# Flow regime prediction in a 3D spouted bed using MFiX-DEM

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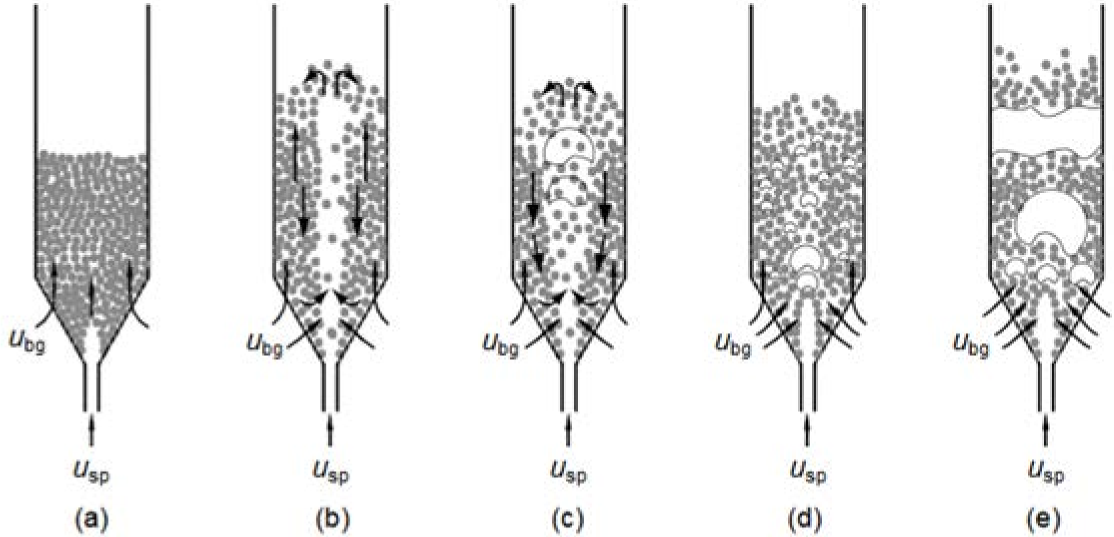
# Background and objectives

- Spout-fluidized beds help suppress de-fluidization and agglomeration, enhance heat and mass transfer, facilitate the adjustment of operating parameters, extend the size range of particles
- The spout is a local high velocity region at the center of the bed where solid particles and voids (bubbles) move in a structured manner with little radial displacement
- Numerical simulations of spouted beds at the particle level are essential to understand flow behaviors that are crucial in the design and operation of systems
- Comparison and validation of numerical predications against experimental readings is necessary to evaluate the accuracy and applicability of computational models for spouted beds

# Flow Regimes in Fluidized Beds



- Different flow patterns depending on operating conditions can be broadly classified into five flow regimes[1]




| Fixed bed/ internal spout | Spouting w/ aeration | Spout-fluidization | Jet in fluidized bed | Slugging |
|---|---|---|---|---|

[1]Zhang, J. & Tang, F. (2006) Prediction of flow regimes in spout-fluidized beds. *China Particuology*, *4*(3-4), 189-193.

# Internal spout

- Spout channel does not penetrate through the bed
- Only particles in the spout channel are moving
- Stable particle configuration
- Mildly fluctuating pressure drop with no periodicity

# Spouting with aeration

- Spout channel penetrates the entire bed
- Only particles in and close to the spout channel are fluidized
- Stable particle configuration
- Slightly fluctuating pressure drop with minimal periodicity

# Spout-fluidization

- Particles in the upper part of the bed are fluidized and move gently
- Spout channel is periodically blocked by particles from the annulus
- Pressure fluctuations are small but regular
- Clear dominant frequency associated with the time taken to remove the blockage

# Jet in fluidized bed

- All particles moving and bubbles are continuously formed in the annulus
- Spout channel present but periodically blocked or diverted through the annulus
- Bubbles are smaller than in the slugging bed regime so the associated frequency is higher
- Frequency spectra can be different for comparable operating conditions based on relative frequencies of bubble formation and spout blockage

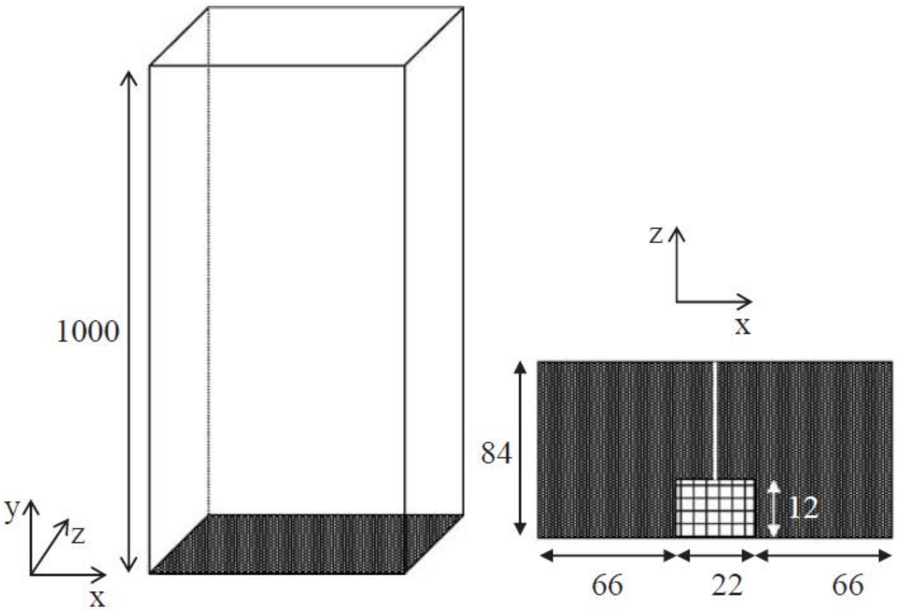
# Slugging bed

- All particles moving and slugs (bubbles with larger diameter than the bed) are continuously formed
- Large pressure drop fluctuations associated with formation of slugs
- Distinct periodic behavior with a low(er) dominant frequency because the slugs take time to form and propagate

