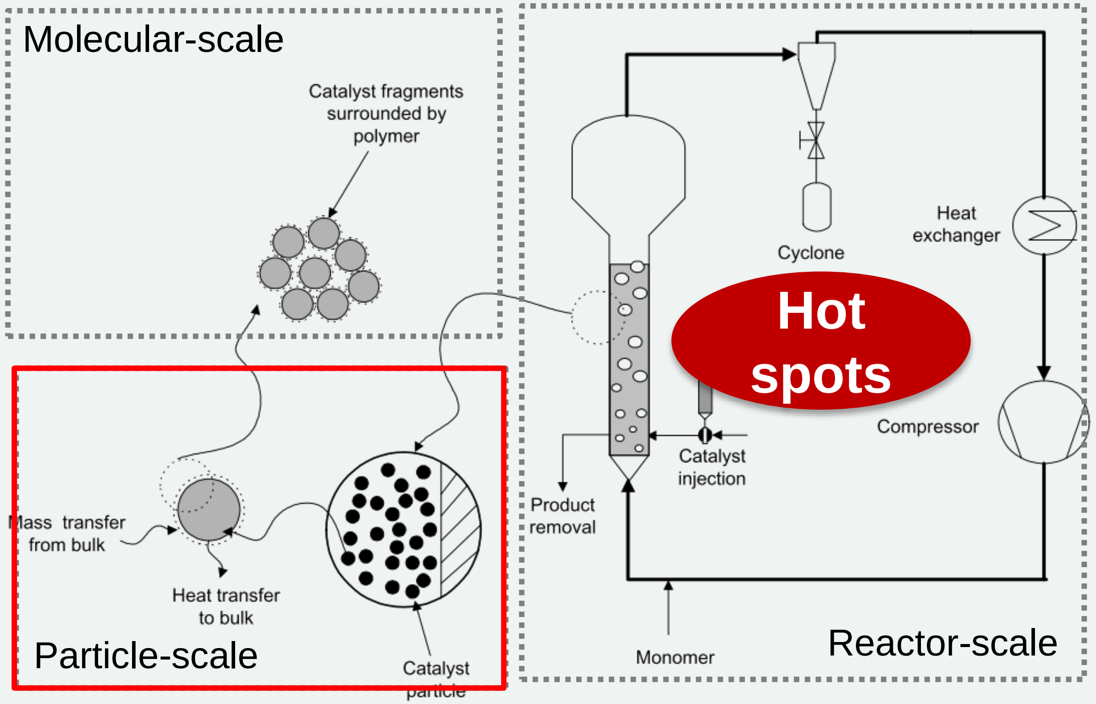
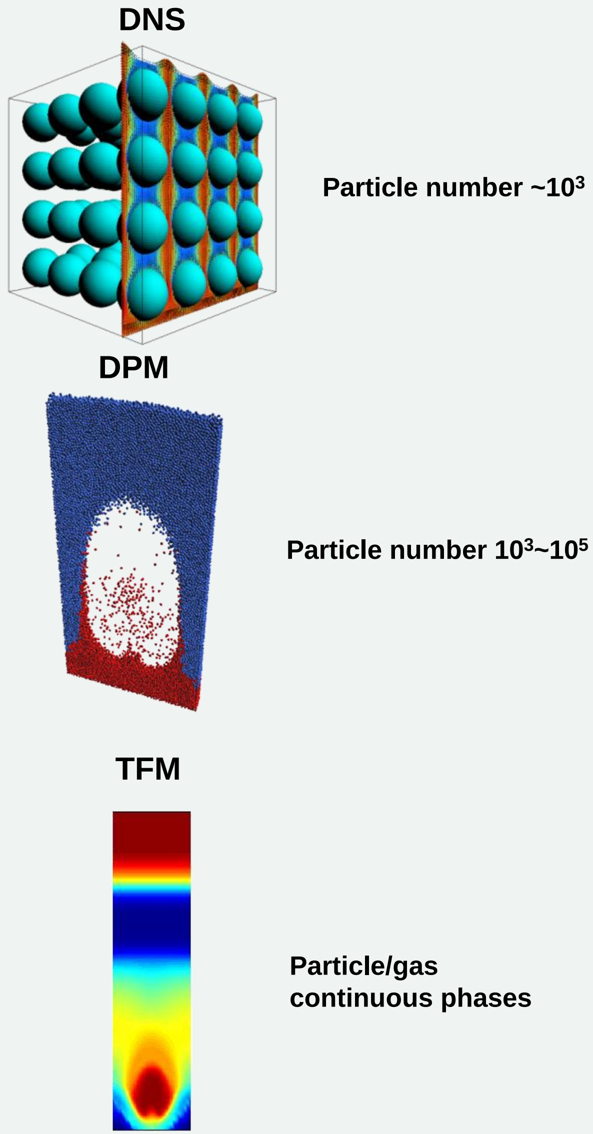
Project background

