



The eighth international conference on
Clean Coal Technologies


Cagliari, Italy
8–12 May 2017



Istituto di Ricerche
sulla Combustione



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DEM simulations of coal particles in entrained-flow slagging gasifiers: particle-particle interaction at different burning levels

Giovanni Tretola, *Francesco Saverio Marra*,
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Entrained-flow gasifiers of new generation are characterized by operating conditions so as to favor ash migration/deposition onto the reactor walls, whence the slag flows.

Historical overview of numerical particle deposition models

Particle viscosity, sticking probability, slagging indices:

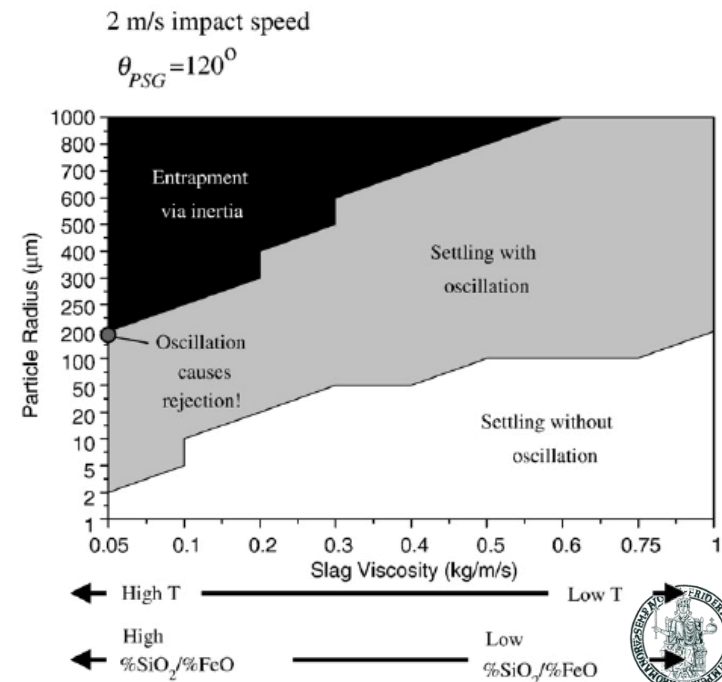
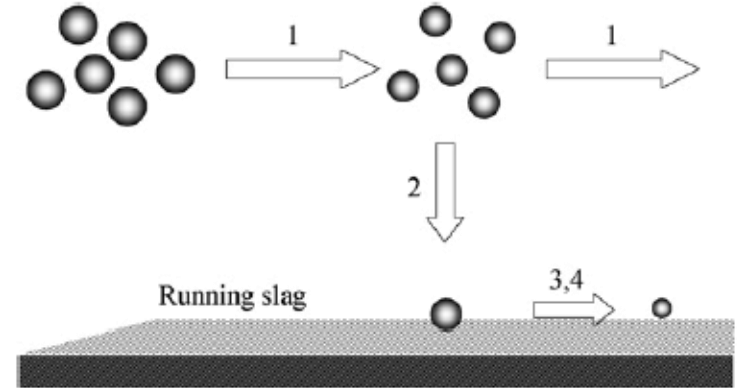
- Baxter and Desollar, Fuel (1993): ADLVIC Sandia National Laboratory model, include a **particle cloud model** with its **interaction with a boundary layer** to estimate deposition rate in function of operative conditions;
- Richards et al. (1993); Lee et al. (1993, 1995); Wang and Harb (1997); Seggiani, Fuel (1998); Tominaga et al. (2000); Barroso et al., Fuel Proc. Tech. (2007); Degereji et al., Fuel (2012), particulate deposition on the wall occurs if either the ash particle or ash layer on the wall has a viscosity lower than a **critical viscosity**
 - Fan et al., Fuel (2001); Fang et al., Fuel Proc. Tech. (2010), **impaction rate and sticking probability**
- Lee & Lockwood, Prog. En. Comb. Sci. (1999); Costen et al., Proc. Comb. Inst. (2000), impaction rate dependent upon **critical velocity to penetrate the boundary layer**.
 - Benyon (2002), a posteriori model, with inertial impact being the dominant form of deposition mechanism. Adhesion depends upon particle temperature, **angle of impact, presence of a liquid slag layer and particle velocity**
- Pyykonen et al. (2002) inertial impaction and turbulent impaction considered separately, impact rate proportional to **turbulent boundary layer structure parameter τ_w**

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Studies concerning the fate of char/ash particles as they impinge the slag have focused on **single particle impacts**, developing deposition criteria based on a *critical viscosity*.

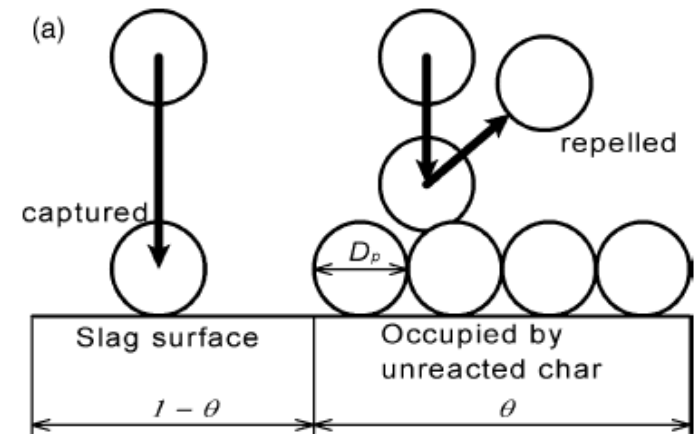
Micro-mechanical inspection of particle-wall interaction

- Wang et al., Comb. Flame 149 (2007); Shen et al., Comb. Flame 166 (2016) take into account burning of suspension and deposited particles
- Shannon et al., Fuel Proc. Tech. 89 (2008) conditions for entrapment or rejection of a particle impacting onto a liquid (slag) surface
- Balakrishnan et al., Energy 81 (2015) bouncing potential



Micro-mechanical inspection of particle-wall interaction

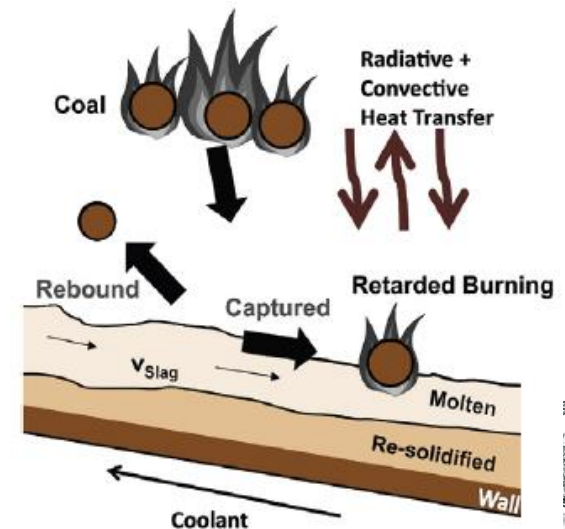
- Shimizu and Tominaga, *Fuel* 85 (2008)
a model of char capture by slag surface that is partially covered by the unreacted char.



- Yong et al. , *Fuel* 92 (2012)
wall particle interaction governed by both sticking and interfacial phenomena.

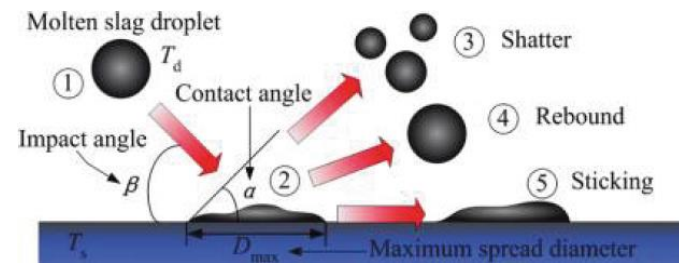
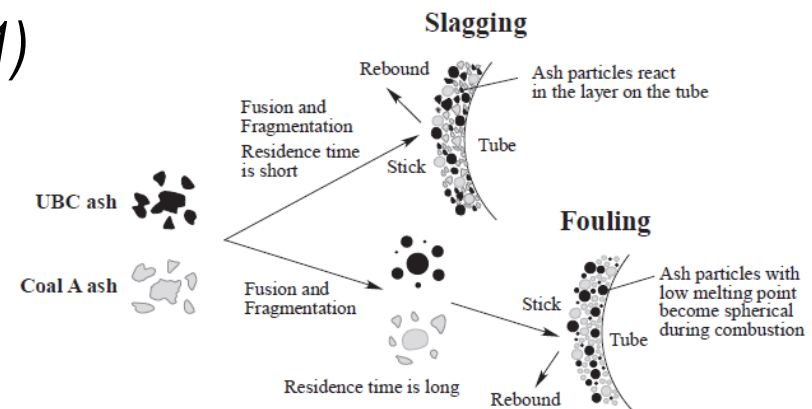
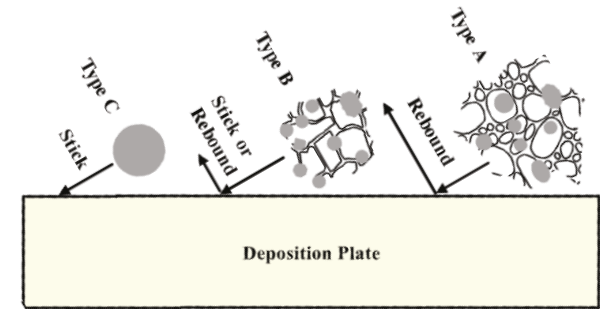
Particle capture criteria.

	Sticky particle		Non-sticky particle	
	$We < We_{cr}$	$We > We_{cr}$	$We < We_{cr}$	$We > We_{cr}$
Sticky wall	Slagging	Slagging	Slagging	Reflect
Non-sticky wall	Fouling	Reflect	Reflect	Reflect



Micro-mechanical inspection of particle-wall interaction

- *Li et al. Energy Fuels 24 (2010)*
different levels of stickiness probability
depending upon conversion rate
- *Akiyama et al. / Fuel Proc. Tech. 92 (2011)*
residence time changes the
deposition mechanism leading
to slagging or fouling
- *Ni et al. Energy Fuels 25 (2011)*
the slag droplet maximum spread diameter,
function of the Reynolds number,
Weber number and contact angle are the
key parameter for the impact process.



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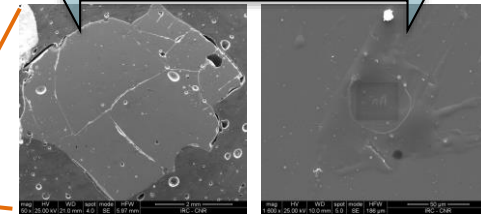
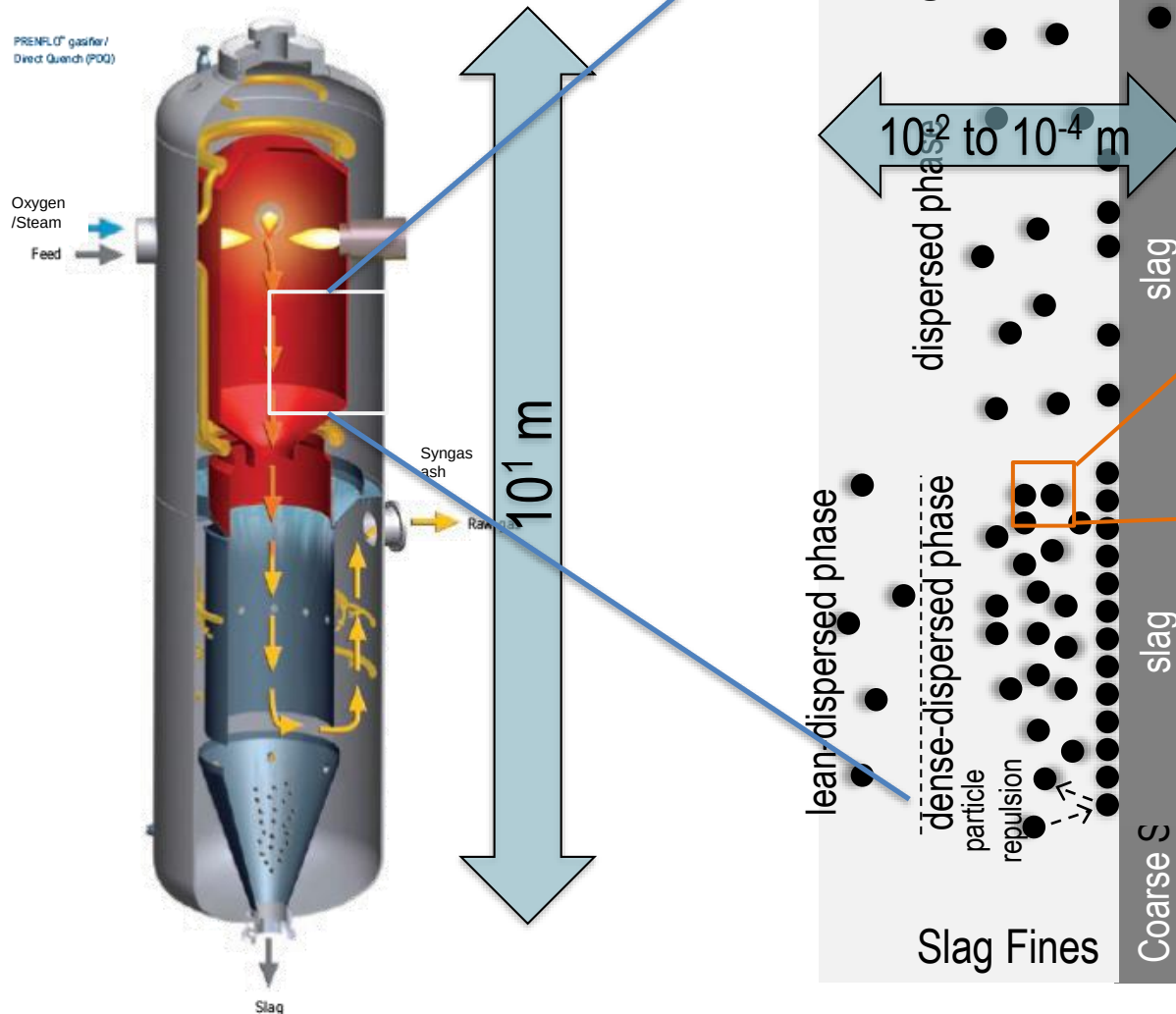
Studies concerning the fate of char/ash particles as they impinge the slag have focused on **single particle impacts**, developing deposition criteria based on a *critical viscosity*.

In previous works from this research group, a different perspective has been adopted to study particle-wall interaction, and several regimes of particle entrapment inside the molten slag or carbon-coverage of the slag layer have been identified.

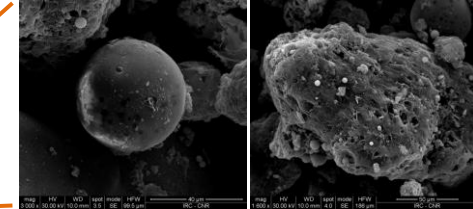
Introduction and Motivations

Montagnaro & al., *En. Fuels* (2011)

Solid wastes supplied by ELCOGAS, from Puertollano (Spain) gasifier.