# Identifying flow regimes by pressure spectra

| Regime | Frequency | Shape | Power |
|---|---|---|---|
| Internal spout | No peak | No peak | Low |
| Spouting with aeration | No peak | No peak | Low |
| Spout-fluidization | High | Narrow (< 0.5 Hz) | High |
| Slugging bed | Low | Broad (> 1 Hz) | High |
| Jet in fluidized bed | Intermediate | Intermediate | High |

# Experimental setup & particle properties




| Property | Experiment[1] | Simulation |
|---|---|---|
| $d_p$ (mm) | 4.04 ± 0.02 | 4.04 |
| $\rho_p$ (kg/m³) | 2,526 ± 1 | 2,526 |
| $u_{mf}$ (m/s) | 1.77 ± 0.03 | 1.97 |
| $e_{n,p\leftrightarrow p}$ | 0.97 ± 0.01 | 0.97 |
| $e_{n,p\leftrightarrow w}$ | 0.97 ± 0.01 | 0.97 |
| $\mu_{p\leftrightarrow p}$ | 0.10 ± 0.01 | 0.10 |
| $\mu_{p\leftrightarrow w}$ | 0.10 ± 0.01 | 0.10 |
| # particles | 44800 | 42840[†] |

[†]Particles automatically in bed generated based on initial specified height

[1]Link, J. M., Cuypers, L. A., Deen, N. G., & Kuipers, J. A. (2005). Flow regimes in a spout–fluid bed: A combined experimental and simulation study. *Chem. Eng. Sci., 60*, 3425-3442.

# Simulation Approach

- Simulations performed in open source code MFiX-DEM[1] – Multiphase Flow with Interphase eXchanges
- Soft-sphere model for particle collisions ($k_n$ = 10,000 N/m, $\eta$ = 0.97)
- Interphase momentum transfer computed using Gidaspow drag law[2] (based on Wen & Yu model[3] and Ergun equation[4])

[1]Garg, R., Galvin, J., Li, T., & Pannala, S. (2012). *Documentation of open-source MFIX–DEM software for gas-solids flow.* Retrieved July 31, 2017, from https://mfix.netl.doe.gov/documentation/dem_doc_2012-1.pdf.

[2]Gidaspow, D. (1992). *Multiphase Flow and Fluidization.* San Diego, CA: Academic Press.

[3]Wen, C. Y., & Yu, H. Y. (1966). Mechanics of fluidization. *Chem. Eng. Prog. Symp. Ser., 62*, 100-111.

[4]Ergun, S. (1952). Fluid flow through packed columns. *Chem. Eng. Prog., 48*, 89-94.

# Determining $u_{mf}$ in simulation

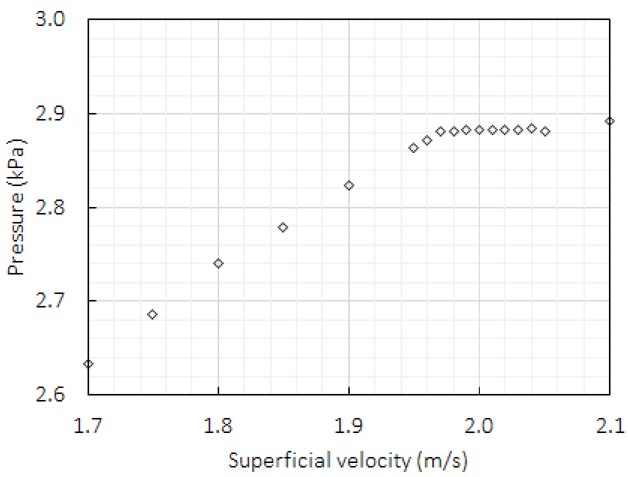
- $u_{mf}$ is the minimum superficial fluid velocity needed to fluidize a bed
- As gas flow into the packed bed is increased, the pressure drop $\Delta p$ across the bed increases until the minimum fluidization condition
- At the minimum fluidization condition the net weight of the bed is exactly balanced by $\Delta p$
- Further increase in the superficial velocity results in no further increase in $\Delta p$
- Bubbles can cause $\Delta p$ to fluctuate but the average value should remain constant