Polymerization process





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



Model introduction

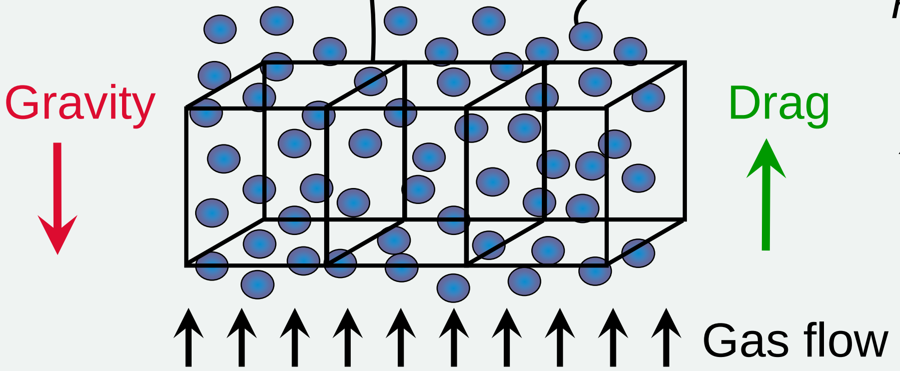
Discrete Particle Model (DPM)

Navier-Stokes equations solved in Eulerian cells

Element movement follows from external and contact forces:

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

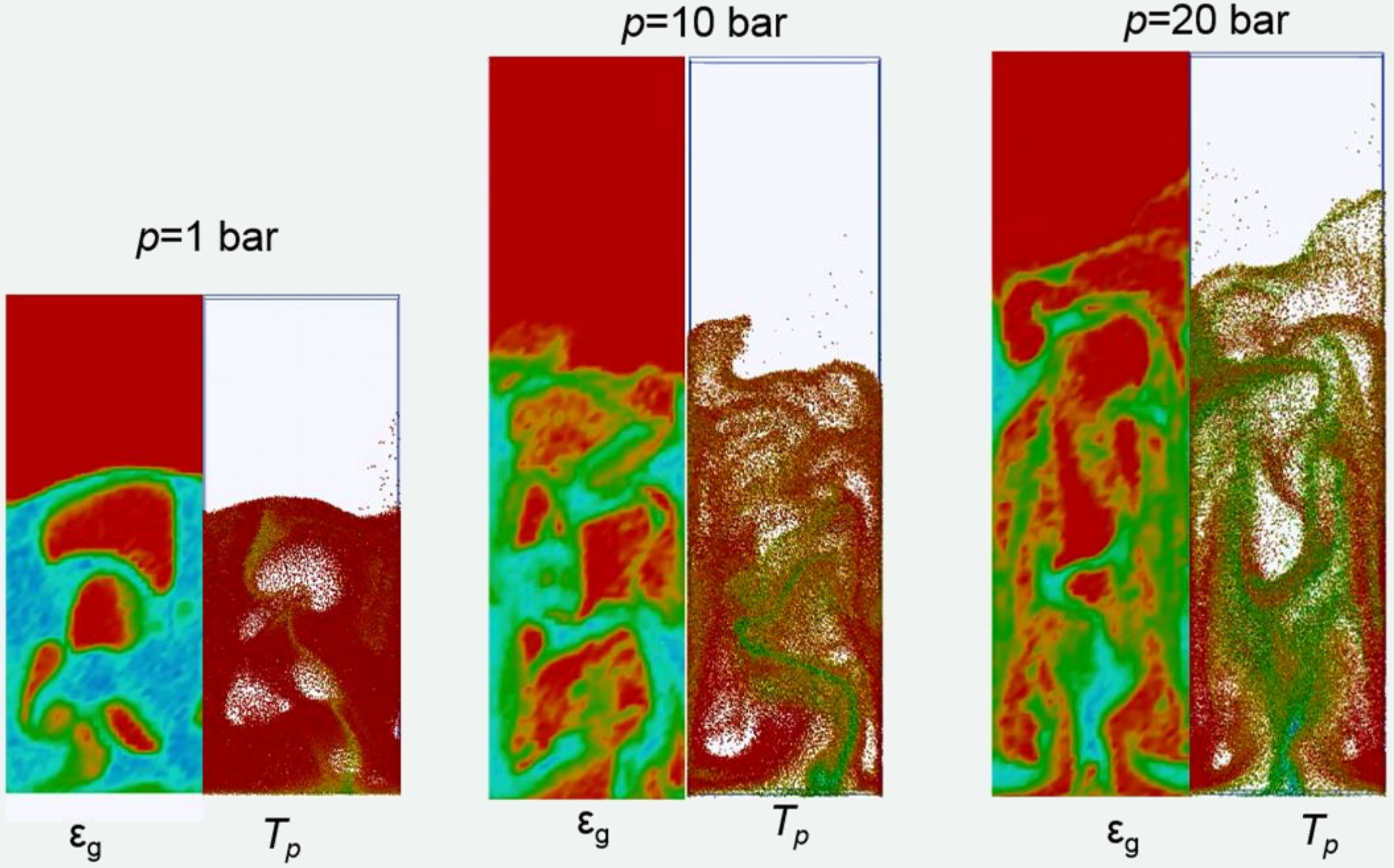
$$\rho_p V_p C_{p,p} \frac{dT_p}{dt} = -hA_p\left(T_{p,a} - T_g\right) + q_v V_p$$