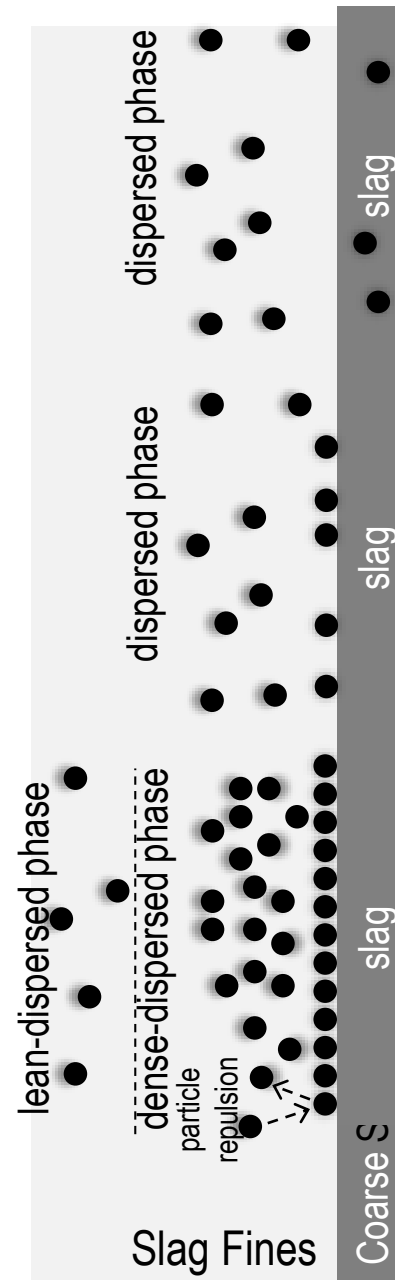
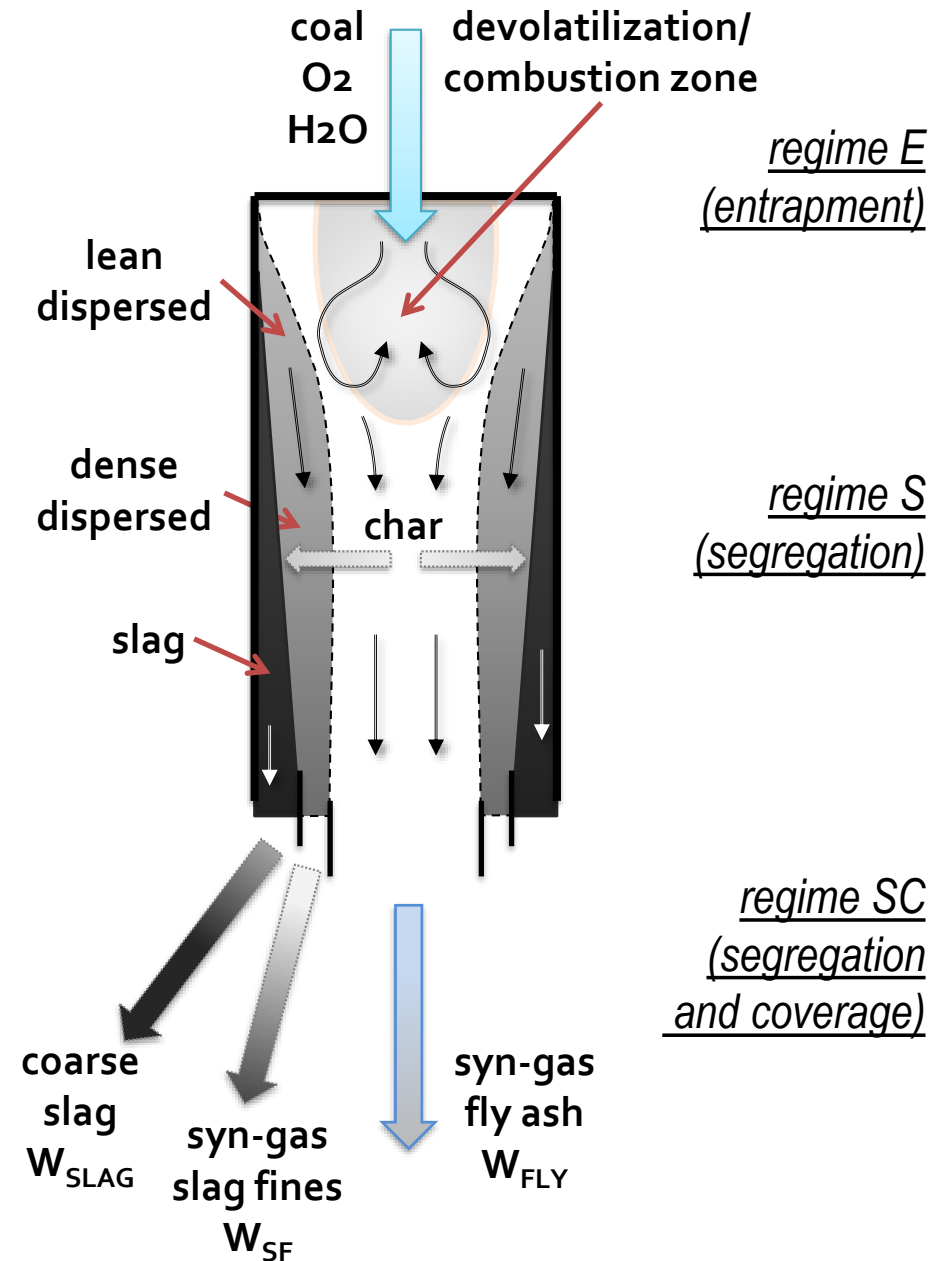
Remarkable carbon content (9.3%) with **patches** having carbon contents **as high as 48.8–54.2%**.



Porous particles, with **carbon content between 82.3 and 86.5%**.

Compact particles with **carbon content between 13.9 and 18.4%**.

Introduction and Motivations



Identification of particle – slag interaction regimes based on particles impacting onto a dense-dispersed phase. **raising the issue of multiple collisions between particles and with the surface.**

Ambrosino et al., Comb. Sci. Tech. (2012);
 Ambrosino et al., Fuel (2013)
 Marra et al., Int. J. Mult. Flow (2017).

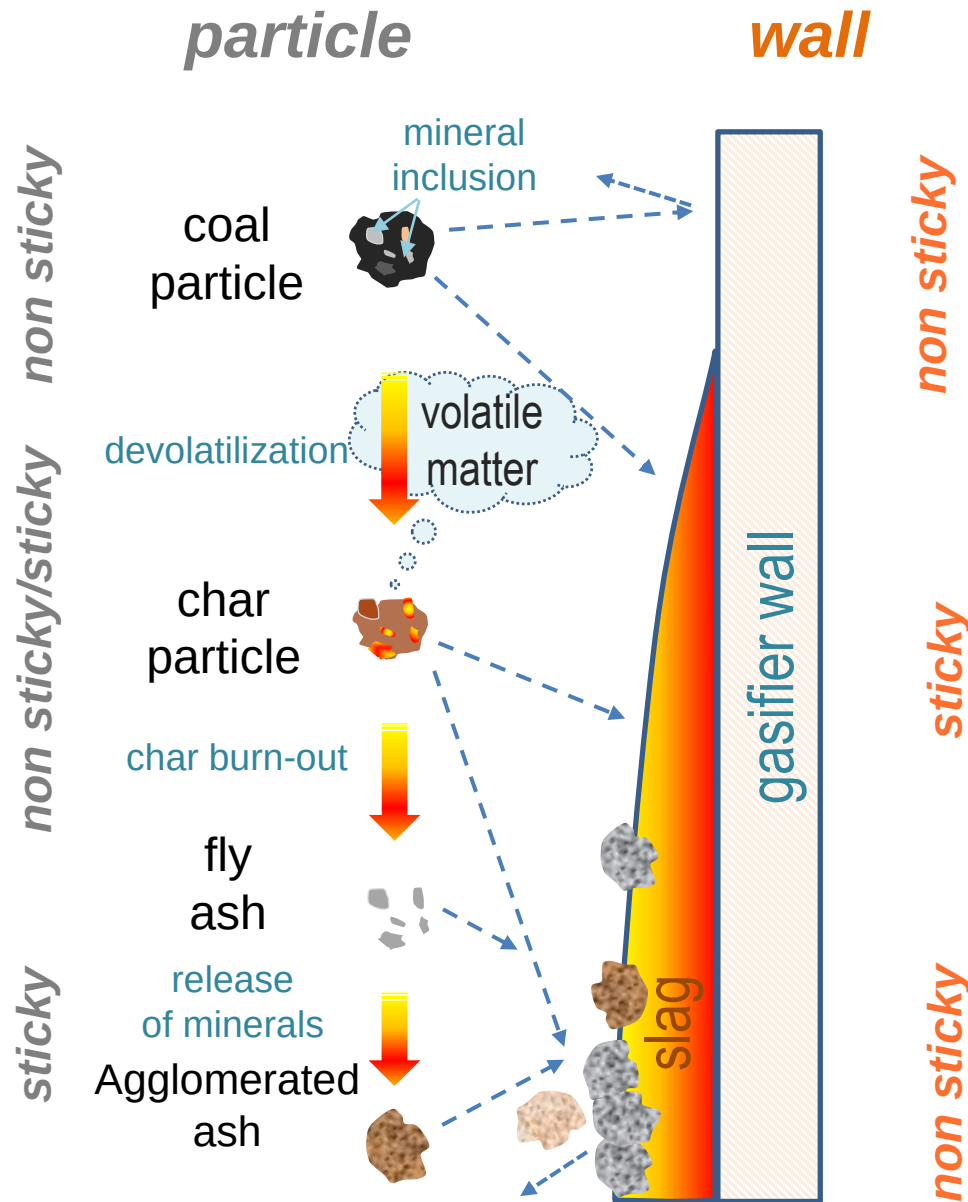
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In this work, the possible role of **particle-particle interaction** close to the wall (and not only there) is investigated by means of numerical simulations.

Limiting particle–wall micromechanical interactions regimes



Different patterns on the basis of the **stickiness degree** of the wall layer and of the impinging char particle.

The material laying on the wall is **sticky** when the wall temperature is so high that the ash is in a molten status (liquid slag layer). In addition, it must not be extensively covered by **non sticky** char particles.

The char particle is **sticky** when its temperature is beyond a critical value and the carbon conversion is beyond a given threshold. If one of these conditions does not apply, the char particle is **non sticky**.

$$m_i \frac{d\mathbf{u}_i}{dt} = \sum_{j=1}^{n_p} (\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij}) + \mathbf{F}_{coh} + \mathbf{F}_V$$

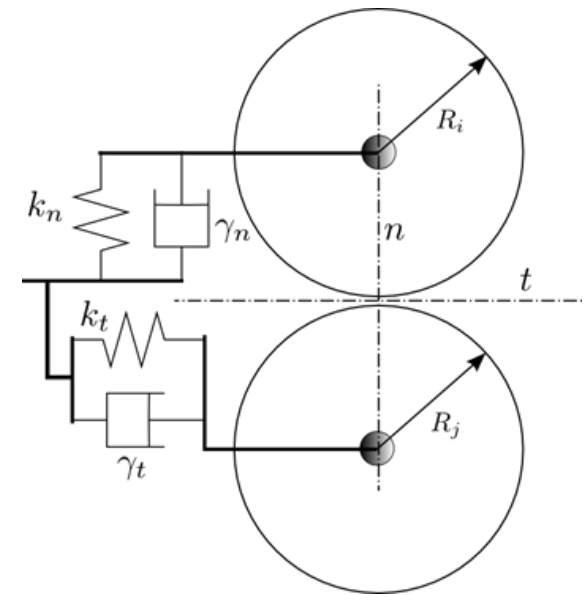
$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{n_p} (\mathbf{T}_{t,ij} + \mathbf{T}_{r,ij})$$

$$\mathbf{F}_{n,ij} = -k_{n,ij} \mathbf{d}_{n,ij} - \gamma_{n,ij} \mathbf{v}_{n,ij} \quad |\mathbf{F}_{t,ij}| < \mu_s |\mathbf{F}_{n,ij}|$$

$$\mathbf{F}_{t,ij} = -k_{t,ij} \mathbf{d}_{t,ij} - \gamma_{t,ij} \mathbf{v}_{t,ij}$$

$$\mathbf{F}_{coh} = c A \mathbf{n}_u \quad c = 10^5 \text{ N m}^{-2}$$

$$\mathbf{T}_{r,ij} = \mu_r |\mathbf{F}_n| \frac{\boldsymbol{\omega}_{rel,ij}}{|\boldsymbol{\omega}_{rel,ij}|} R_i$$



Soft sphere spring-dashpot
Hertzian contact model.

Discrete Element Method

$$k_{n,ij} = \frac{4}{3} Y^* \sqrt{R^* \delta_{n,ij}}$$

$$k_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}}$$

$$\gamma_{n,ij} = -2 \sqrt{\frac{5}{6}} \beta \sqrt{m^* S_n}$$

$$\gamma_{t,ij} = -2 \sqrt{\frac{5}{6}} \beta \sqrt{m^* S_t}$$

$$\frac{1}{Y^*} = \frac{1 - \nu_i^2}{Y_i} + \frac{1 - \nu_j^2}{Y_j}$$

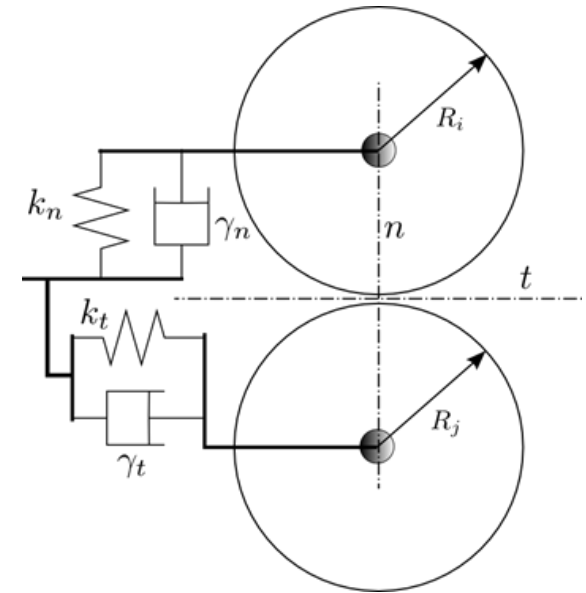
$$\frac{1}{G^*} = \frac{2(2 + \nu_i)(1 - \nu_i)}{Y_i} + \frac{2(2 + \nu_j)(1 - \nu_j)}{Y_j}$$

$$\frac{1}{R^*} = \frac{1}{R_i} + \frac{1}{R_j} \quad \frac{1}{m^*} = \frac{1}{m_i} + \frac{1}{m_j}$$

$$\beta = \frac{\ln(\varepsilon)}{\sqrt{\ln^2(\varepsilon) + \pi^2}}$$

$$S_n = 2Y^* \sqrt{R^* \delta_{n,ij}}$$

$$S_t = 8G^* \sqrt{R^* \delta_{n,ij}}$$



Soft sphere spring-dashpot
Hertzian contact model.