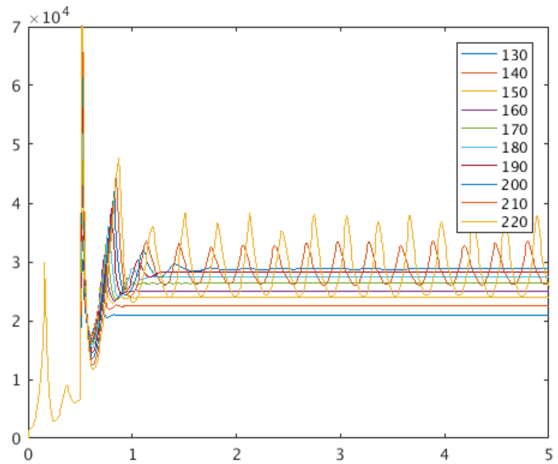
# Determining $u_{mf}$ in simulation

- Minimum fluidization occurs at intersection of linearly increasing pressure and constant pressure
- At minimum fluidization,

$$\frac{\Delta p}{L} = (1 - \varepsilon_{mf})(\rho_s - \rho_f)g$$

$$u_{mf} = 1.97 \text{ m/s}$$
$$\varepsilon_{mf} = 0.365$$



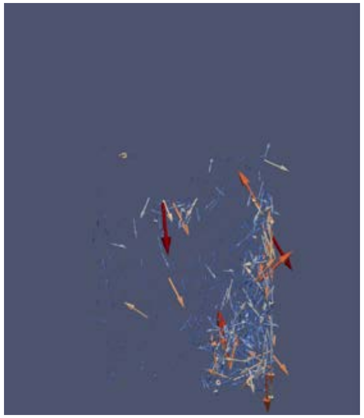



# Confirming $u_{mf}$ by visualization

- Particles are visualized by their motion at $u$ = {1.96, 1.97, 1.98 m/s}
- Only few individual particles exhibit motion at 1.96 m/s
- Significant number of particles fluidized at 1.97 m/s