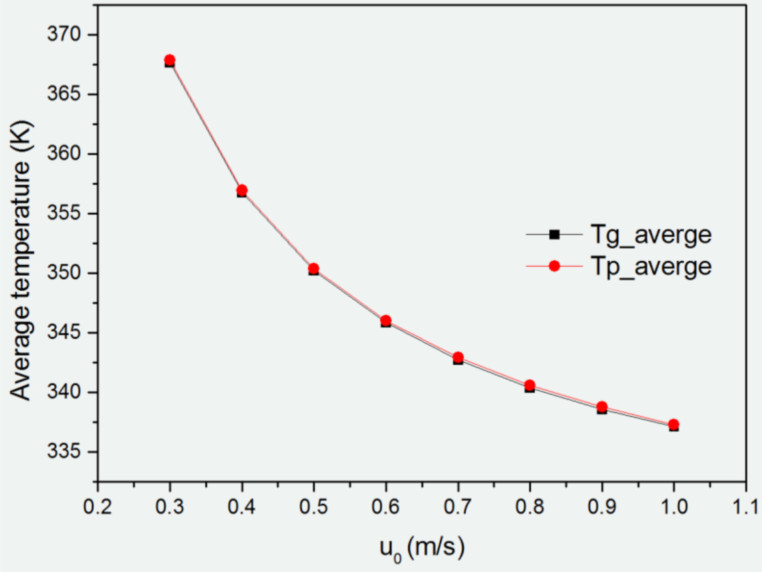
$$\frac{\partial}{\partial t}\varepsilon\rho_g\mathbf{u} + \nabla\cdot\varepsilon\rho_g\mathbf{uu} = -\varepsilon\nabla p - \nabla\cdot\varepsilon\boldsymbol{\tau}_g - S_p + \varepsilon\rho_g\mathbf{g}$$