Regime “i-j”	$\varepsilon_{i,j}$ [-]	$\mu_{s,ij}$ and $\mu_{r,ij}$ [-]	ρ [kg m ⁻³], Y [GPa], ν [-]
NSP-NSW	0.9 (any interaction)	0.3 (any interaction)	1100, 3, 0.37 (any regime)
NSP-SW	0.9, 0.1, 0.1, 0.1	0.3, 5×10^{-3} , 5×10^{-3} , 5×10^{-3}	
SP-NSW	0.1, 0.9, 0.9, 0.9	5×10^{-3} , 0.3, 0.3, 0.3	
SP-SW	0.1 (any interaction)	5×10^{-3} (any interaction)	

Coefficient of restitution ε
considered as the main
parameter:

non sticky $\rightarrow \varepsilon = 0.9$

sticky $\rightarrow \varepsilon = 0.1$

Numerical configuration

LIGGGHTS DEM solver

(open source, CFDEMresearch GmbH, Austria)

$$R_{cyl} = 0.02 \text{ m}$$

$$H = 0.3 \text{ m}$$

(the geometry mimic the experimental cold flow reactor laboratory apparatus adopting solid or molten wax, Troiano et al., Fuel (2014))

$$\text{Time step} = 10^{-8} \text{ s} \quad (10^{-8} \text{ s for SW-SP})$$

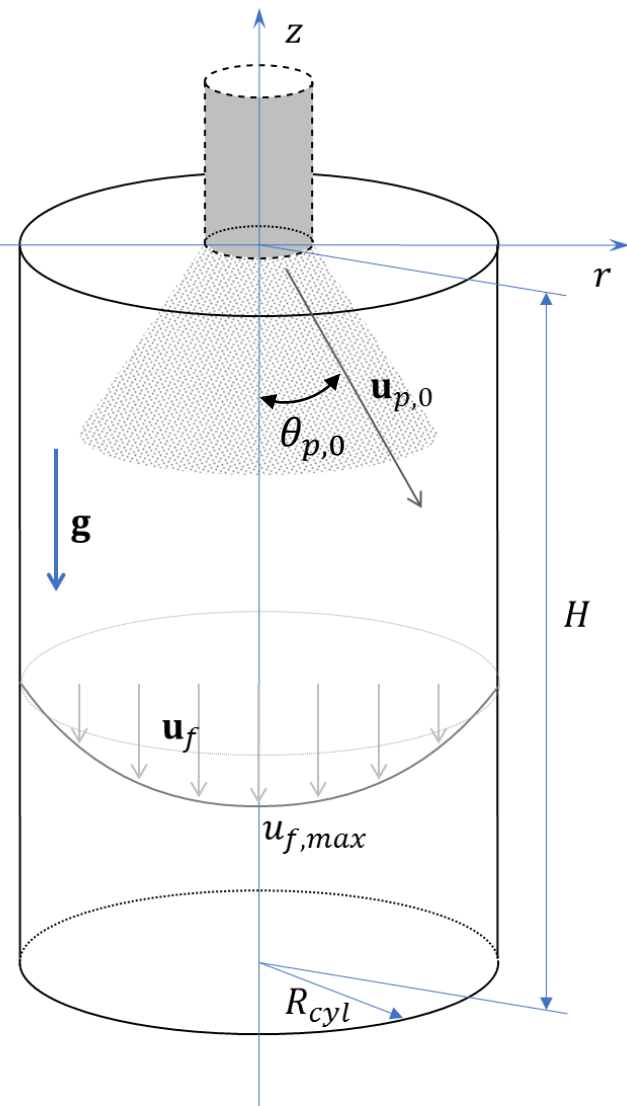
N_p contemporary in the domain at steady state:
from 1.8×10^5 to 2.6×10^5

Volume fraction at insertion = 0.04

$$u_{p,0} = 2.5 \text{ m s}^{-1} \quad \theta_{p,0} = 28^\circ$$

$$u_{f,max} = 0.04 \text{ m s}^{-1}.$$

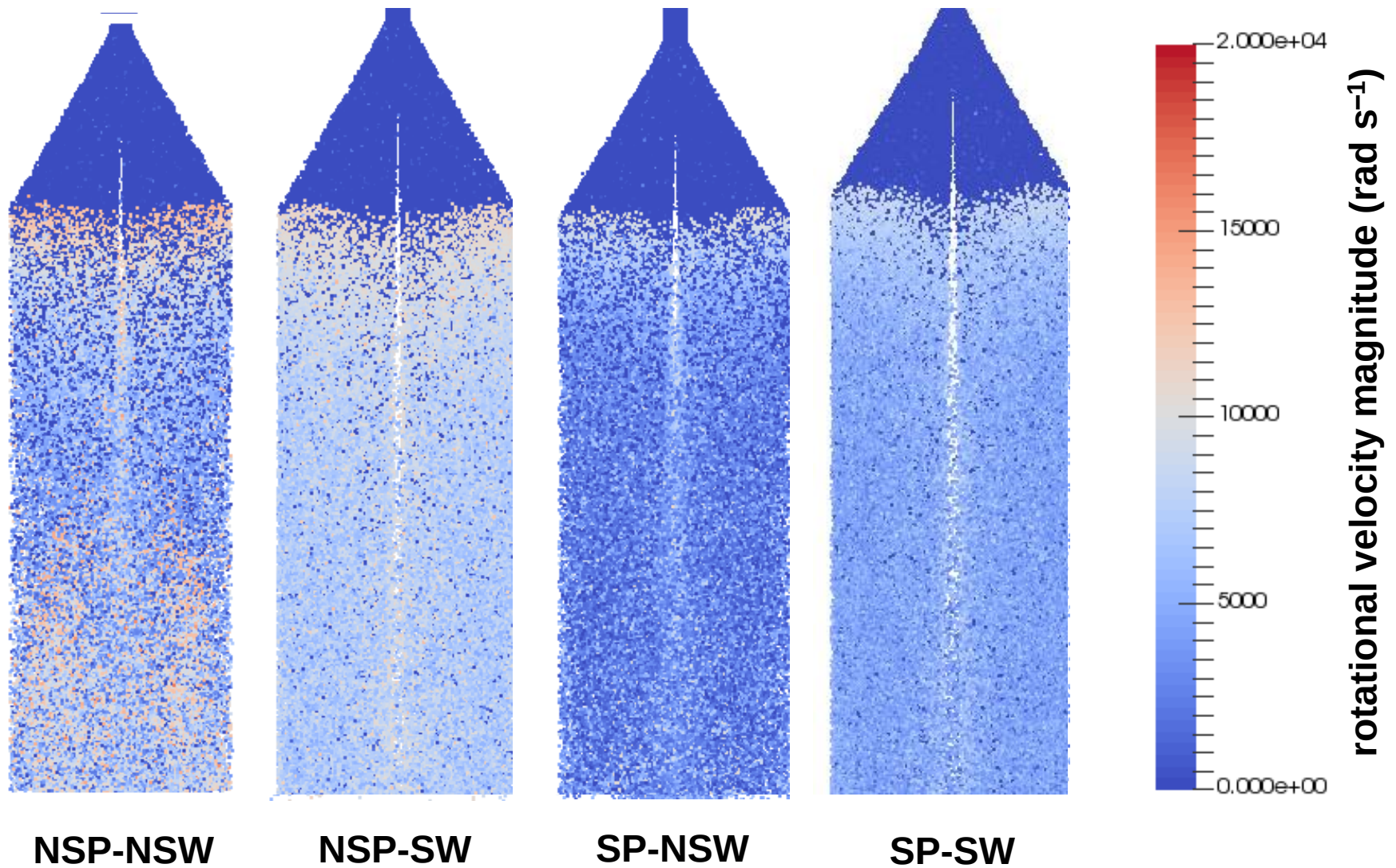
Particle flux in the area of first impact of about
 $30 \times 10^6 n_p \text{ m}^{-2} \text{ s}^{-1}$



$$\mathbf{F}_V = m_p \mathbf{g} + \mathbf{F}_{drag}$$

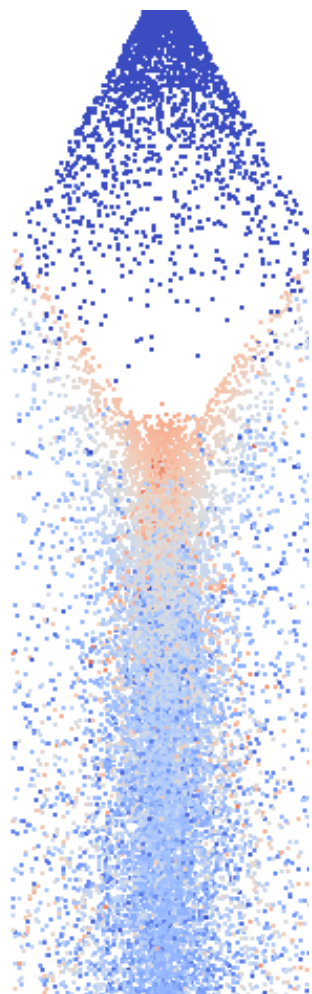
$$\mathbf{F}_{drag} = \frac{3}{4} \frac{\rho_f}{\rho_p} \frac{m_p}{D_p} C_D (\mathbf{u}_f - \mathbf{u}_p) |\mathbf{u}_f - \mathbf{u}_p| \quad C_D = \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) \quad Re_p = \frac{\rho_f |\mathbf{u}_f - \mathbf{u}_p| D_p}{\mu}$$

