Summary of Non-rectangular Wall and Internal Surface Boundary Conditions Treatment in MFIX-DEM

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In this document, the implementations of non-rectangular wall boundary and internal surface in MFIX-DEM are briefly summarized. To model the wall and internal surface in the domain, the fluid cells close to walls or internal surfaces are located with subroutine *cell_near_wall* first. The particle-wall contact checking in *calc_force_des* is performed only particles on those cells identified in *cell_near_wall*. In MFIX, a typical inclined wall is approximated using stair-stepping as shown in figure 1. It is possible that a particle contacts with a wall through the edge. To take care of this situation, a wall particle is generated and its center is located at a particle radius away from the edge of wall. Similar technique is used when the particle contacts the wall through one node. In the current implementation, **only one contact** with the edge or node of wall cell for a particle is allowed since the particle size is smaller that the size of control volume. All these changes are triggered only when the variable 'non_rect_bc' is set to true in the mfix.dat.

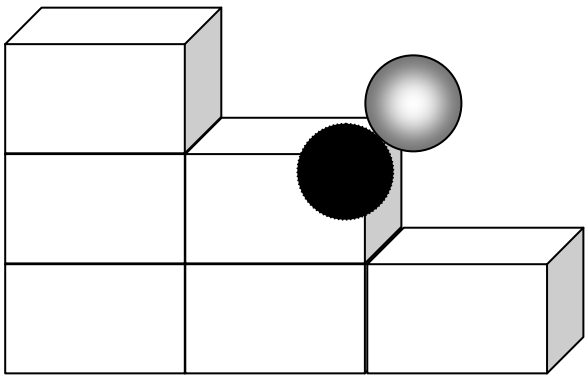

Figure 1. Particle-wall interaction

The new subroutines as well as those that have been modified to accommodate the new wall-particle treatment are listed in table 1, with a brief description.

Table 1. New and modified subroutines

New	Description
cell_near_wall	Find the cells that are in the neighborhood of the walls or internal surfaces
wallfacecontact	Check if a particle contacts with the face of wall cell and generate the wall particle

walledgecontact	Check if a particle contacts with the edge of wall cell and generate the wall particle
wallnodecontact	Check if a particle contacts with the node of wall cell and generate the wall particle
Modified	
calc_force_des	Perform wall-particle contact check
Des_allocate_arrays	Allocate variables for *cell_near_wall*
Discretelement	Add declaration of variable for *cell_near_wall*
drag_fgs	Gas pressure interpolation near walls and internal surfaces
make_arrays_des	Call *cell_near_wall*

Test case:

A simple two dimensional test case has been run to validate the implementation. More validations are necessary to make sure it works for both two and three dimensional cases. In this test case, a two dimensional spouted bed with conical bottom and two draft plates is simulated. A snapshot of the simulation result is shown in figure 2.

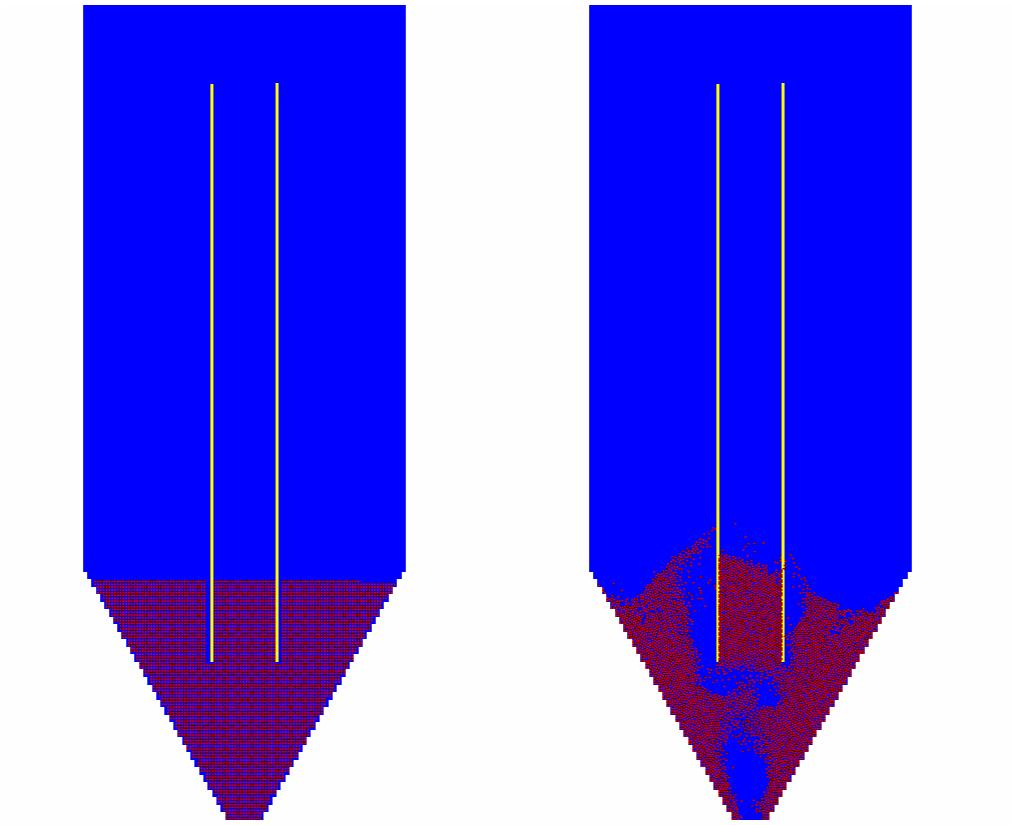

Figure 2. Simulation snapshot of a 2D spouted bed with draft tube plates