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

Simulations with mono-dispersed particles



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

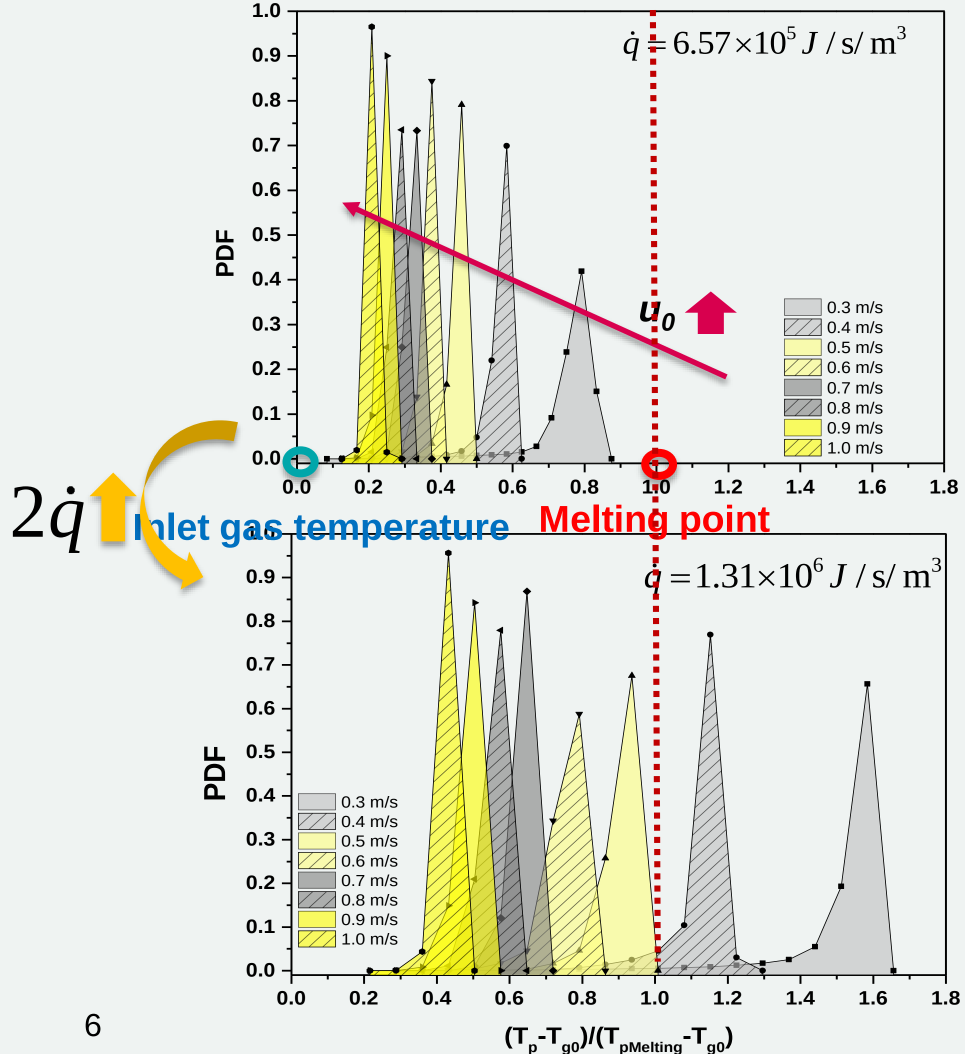


Simulations with mono-dispersed particles
Particle temperature distribution

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

- Definition:

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



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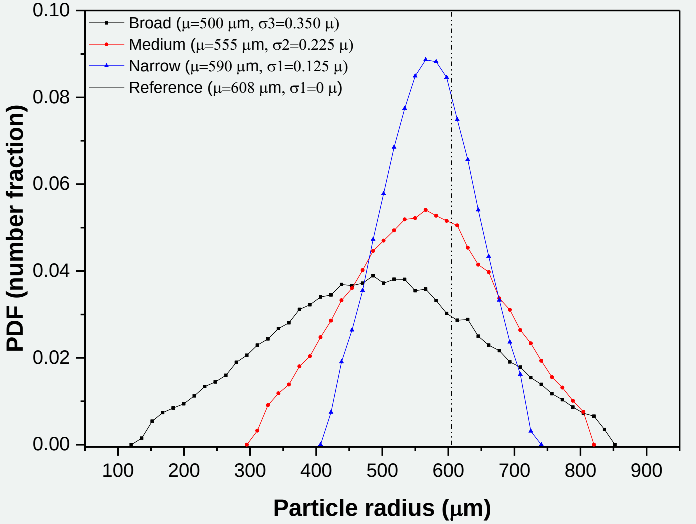
Simulations with poly-dispersed particles