Computed particles distribution patterns



Surface distribution

Computed particles distribution patterns



NSP-NSW



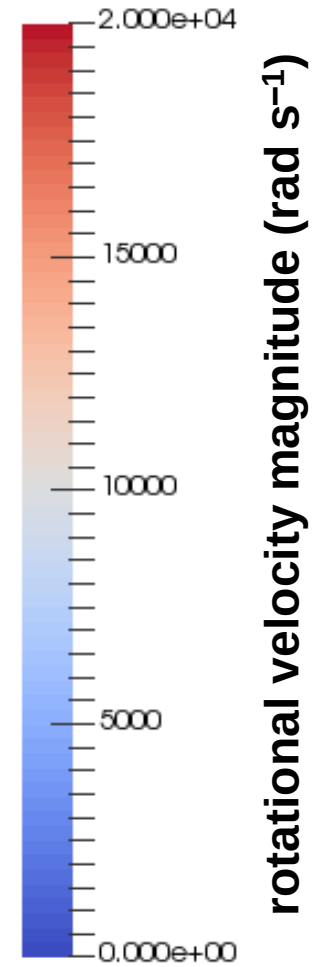
NSP-SW



SP-NSW

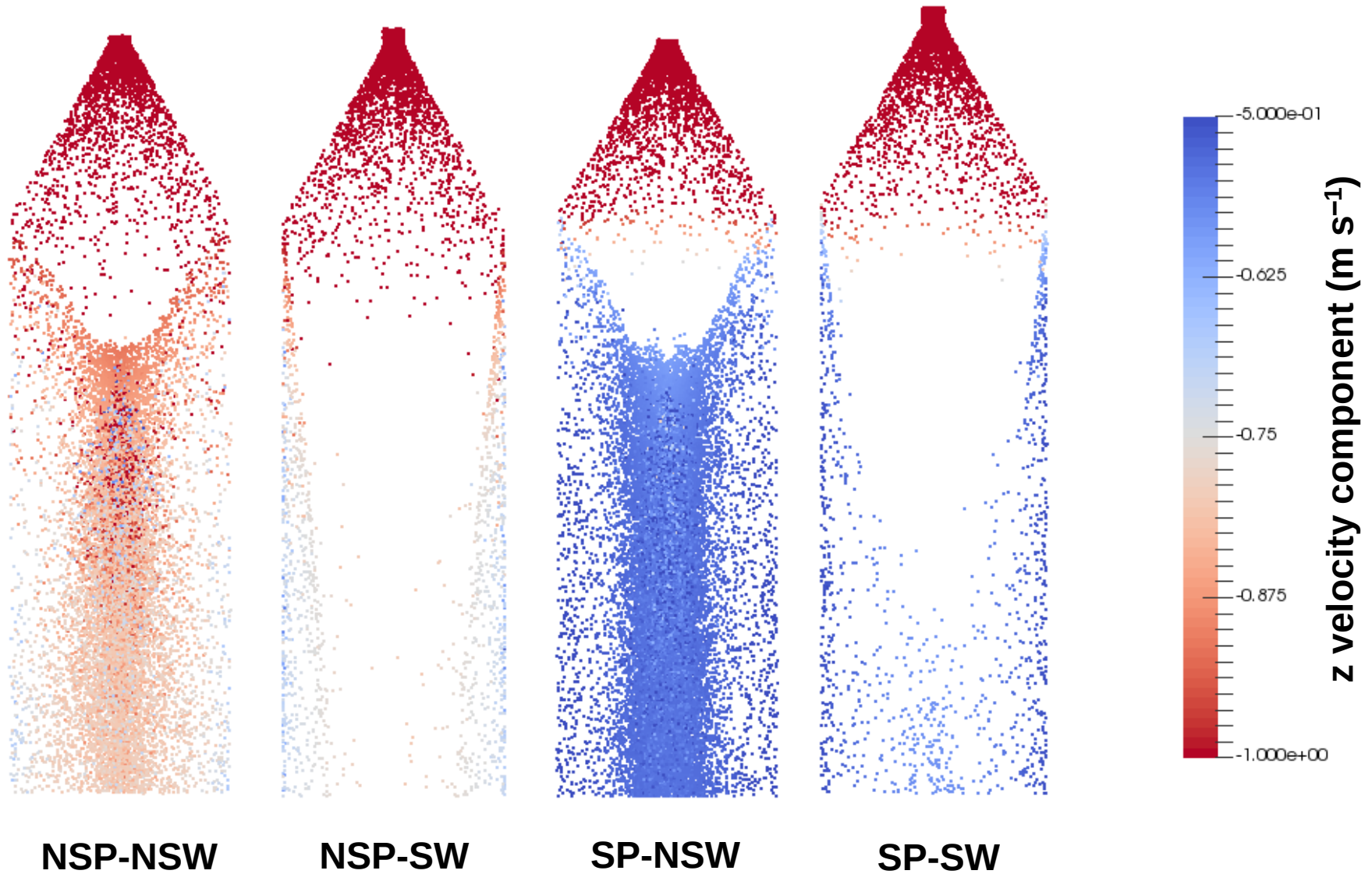


SP-SW



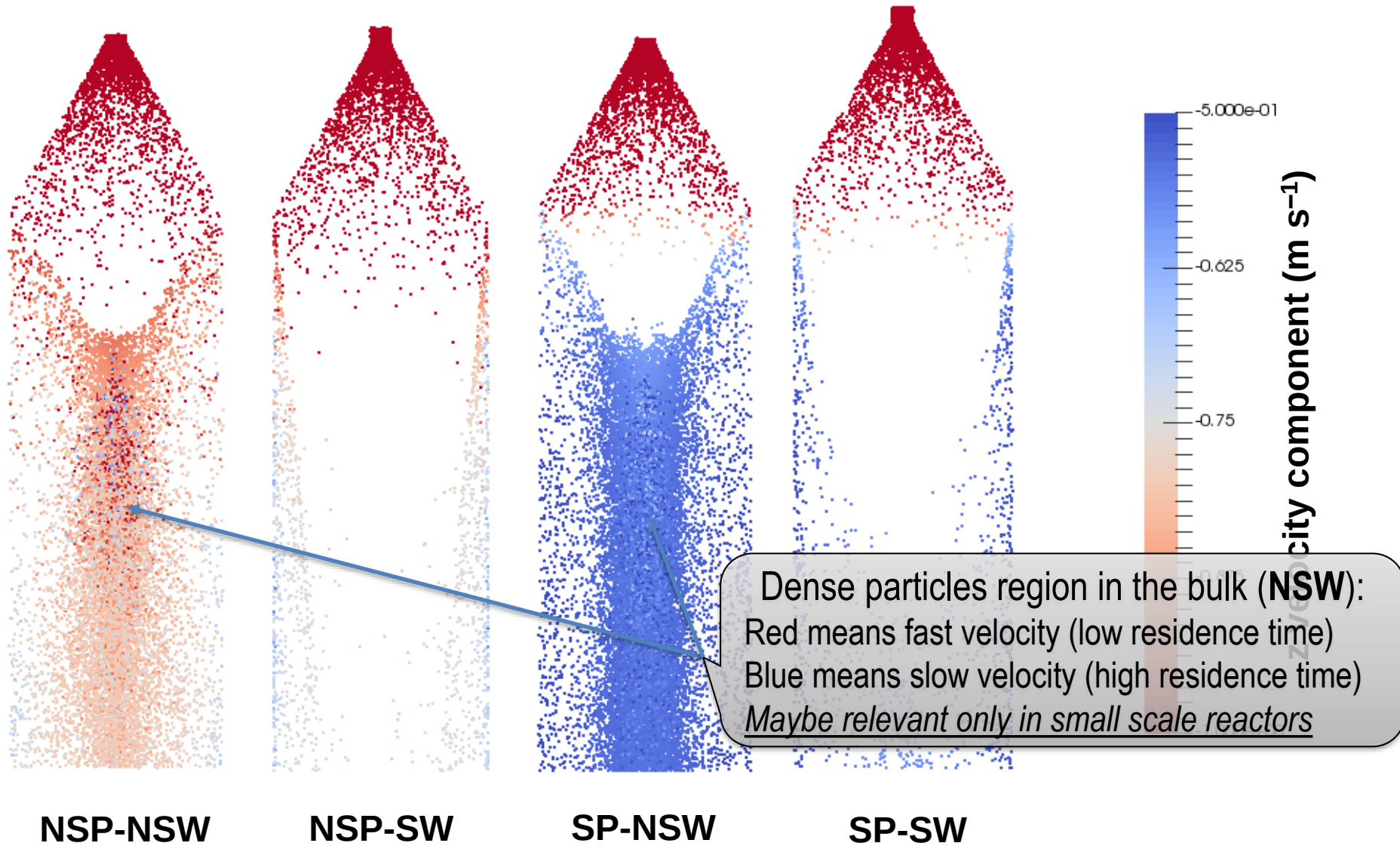
Inside distribution

Computed particles distribution patterns



Inside distribution

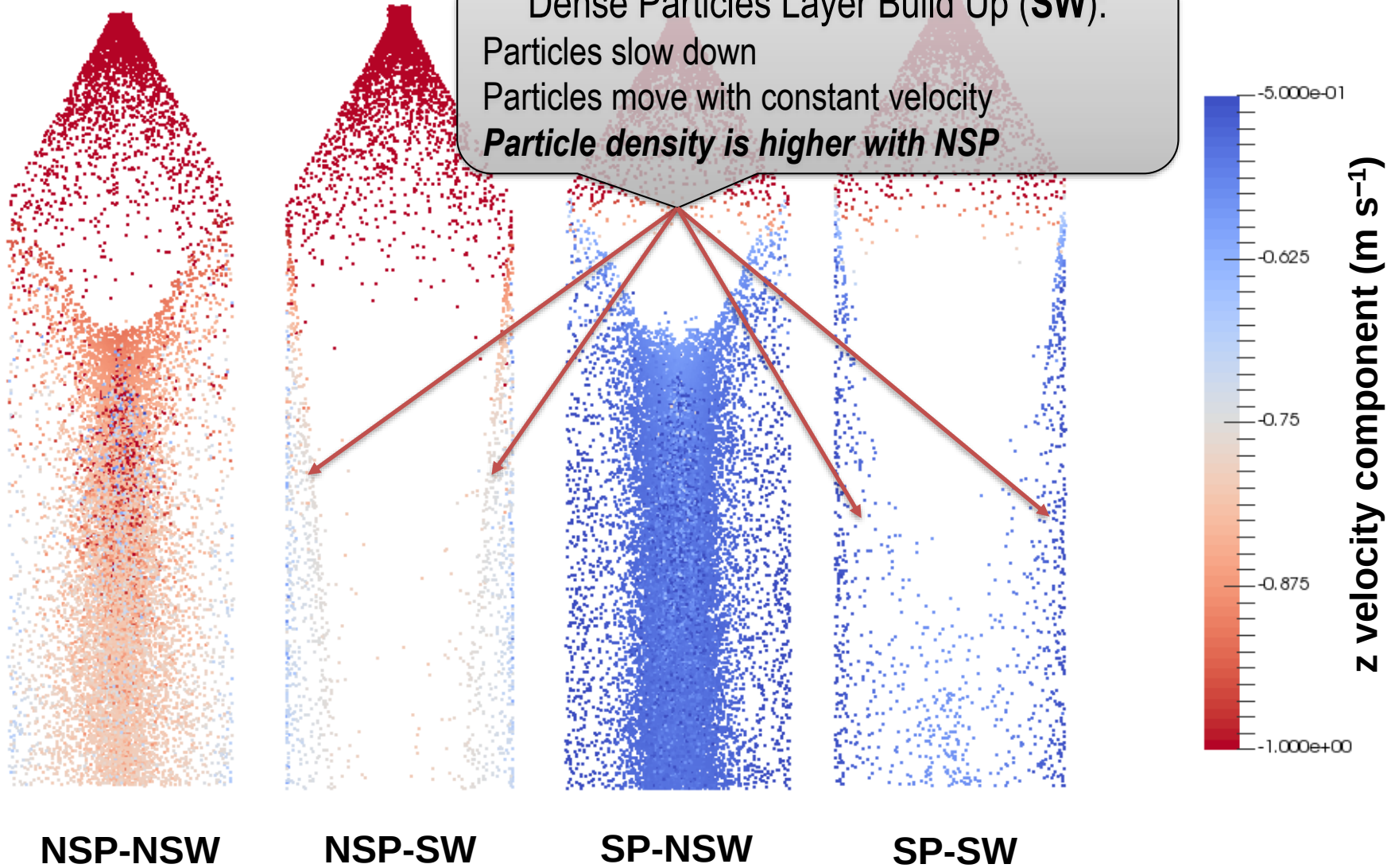
Computed particles distribution patterns



Inside distribution

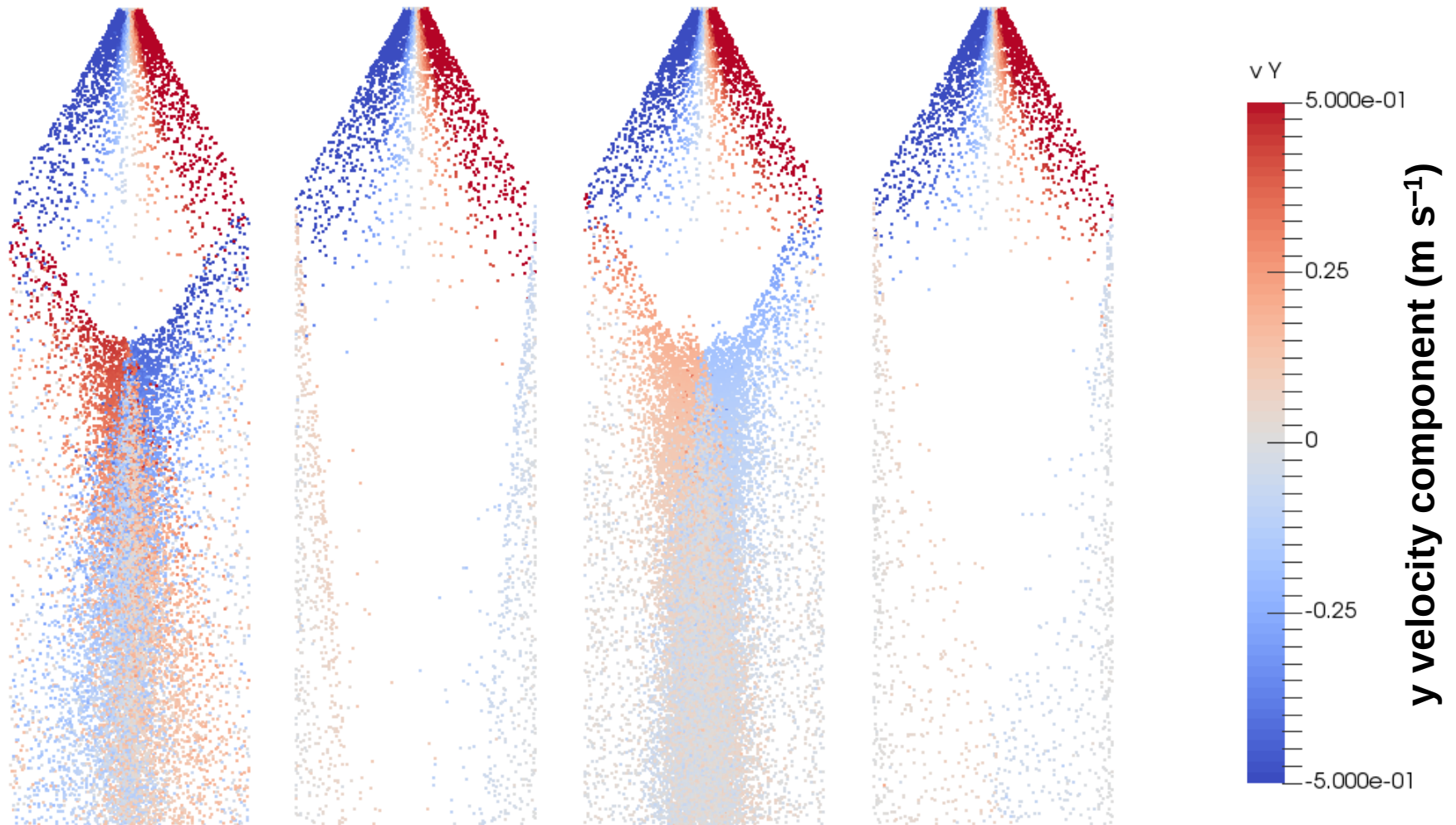
Computed particles distribution patterns

Dense Particles Layer Build Up (SW):
Particles slow down
Particles move with constant velocity
Particle density is higher with NSP