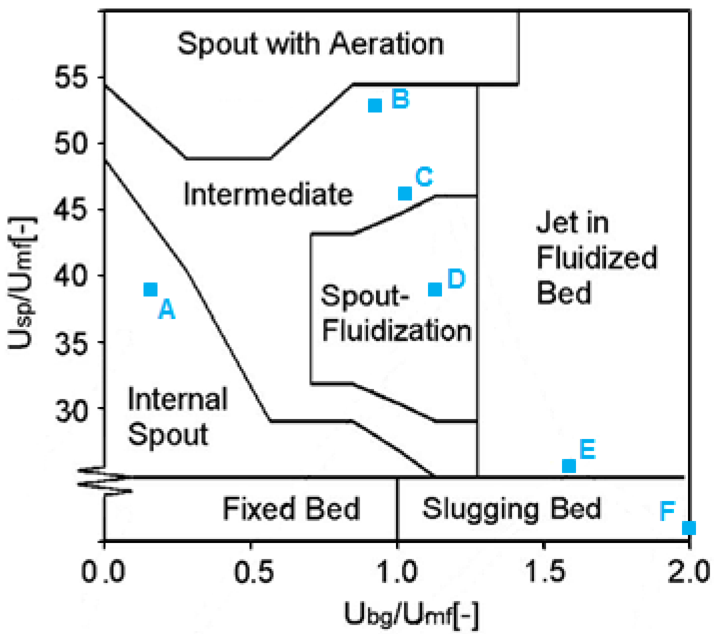
$u$=1.96 m/s

$u$=1.97 m/s



$u$=1.98 m/s

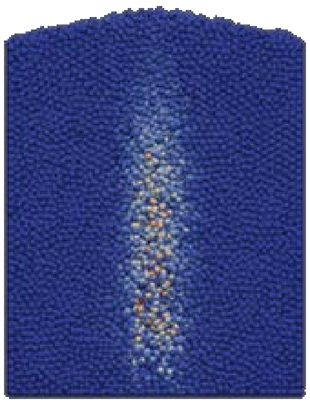
# Simulation test cases

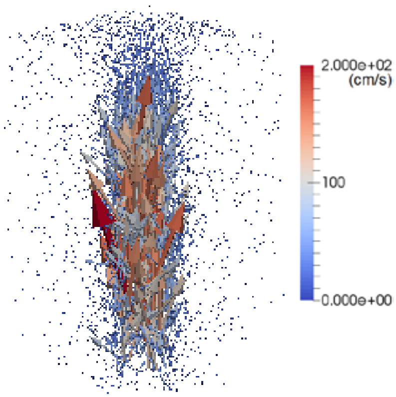


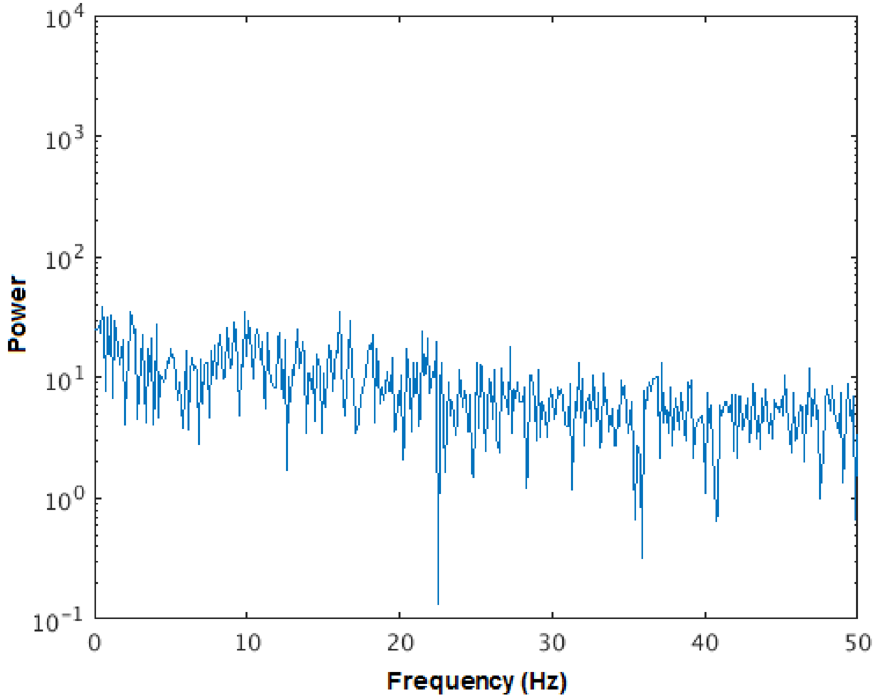

| Case | $u_{bg}$ (m/s) | $u_{bg}/u_{mf}$ | $u_{sp}$ (m/s) | $u_{sp}/u_{mf}$ |
|---|---|---|---|---|
| A | 0.3 | 0.15 | 76 | 39 |
| B | 1.8 | 0.9 | 103 | 53 |
| C | 2.0 | 1.0 | 90 | 46 |
| D | 2.2 | 1.1 | 76 | 39 |
| E | 3.1 | 1.6 | 41 | 34 |
| F | 3.9 | 2.0 | 3.9 | 2.0 |

# Results and discussion – Case A

- Spout channel is evident but does not penetrate bed
- Kinetic energy of particles goes towards loosening the original closely packed configuration
- Frequency spectrum of pressure drop shows no periodicity