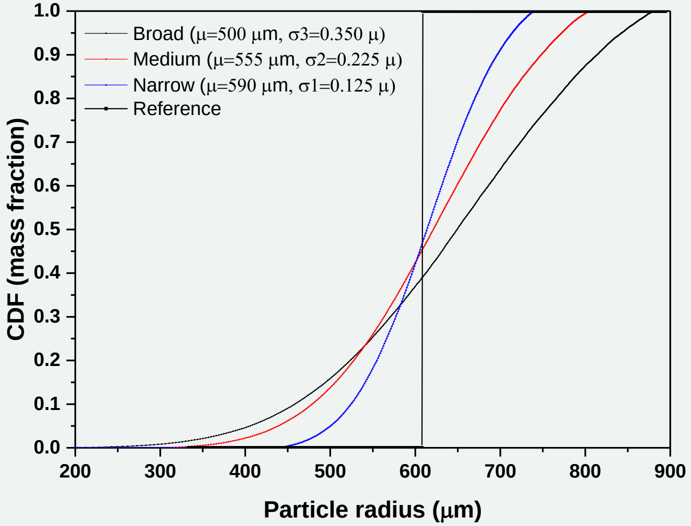
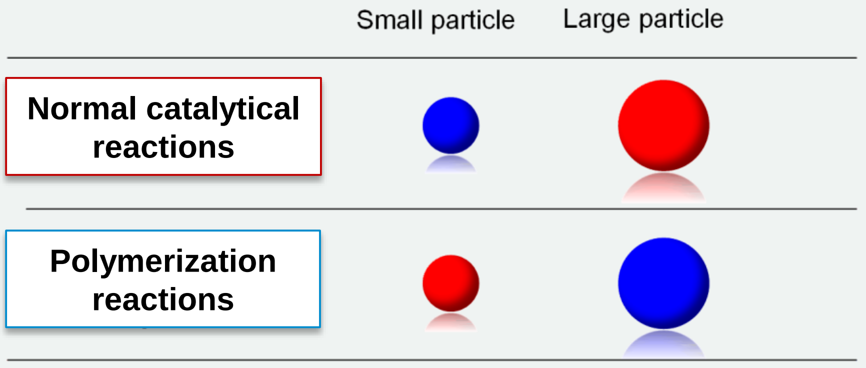


Table. Particle properties

	Mean radius (μm)	Standard deviation (μm)	Sauter mean radius (μm)	Mass of the bed (g)	Particle number
Reference	608	0	608	35.6	56,601
σ1 (narrow)	590	75	608	35.6	59,908
σ2 (medium)	555	125	608	35.6	66,807
σ3 (broad)	500	175	608	35.6	80,000



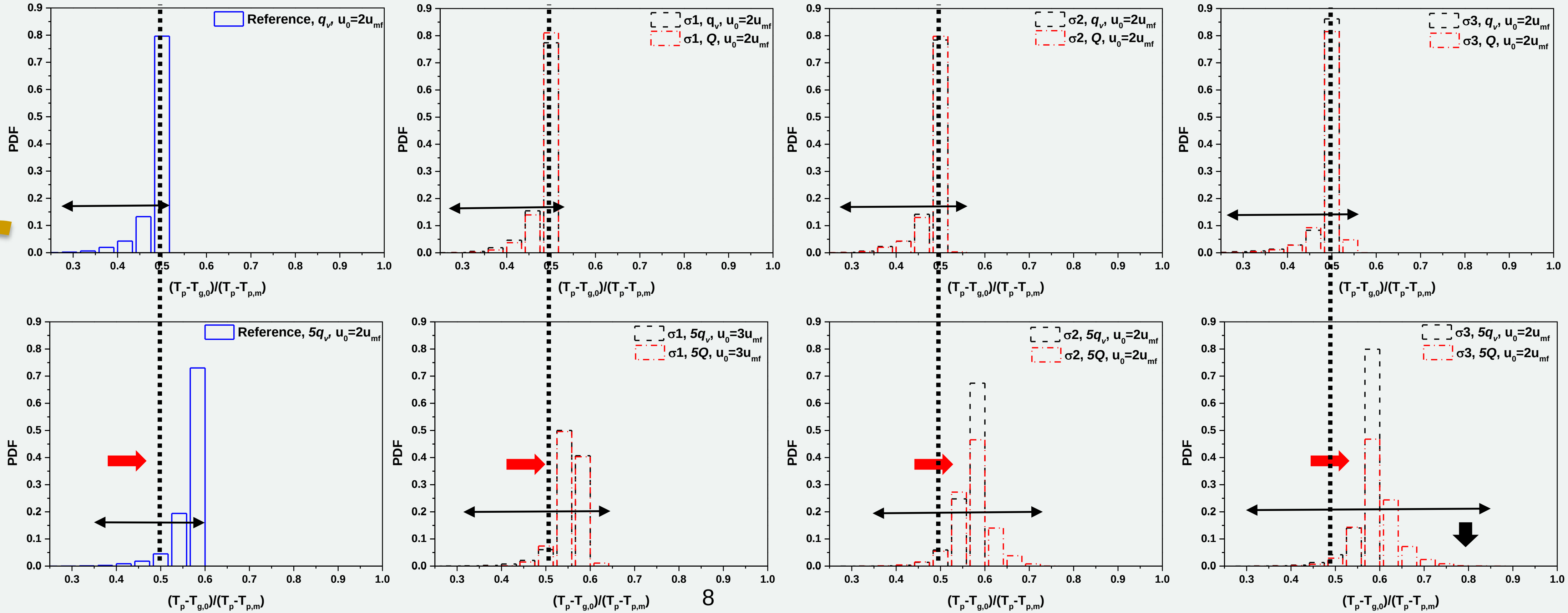
Simulations with poly-dispersed particles
- Particle temperature PDF