Inside distribution

Computed particles distribution patterns



NSP-NSW

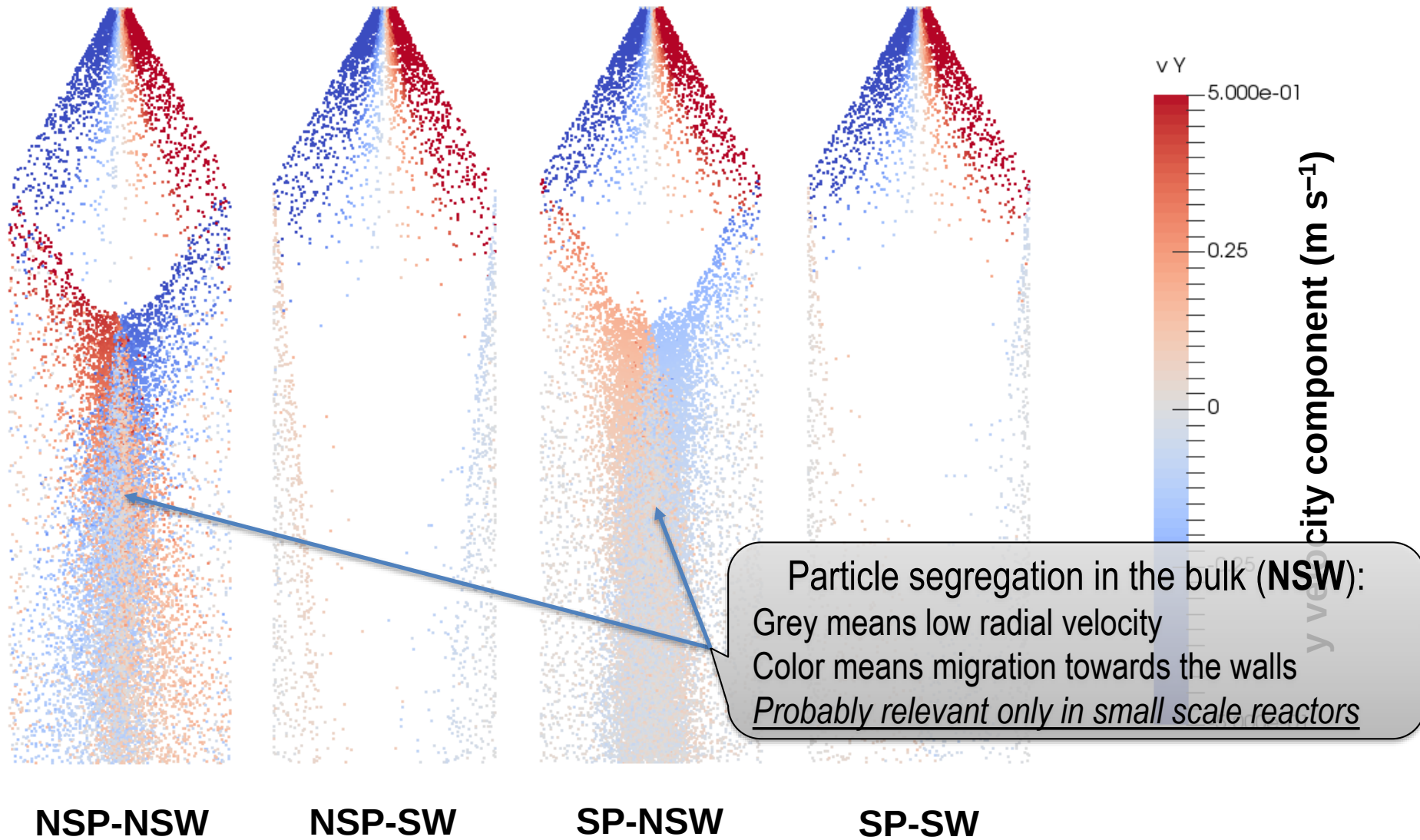
NSP-SW

SP-NSW

SP-SW

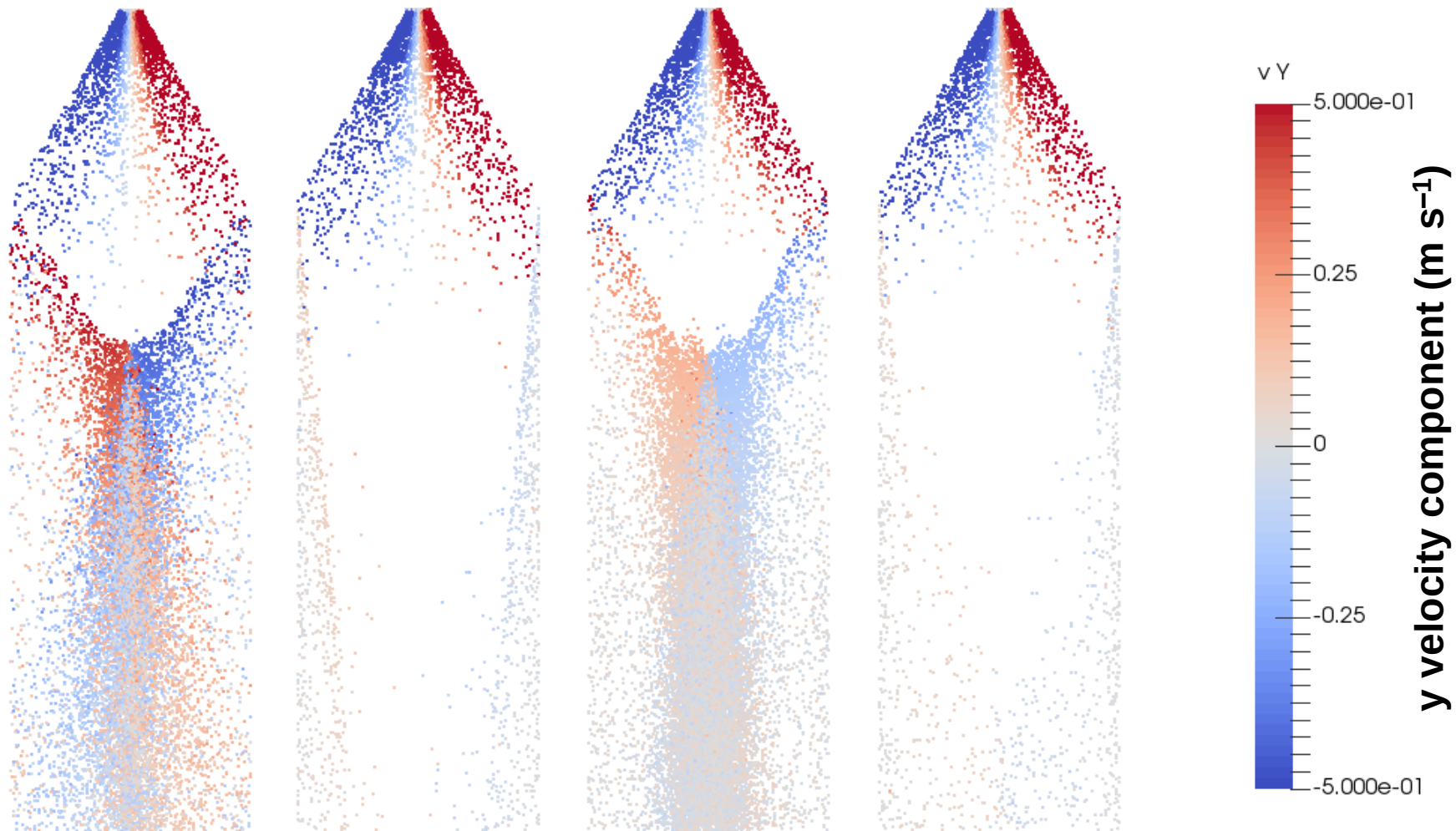
Inside distribution

Computed particles distribution patterns



Inside distribution

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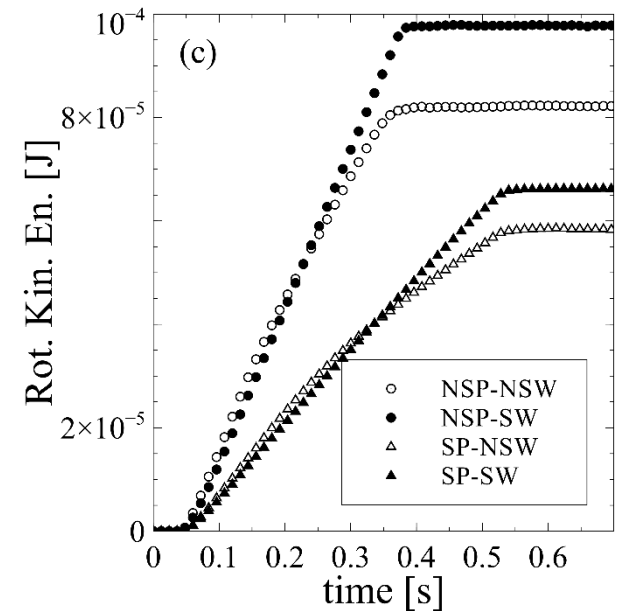
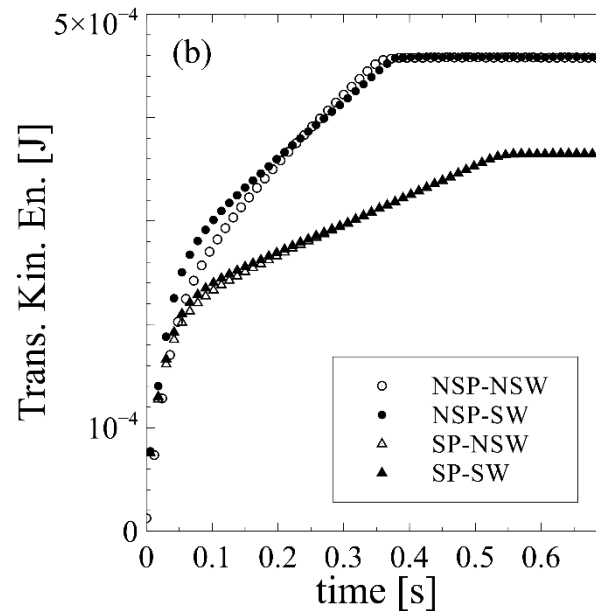
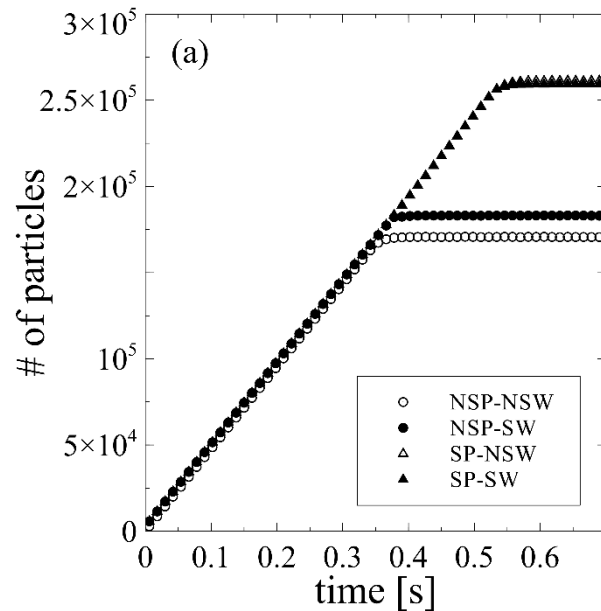
NSP-NSW

NSP-SW

SP-NSW

SP-SW

Inside distribution

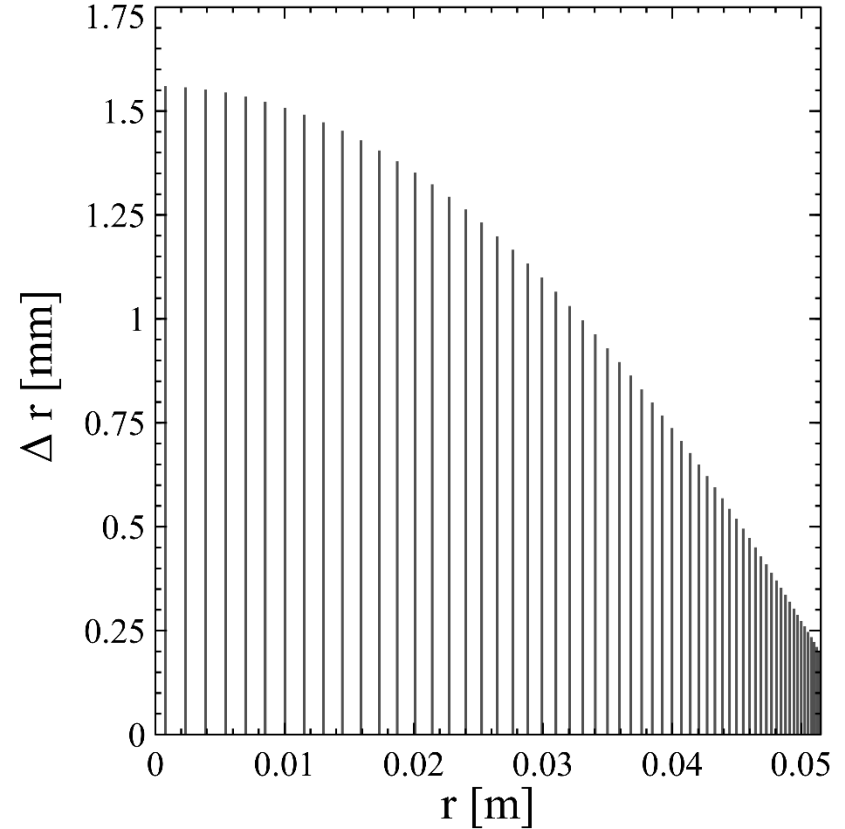


Total number of particles increases with increasing overall stickiness, especially that of walls

Kinetic energies equilibrate at different intensities and within different times:

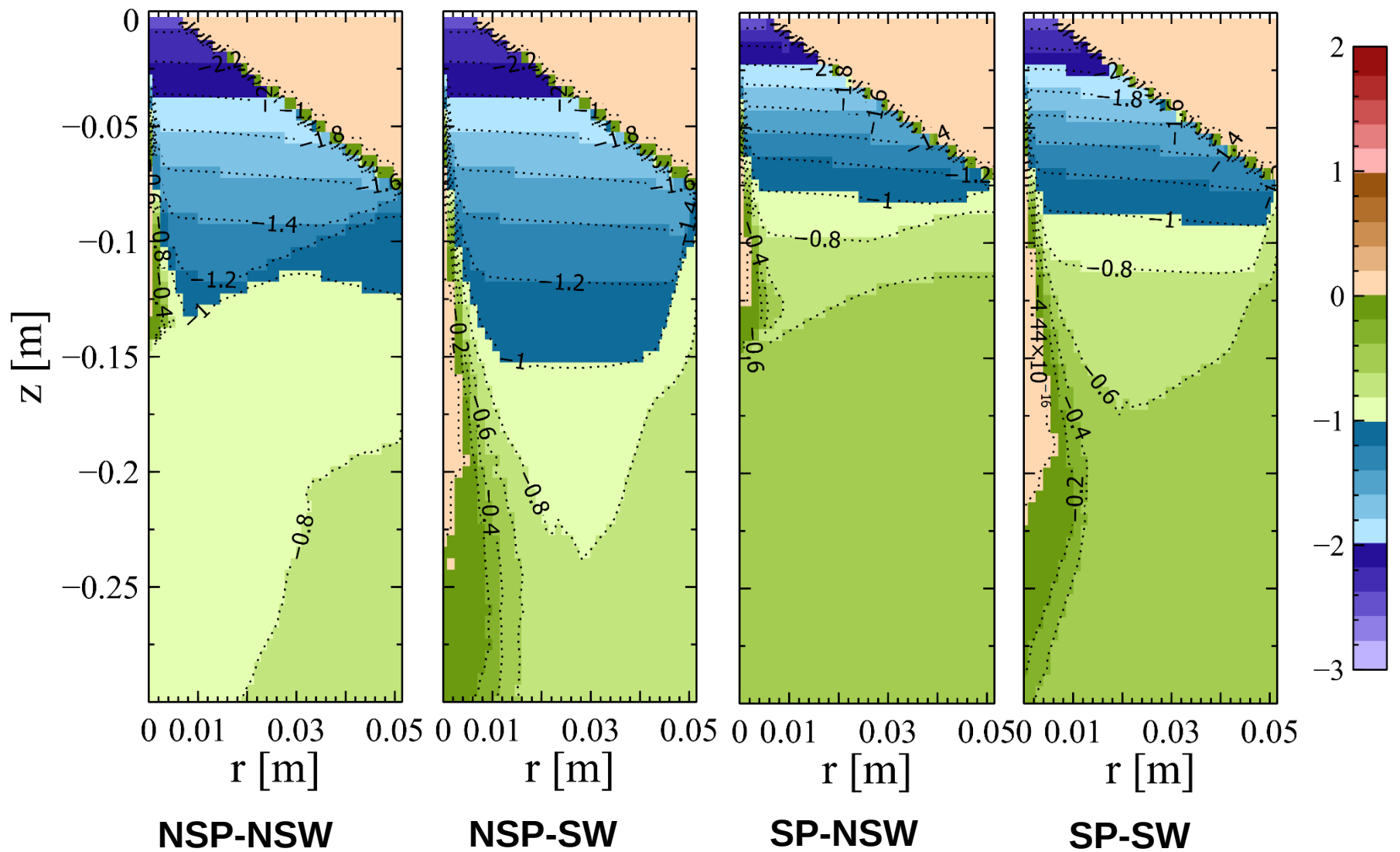
- Translational: **NSP high; SP low**
- Rotational: different levels for all interactions

- 1000 snapshots during 1 sec of collection in fully developed conditions
- 60x60 annular volumes $V_{i,j}$
- Non uniform along radius (see figure)
- Uniform along the axis