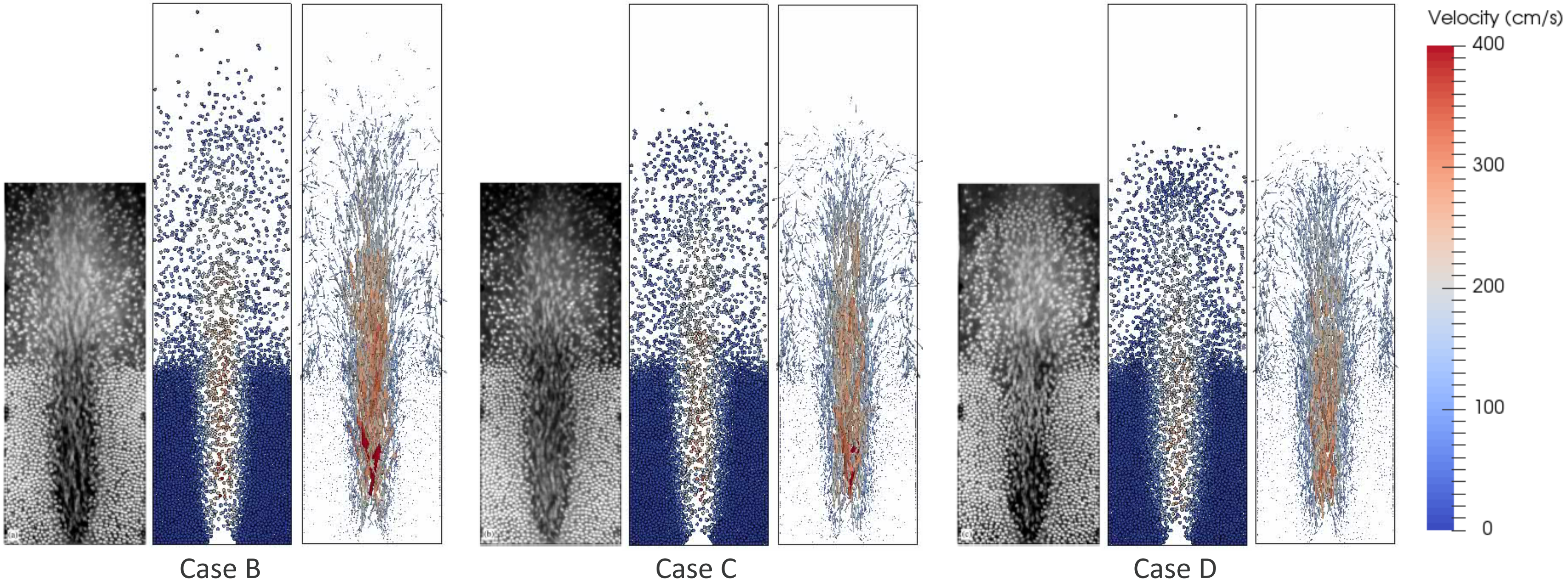




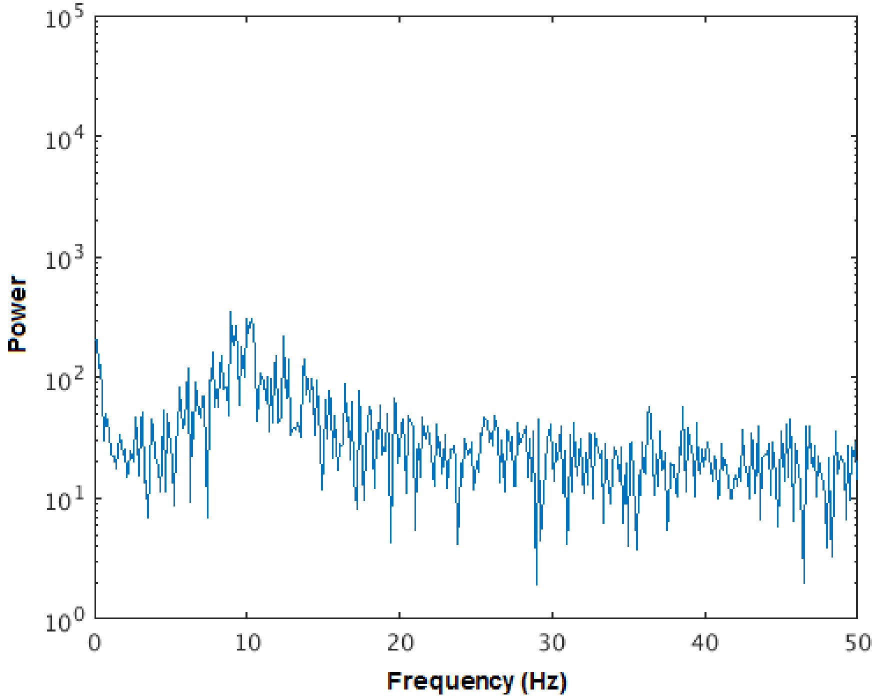
# Results and discussion – Cases B,C,D

- All three cases exhibit spouting behavior and have a similar overall shape
- Pressure spectra and particle velocities can differentiate the flow regimes between these configurations



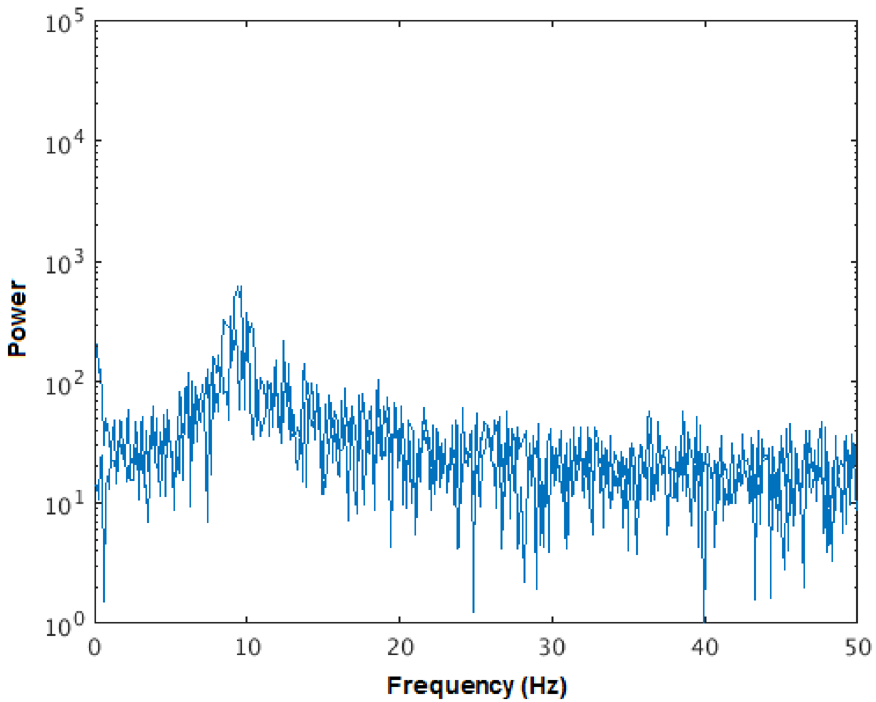
# Results and discussion – Case B

- Very fast spout with no fluidization in the annulus
- Discernible 'peak' with low power at a relatively high frequency
- Despite the slight periodicity, this configuration lies in the spouting with aeration regime



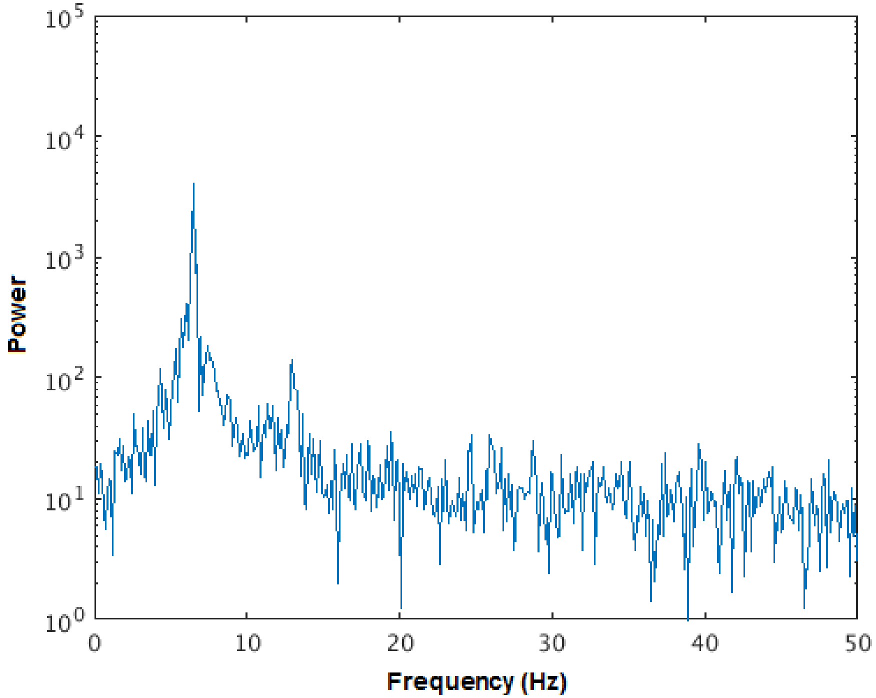
# Results and discussion – Case C

- Reduced spout velocity and more movement in annulus
- Peak is more distinct – narrower and with higher power
- Increased periodicity associated with intermittent blockage of spout by entrained particles from annulus but no clear dominant frequency
- Characterizes an intermediate regime between spouting with aeration and spout fluidization