mono | narrow | medium | broad

Small heat production

5

Large heat production

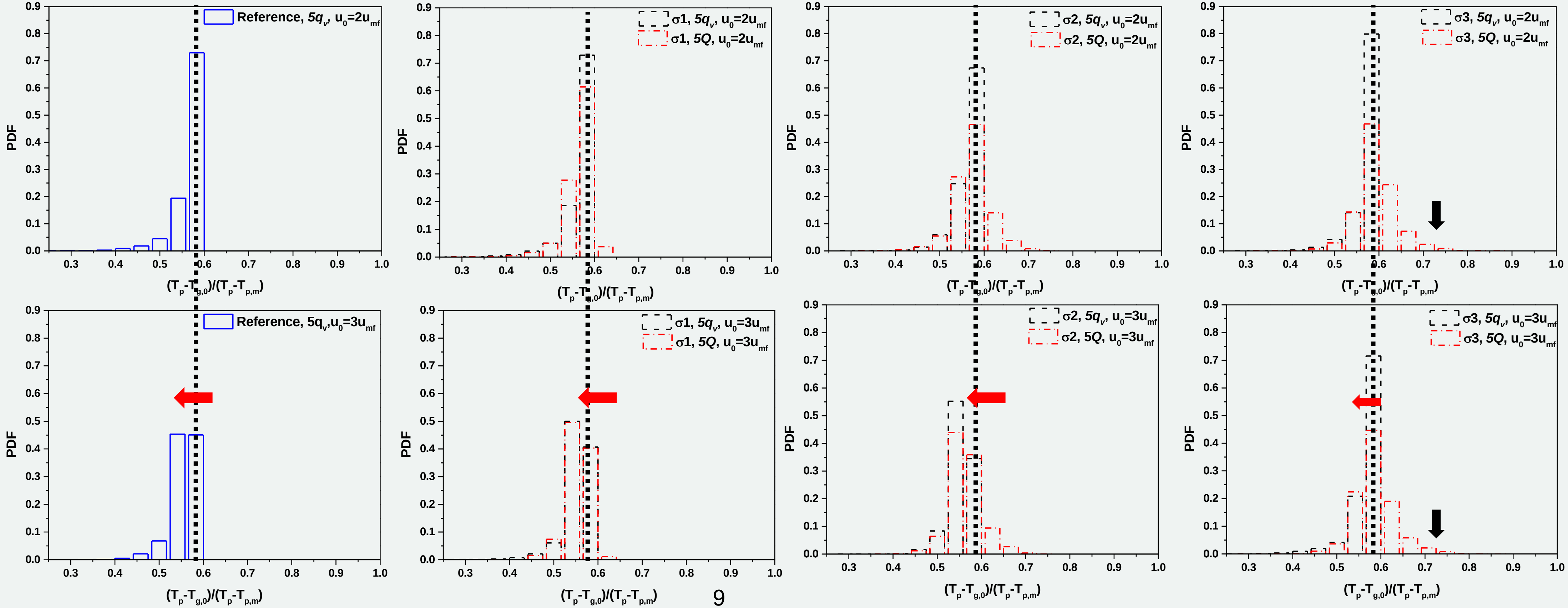


Simulations with poly-dispersed particles
- Particle temperature PDF

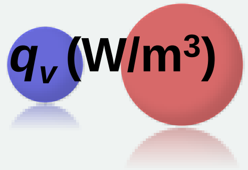
mono | narrow | medium | broad