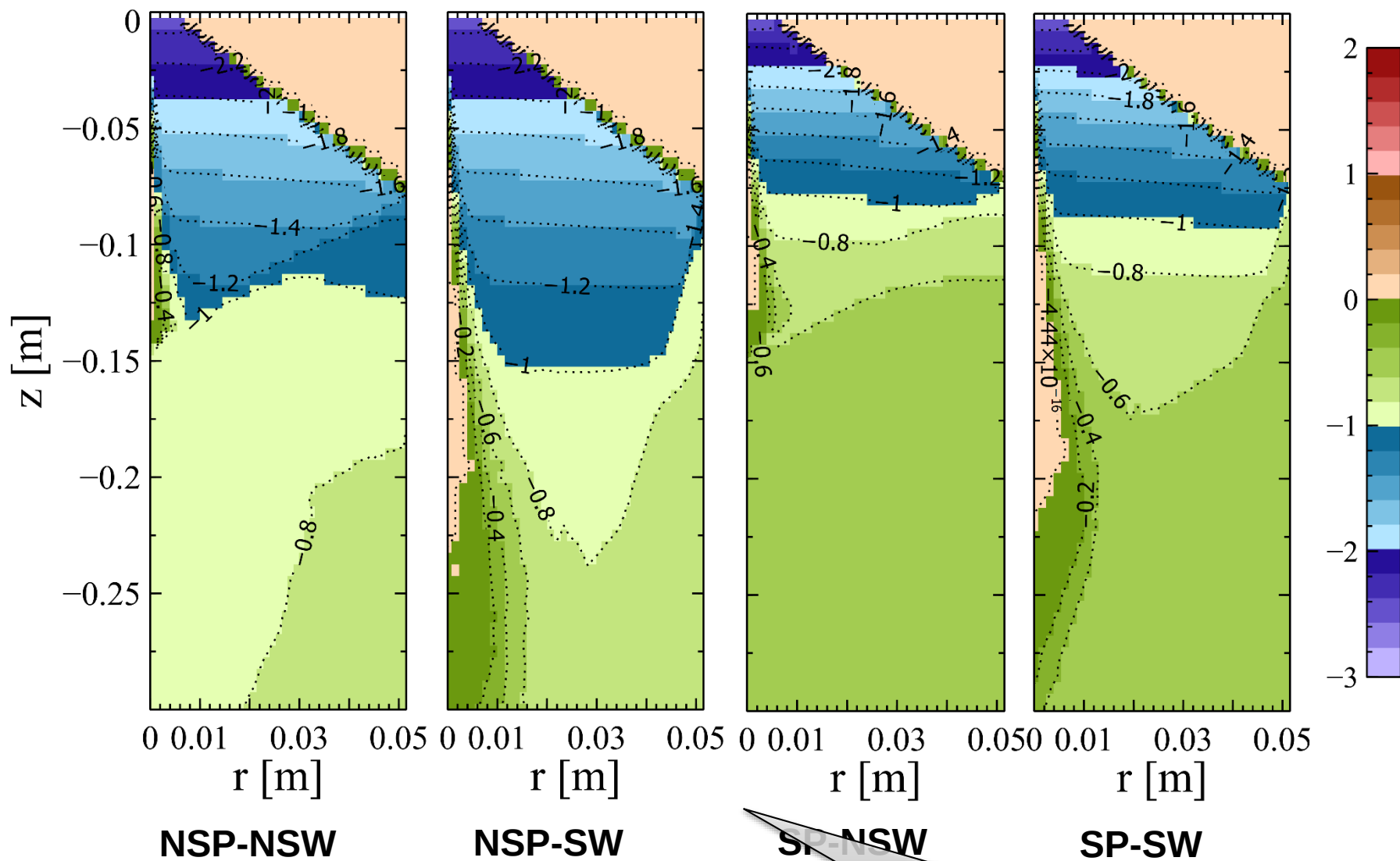
$$\bar{\varphi}_{z;i,j} = \frac{1}{N_t} \sum_{k=1}^{N_t} \frac{1}{N_p(k,i,j)} \sum_{p_{i,j}} \varphi(p_{i,j}, k)$$

Computed particles average fields



Average axial velocity of particles (half plane section)

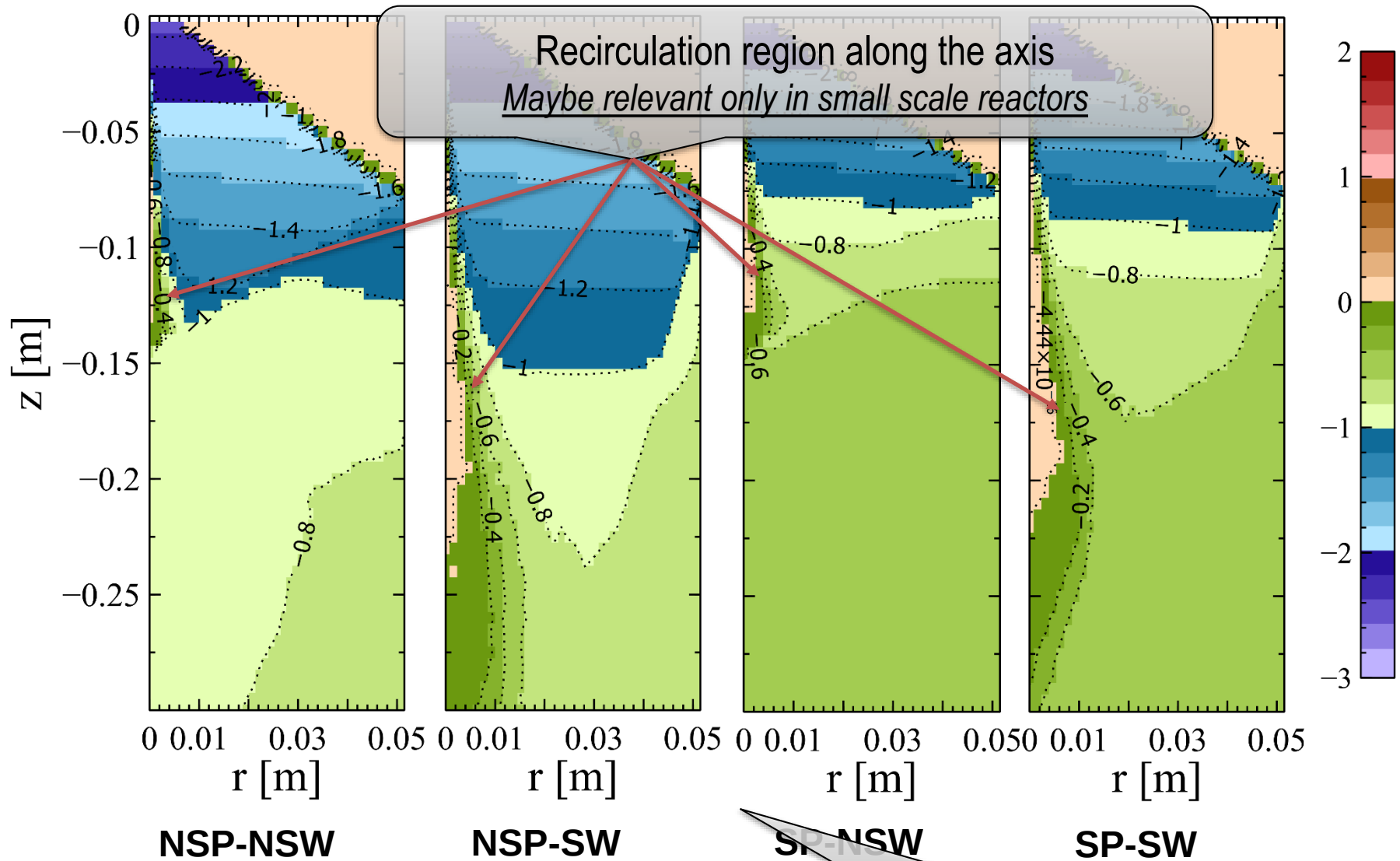
Computed particles average fields



Average axial velocity of particles (half plane section)

Decreasing axial velocity

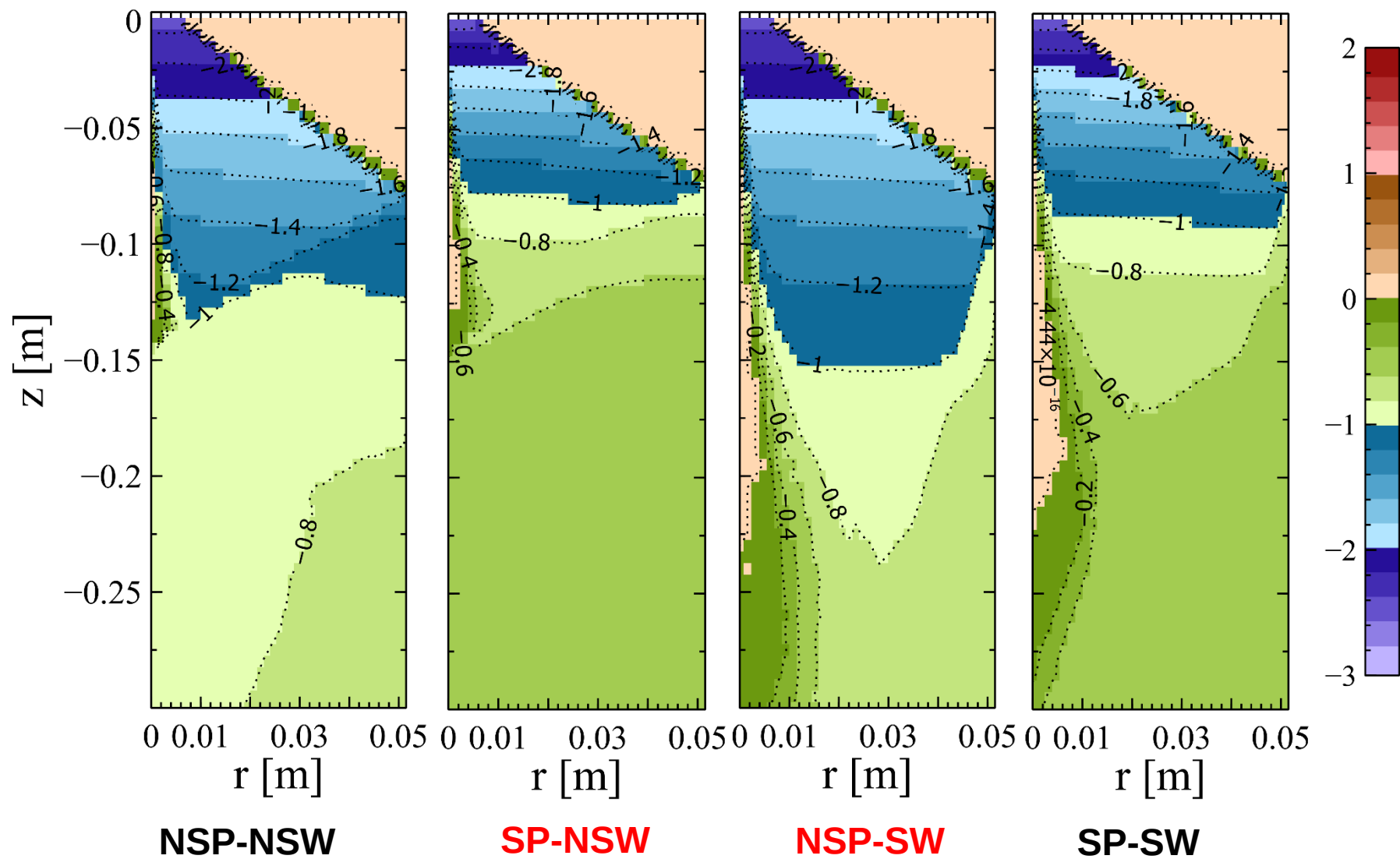
Computed particles average fields



Average axial velocity of particles (half plane section)

Decreasing axial velocity

Computed particles average fields

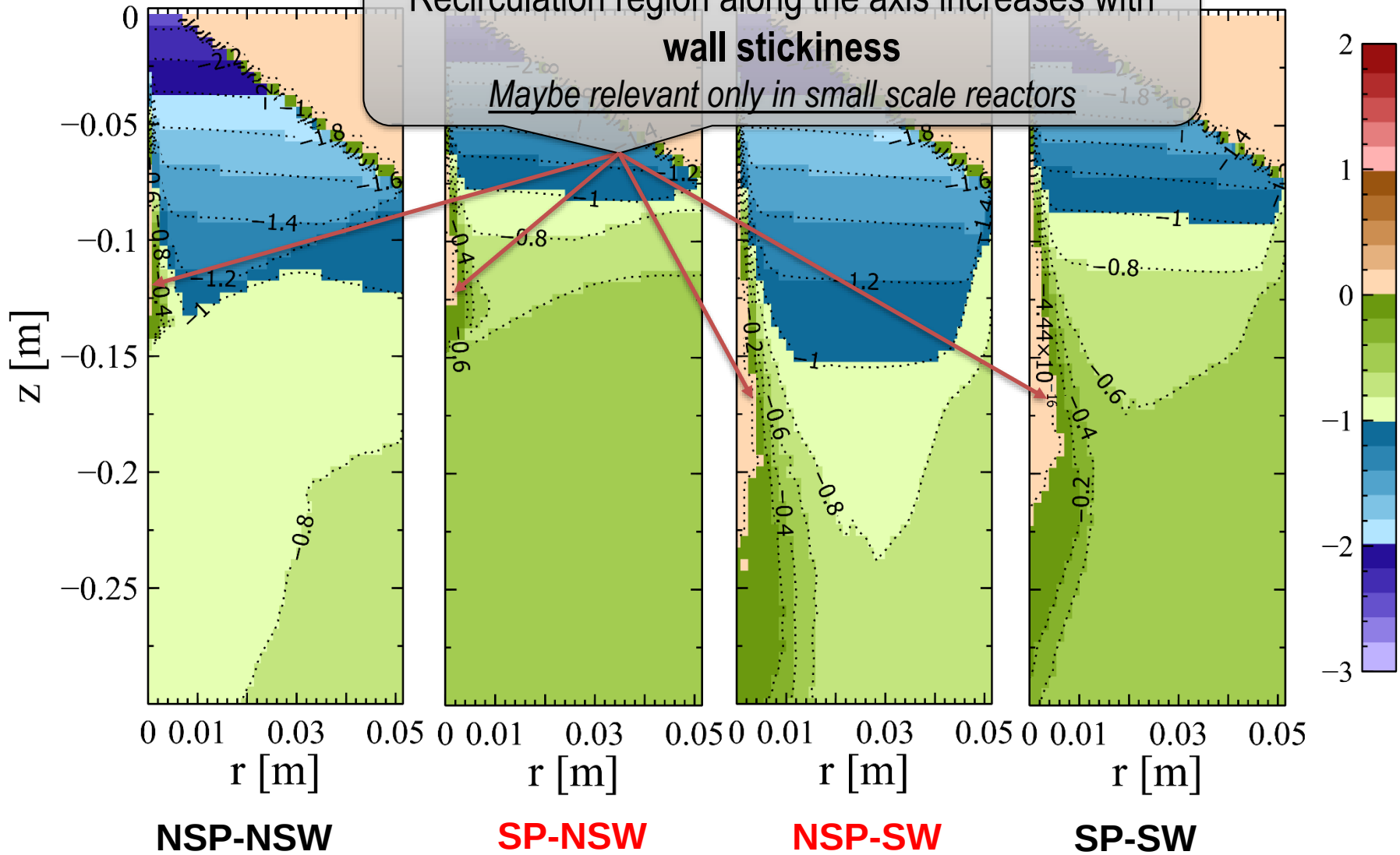


Average axial velocity of particles (half plane section)