# Results and discussion – Case D

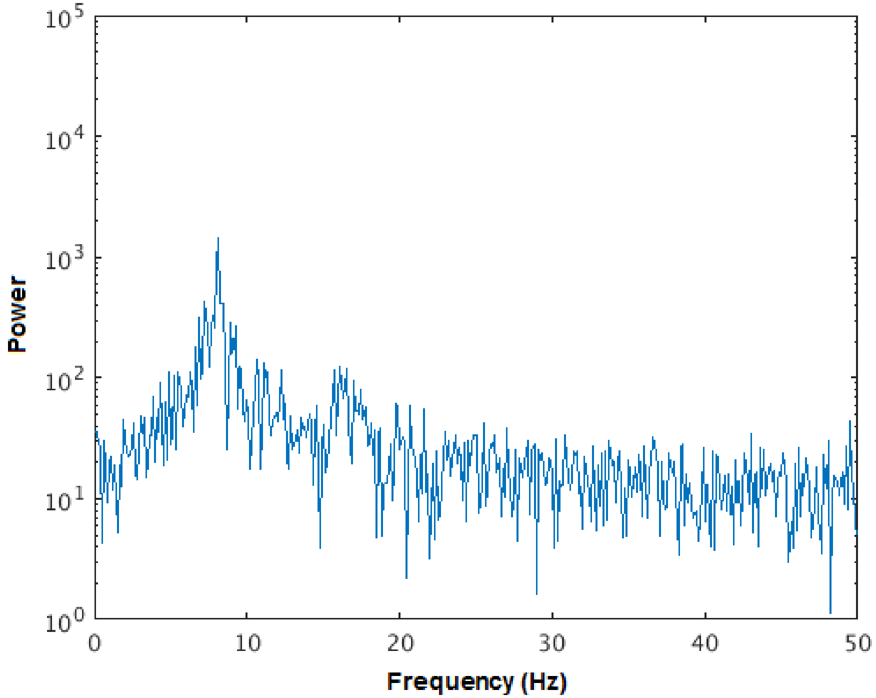
- Further reduced spout velocity reflects in maximum bed height; annulus shows more particle movement
- Sharp peak shows clear dominant frequency at 6.5 Hz with very high power
- Second harmonic peak also visible
- Definitely in the spout-fluidization regime
- Dominant frequency is in excellent agreement with experimental data



# Results and discussion – Case D*

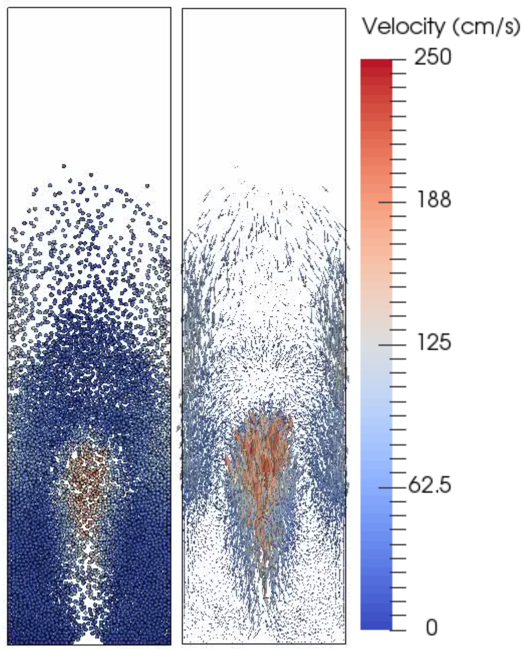
$u_{sp}$ increased to 86 m/s with same $u_{bg}$

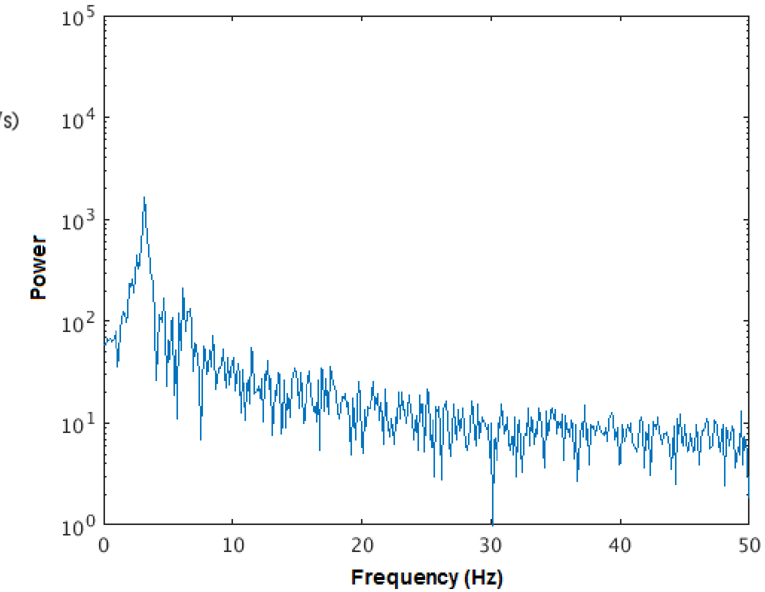
- Increased fluidization in annulus and lower velocity in spout are both essential for spout-fluidization
- Peak becomes broader and shifts to the right
- Behavior closer to the intermediate regime