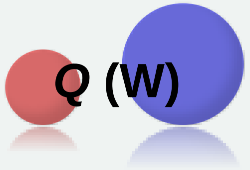
$u_0=2u_{mf}$

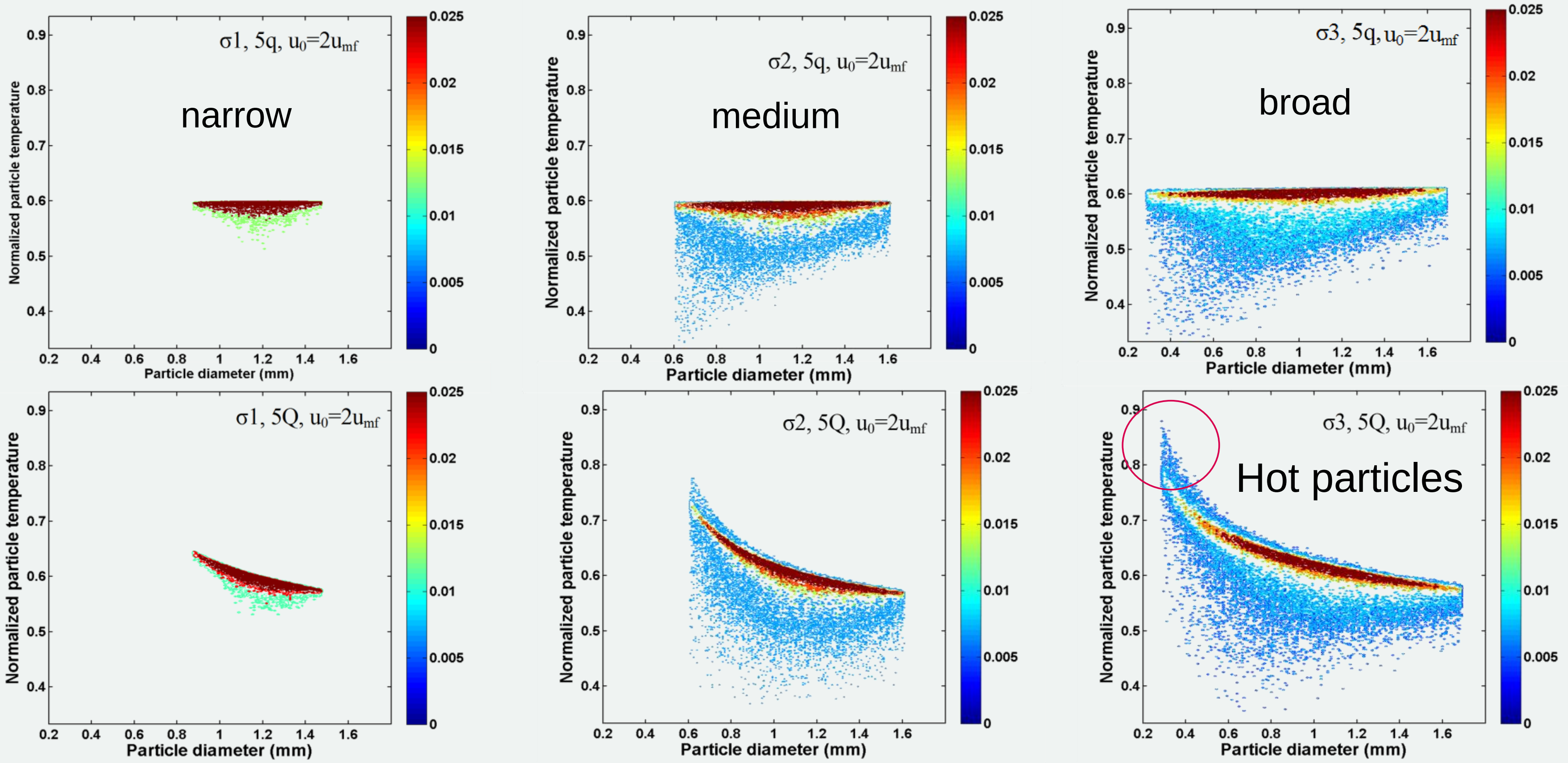
$u_0=3u_{mf}$



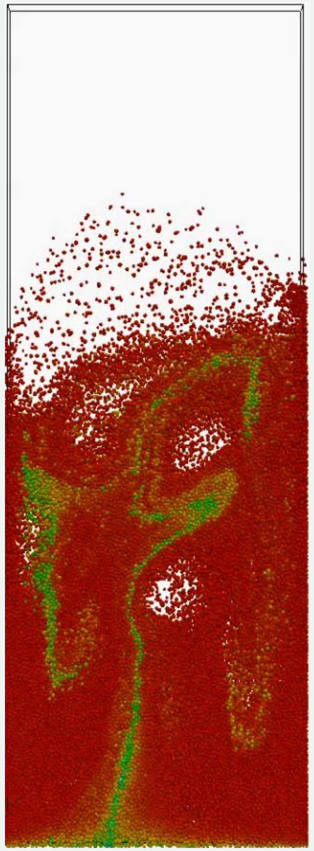
Simulations with poly-dispersed particles
- Temperature contour

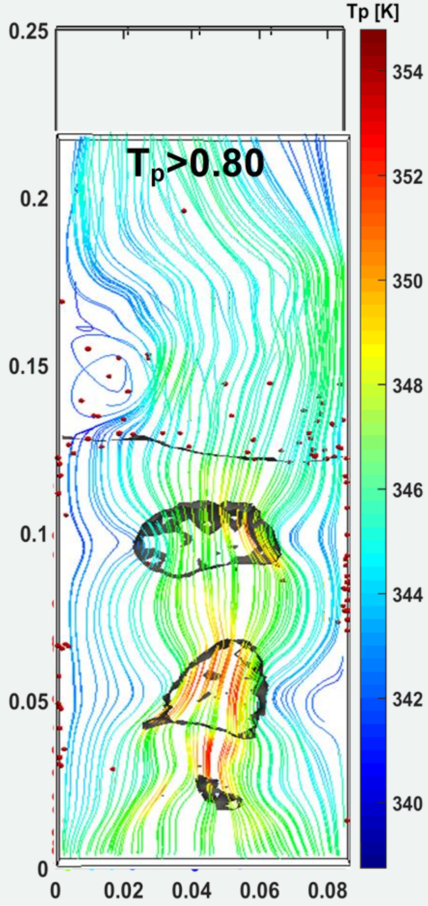