Computed particles average fields

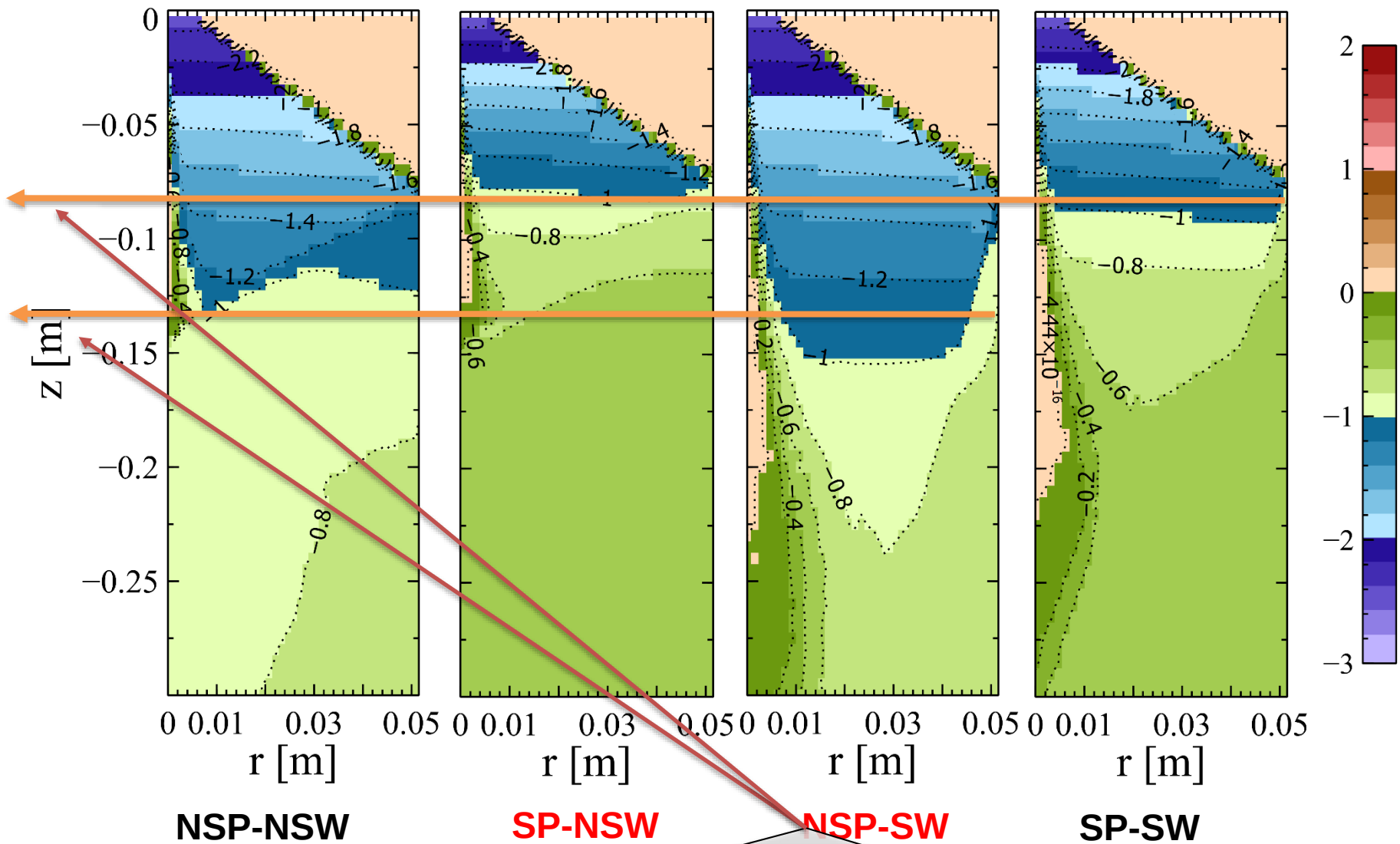
Recirculation region along the axis increases with
wall stickiness

Maybe relevant only in small scale reactors



Average axial velocity of particles (half plane section)

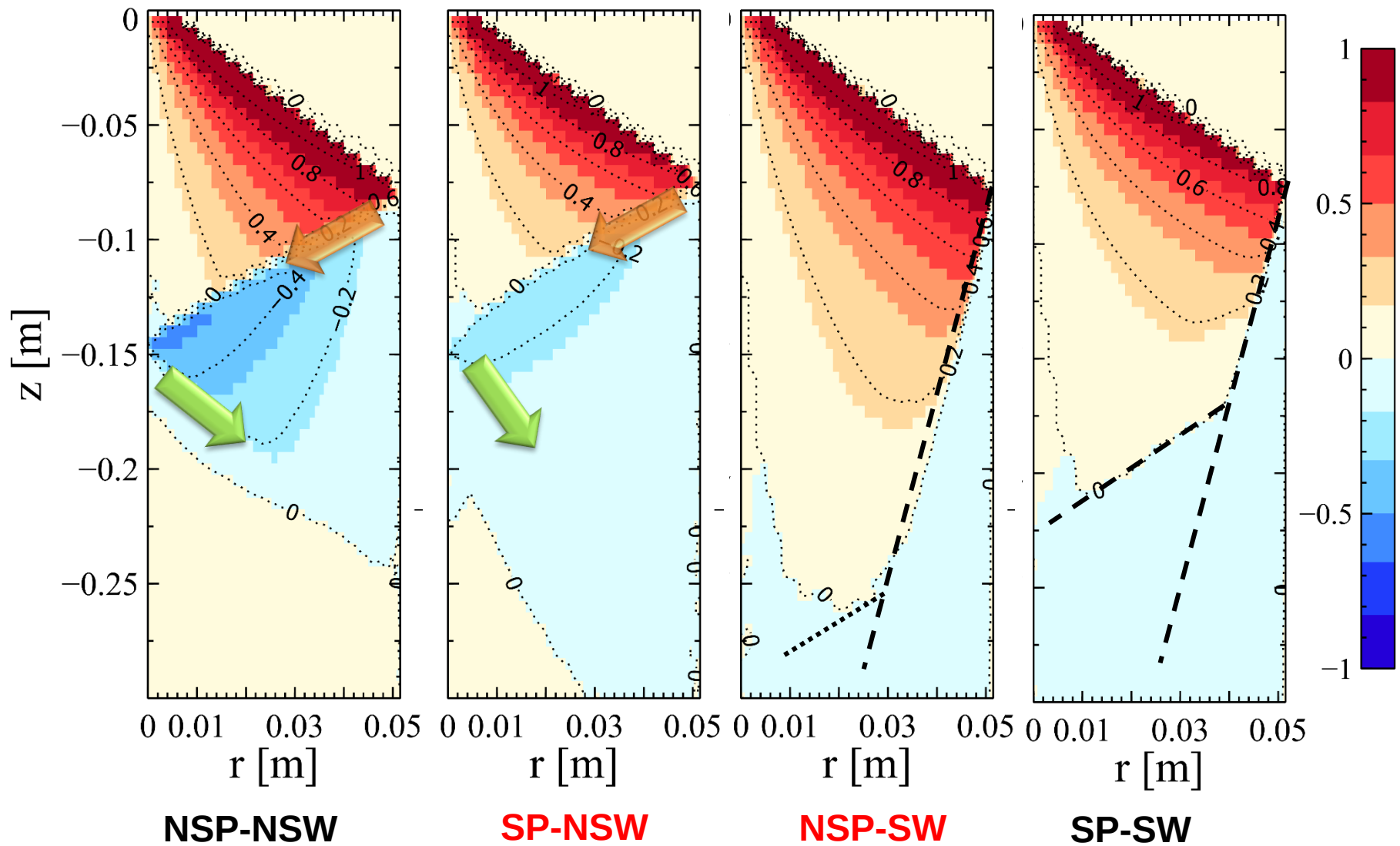
Computed particles average fields



Average axial velocity of

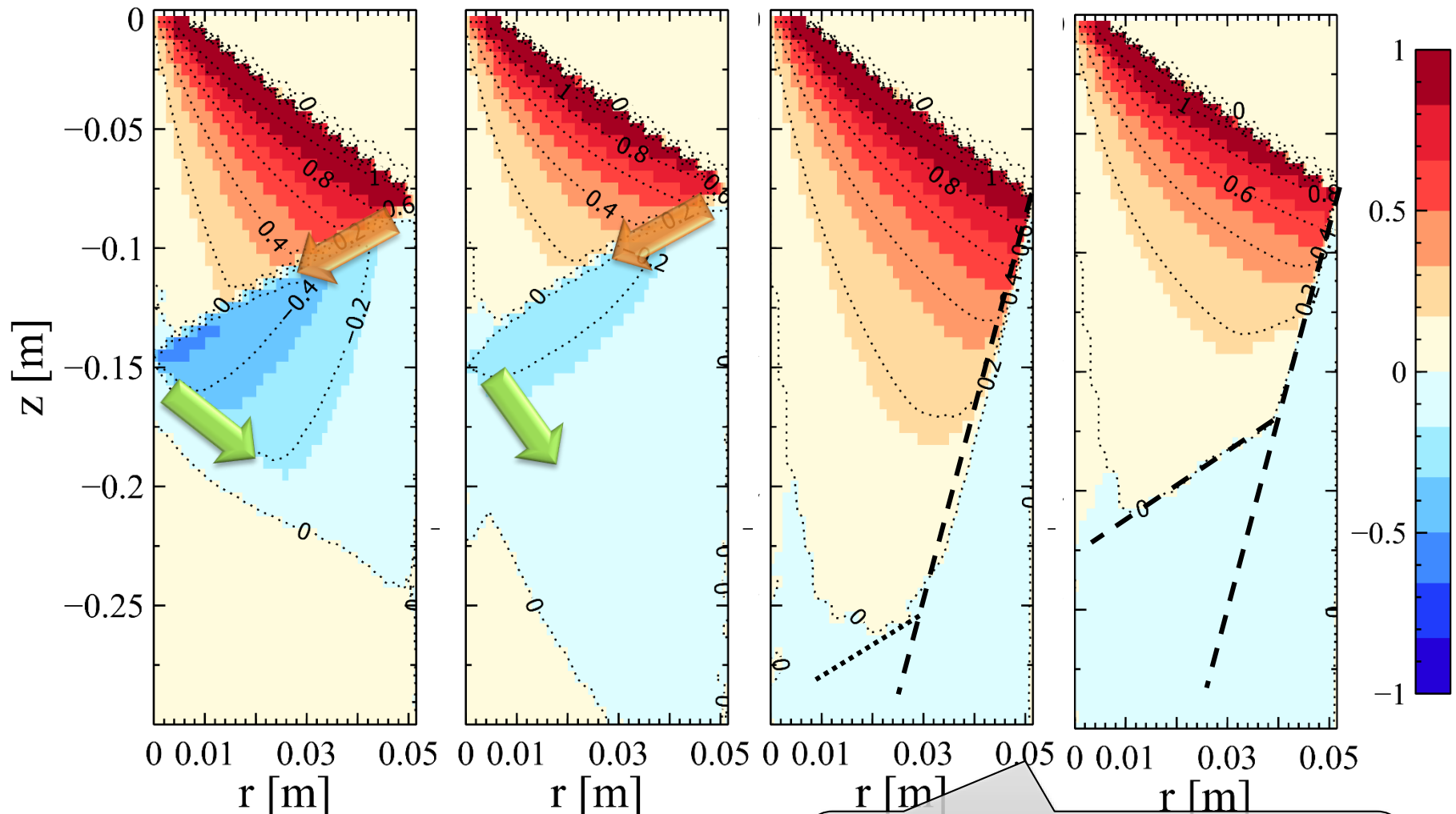
Initial jet penetration changes with particles stickiness (slightly increases with wall stickiness)

Computed particles average fields



Average radial velocity of particles (half plane section)