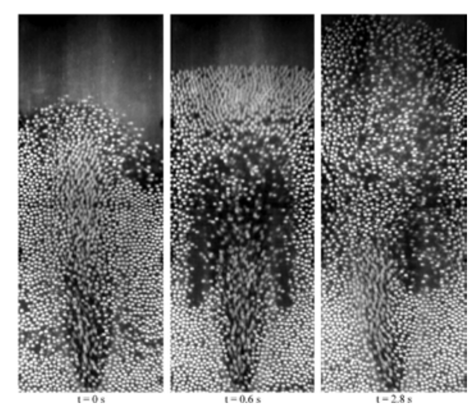


# Results and discussion – Case E

- Annulus is completely fluidized and starts to bubble
- Spout channel period-ically diverted through annulus
- Flow configuration is an overlap of a spout-fluidized bed and a bubbling bed
- Somewhat wide peak at 3 Hz with power of 1600

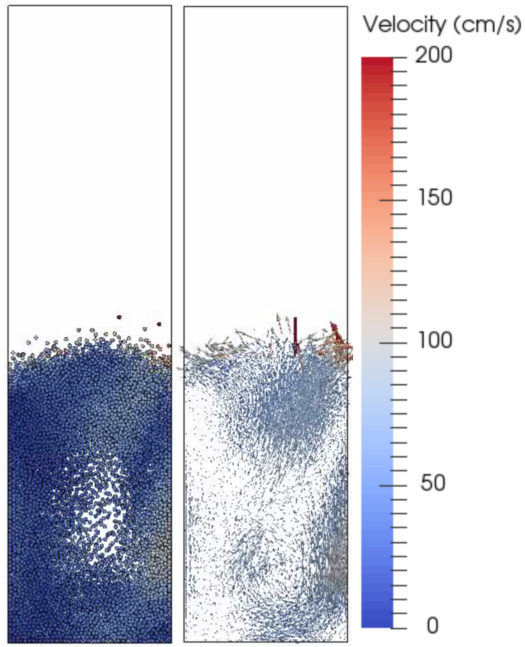


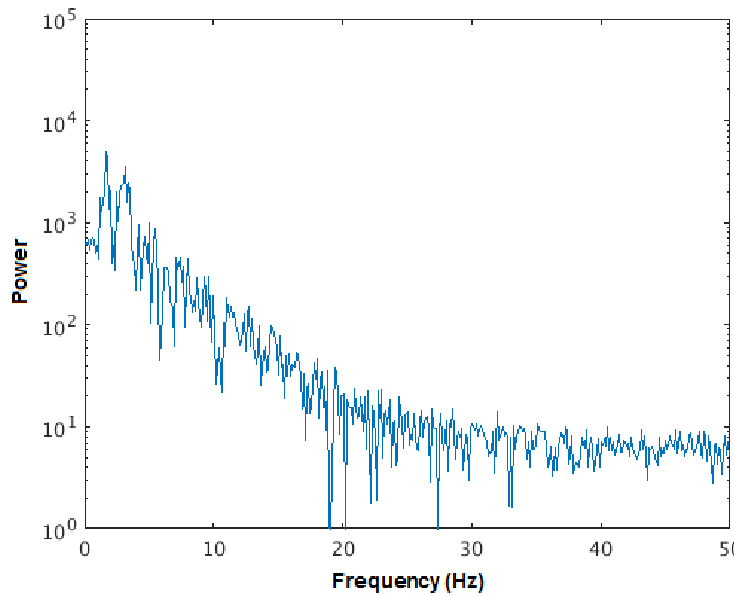



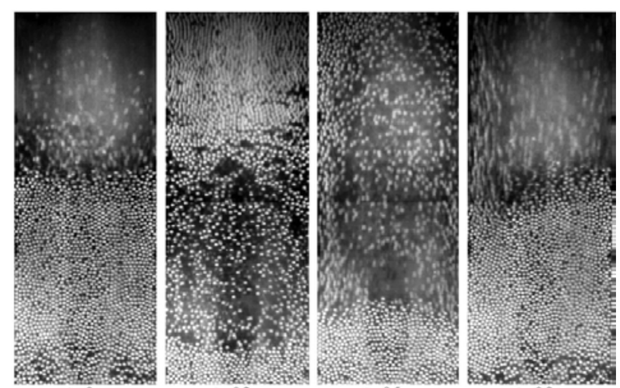



# Results and discussion – Case F

- Particles across the bed shoot up rapidly forming bubbles larger than the bed width known as slugs
- Time scale of slug formation matches experiment
- Low frequency of 1.6 Hz agrees with experiment (but twin peaks instead of one wide peak)