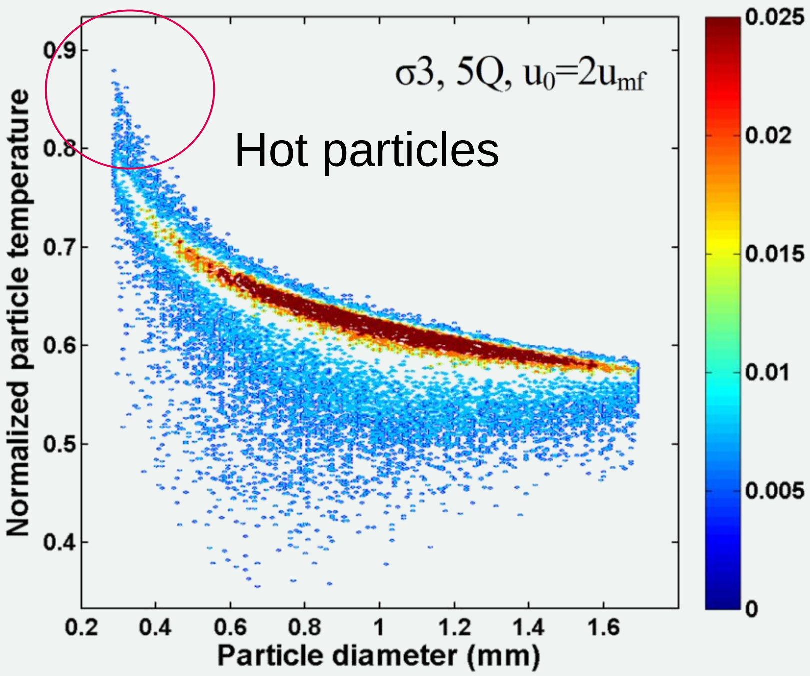




Mechanism of hot spots formation







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

This research is part of research programs of Dutch Polymer Institute (DPI) as project #751.

Thanks for your attention!