Computed particles average fields



NSP-NSW

SP-NSW

NSP-SW **Sticky Walls** SP-SW

NSP: build up and slow dispersion

SP: build up and rapid dispersion

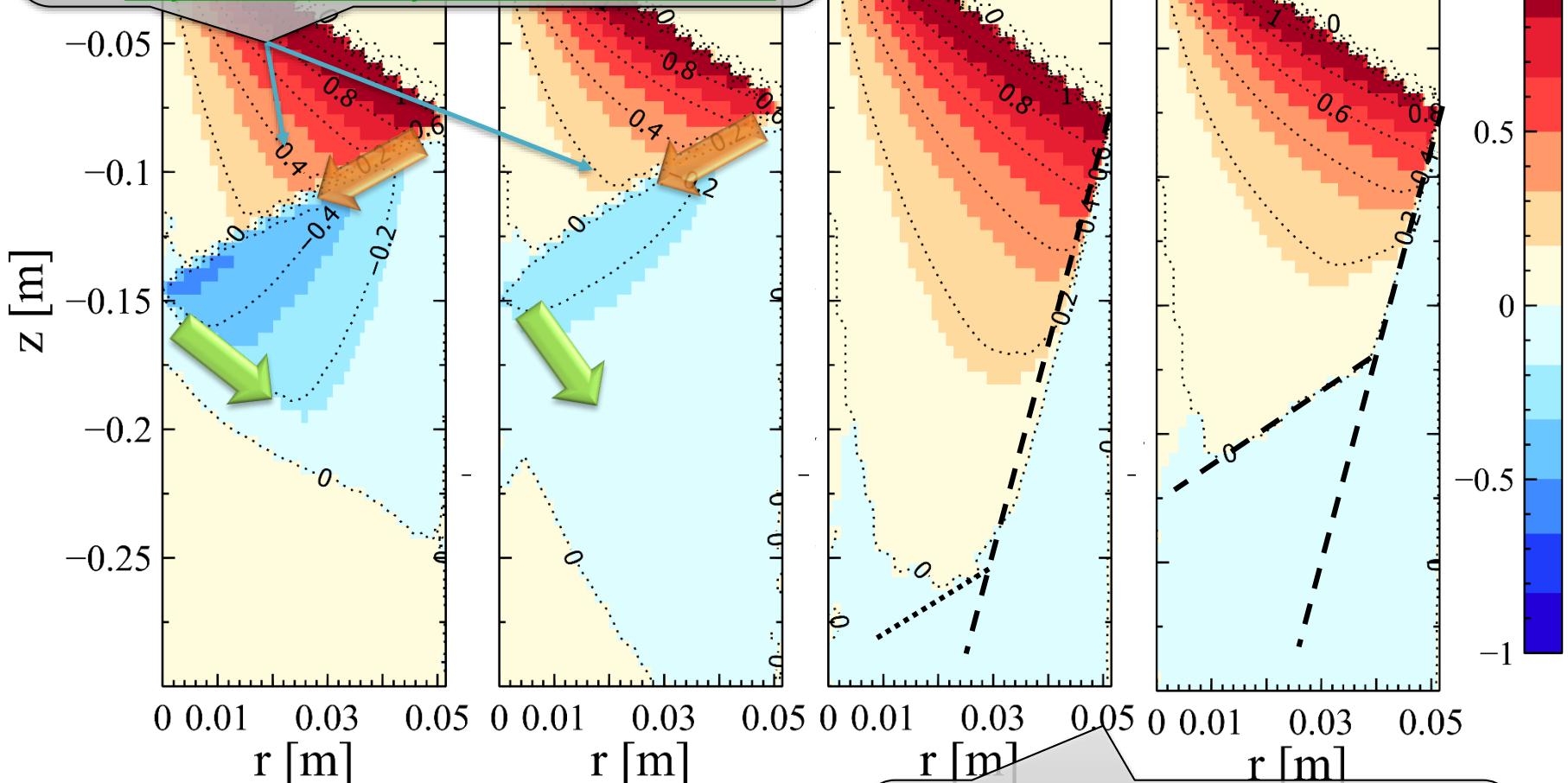
Average radial velocity of particles (

Non Sticky Walls

1) First reflection on wall

2) Second reflection on axis

Maybe relevant only in small scale reactors



NSP-NSW

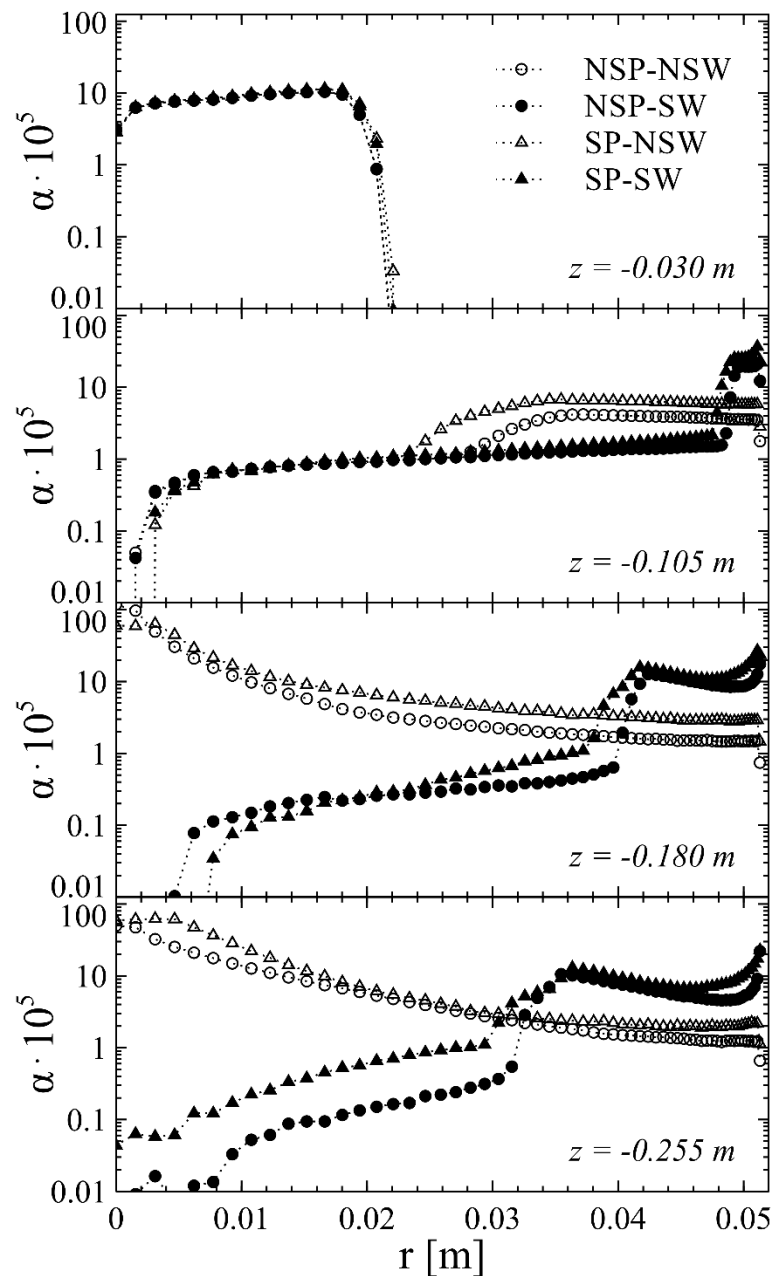
SP-NSW

NSP-SW Sticky Walls

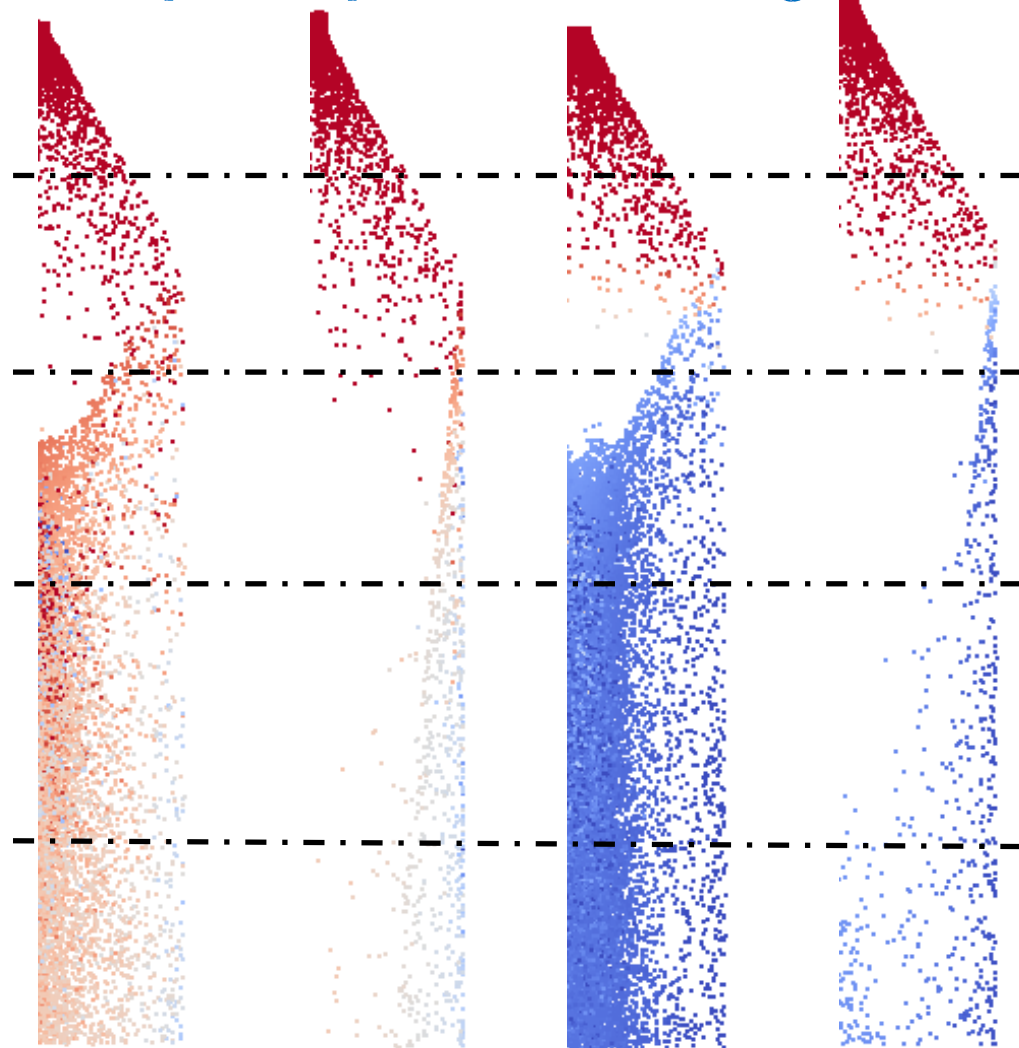
NSP: build up and slow dispersion

SP: build up and rapid dispersion

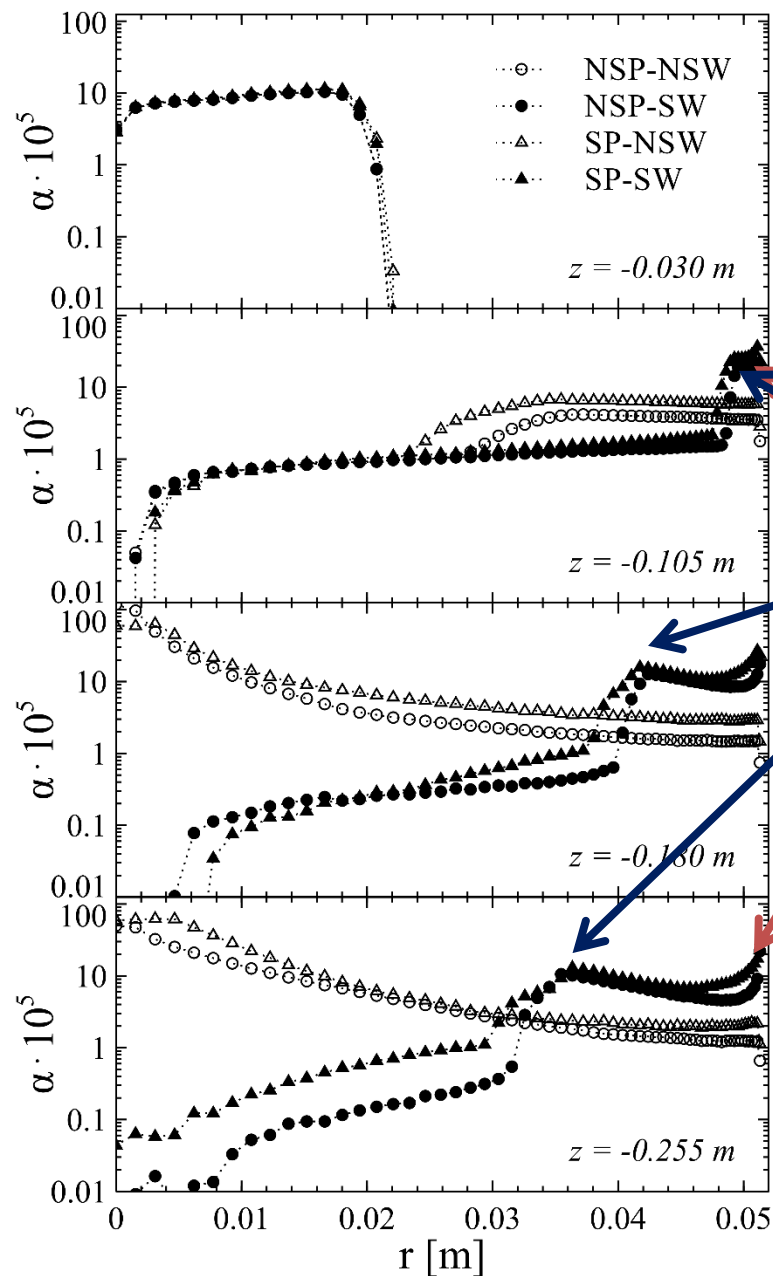
Average radial velocity of particles (m/s)



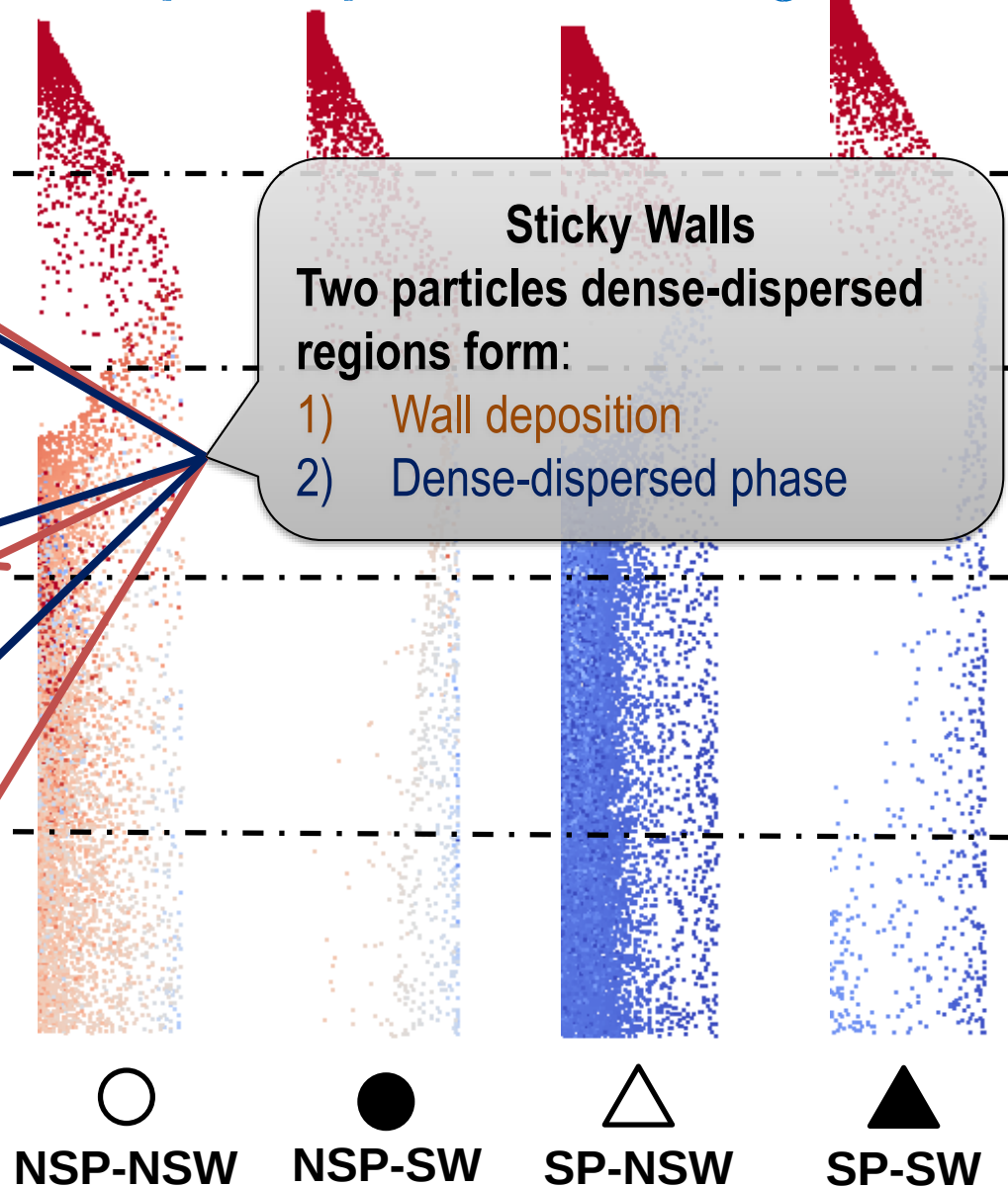
Computed particles average fields



Average radial particles concentration profiles



Computed particles average fields



Average radial particles concentration profiles

Detailed DEM numerical simulation of collision effects of non sticky (unconverted char) and sticky (molten ash) particles has been carried out.

Dynamics of intra-particles collision strongly affects the effective distribution patterns.

Numerical simulations indicate that a segregation and coverage regime can likely occur on sticky walls (walls covered by a slag layer).

This hypothesis is enforced by the behavior of sticky particles that on average **keep floating** above the surface of a sticky wall.

Stickiness associated with changes in restitution coefficient:

non sticky $\rightarrow \varepsilon = 0.9$; sticky $\rightarrow \varepsilon = 0.1$

is this really the only parameter to take into account (what about friction coefficients, cohesion, PSD)?

Effect of velocity and angle of impact

Effect of particle's Stokes numbers

Effect of particle flux intensity (number of particles $\Leftrightarrow$ number of collisions)

Effect of geometry size

Effect of injection type (tangentially fired, top fired, cross fired, ...)



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sviluppo per il sistema elettrico nazionale”,
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The benefits of Clean Coal Technologies

Two pink flamingos standing on a small patch of ground.
Cagliari, Italy
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Thank you for your kind attention



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