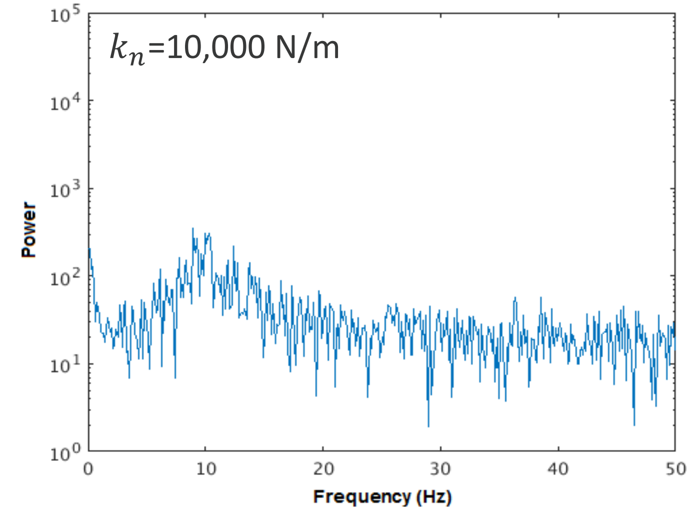



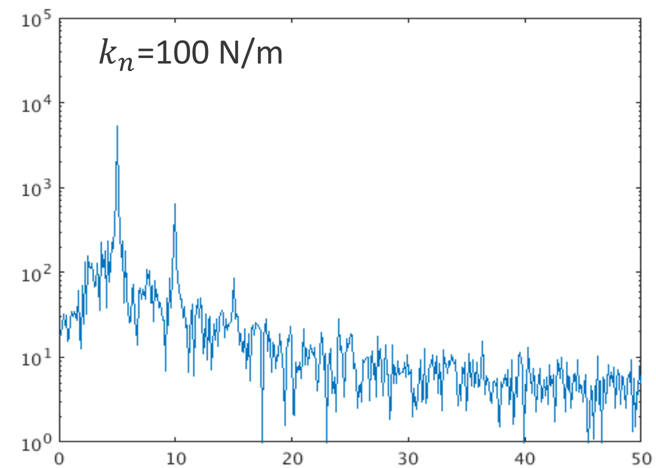



t = 0 s t = 0.2 s t = 0.5 s t = 0.8 s

# Parameter study: spring stiffness

- Many model parameters are indeterminate[1]
  - $e_t$, $k_t$ cannot be derived
  - Physical values of $k_n$ cannot be used
- Little to no effect on $u_{mf}$ so differences in flow regimes cannot be attributed to differing $u_{sp}/u_{mf}$ and $u_{bg}/u_{mf}$ ratios
- Investigate effects in spouting with aeration regime as it has largest particle velocities (collision forces largest)
- Spring stiffness is reduced to $k_n$ = 100 N/m
  - Clear dominant frequency at 5.0 Hz with high power of 5,300
  - Additional harmonic frequencies present




[1]Bakshi, A. et al. Multivariate sensitivity analysis of CFD-DEM: Critical model parameters and their impact on fluidization hydrodynamics, *2017 AIChE Annual Meeting*, October 29-November 3, Minneapolis, MN.

# Conclusions

- Detailed numerical simulation of spouted bed experiment over a range of flow conditions corresponding to different flow regimes
- Spectral analysis of the pressure fluctuations are used to characterize the flow regimes accurately
- Flow regimes predicted by simulation are in excellent agreement with the experiment including good quantitative matches where applicable
- MFiX-DEM is a powerful tool for predicting key performance parameters for effective design, tuning and optimization of spout-fluidized systems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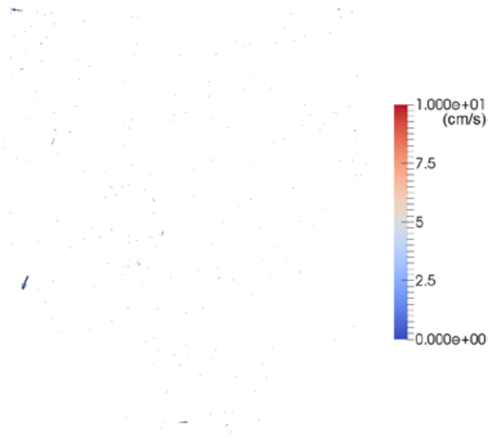
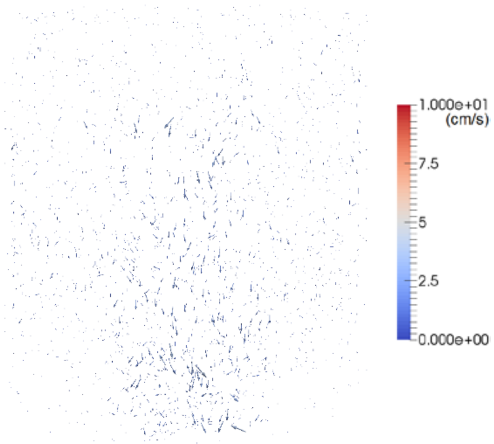
# Backup Slides – Fluidization Snapshots




$u$=1.96 m/s

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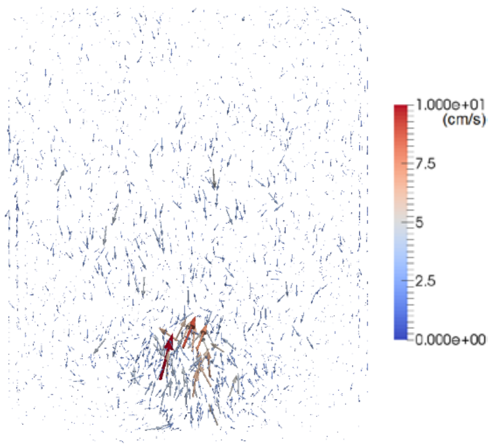


$u$=1.98 m/s

# Backup Slides – Bed Snapshots