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Electrically Conducting Fluid/Solid Boundaries

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Problem

A weakly conducting fluid containing a positive electric charge is entering a pipe with conducting solid walls. The pipe is assumed to be grounded on its outside surface (to insure this, a separate solid was wrapped around the outside and defined to be a perfect conductor at zero potential). This problem was originally investigated by a *FLOW-3D* user, Harold Walmsly, who raised questions about simulation results when the solid/fluid boundary is, or is not, coincident with a mesh/grid line. When coincident, grid elements contain either pure fluid or pure solid. Alternatively, the boundary could be within a grid element creating a “mixed” cell containing both fluid and solid. The question raised was why there are differences in the computational results and is this some problem associated with the **FAVOR**TM method? This note addresses these questions and describes a code change to improve the electrical treatment of mixed cells.

Two basic options are available for simulating this arrangement. Either the solid can be considered a perfect conductor having a specified potential (an “electrode”) or it can have a finite conductivity in which case the simulation will compute potentials and charge densities in the solid.

Thus, having a mixed cell boundary, or not, and allowing for currents in the solid pipe, or not, constitutes a set of four possible arrangements whose results can be compared.

Code Notices

Before making these comparisons it is important to mention that there was a programming error in the Version 10 as well as in the initial release of Version 11. This error has been corrected in the patch release of Version 11.1. Furthermore, this study has resulted in another small change in the program to better account for mixed solid/fluid cells.

In the following discussion it will be useful to know how electrical properties are located and stored in the computational grid. Physical property data includes dielectric constant, conductivity and charge mobility and these are assigned to each grid element. Electric potential is either specified or computed and is assigned to the center of each grid element. Electric field components are computed as the negative gradient of the potential so are most conveniently located at the sides of the elements, e.g., the x-components of the electric field (\mathbf{E}_x) are located at

grid boundaries between neighboring elements in the x-direction, E_y values are located at the boundaries between neighboring elements in the y-direction, etc.

Physical Considerations

In the pipe there is an electric field generated by the charge in the fluid and this field is directed into the wall of the pipe. As the pipe is a good conductor (relative to the fluid) and has no, or almost no, spatial variation of the potential and hence no significant field in its interior. However, there must be a non-zero free charge on the surface of the conducting pipe wall as a consequence of Gauss' law relating the electric field and the charges. This requirement has consequences for those simulations where the solid is given a finite conductivity, because the surface charge must then be accounted for. If the solid is simply treated as a perfect conductor with a fixed potential, then there is no need to consider a surface charge on the conductor.

Simulation Results and Comparisons

The simplest case has the solid pipe boundary coincident with grid lines and the pipe is a constant potential "electrode" set at a zero value. All results to be displayed in this note correspond to a simulation time of 0.25s, which is somewhat beyond the time at which fluid completely fills the section of pipe simulated. Figure 1 shows the entire pipe used in the simulation, while Fig 2a shows only a central region with the grid overlaid to emphasize the location of the solid/fluid boundary with respect to the grid.

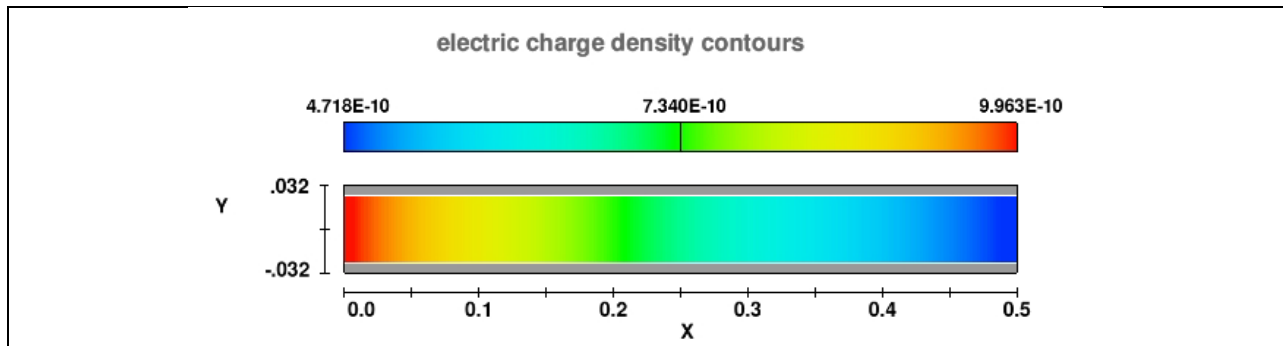
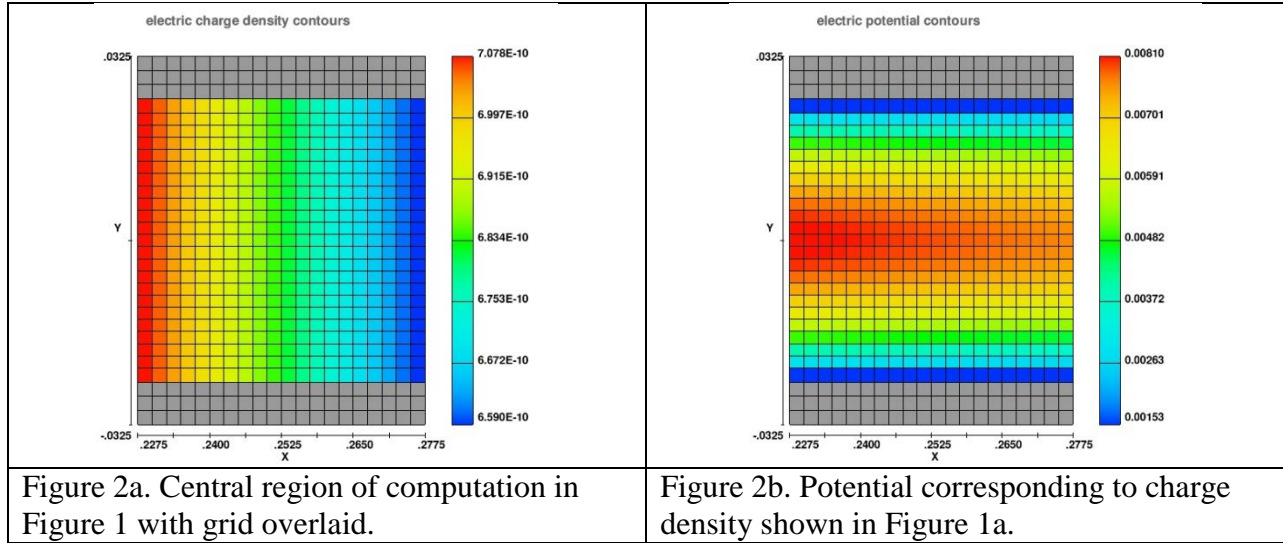


Figure 1. Computed fluid charge density at $t=0.25s$. Solid is at a constant potential of zero.

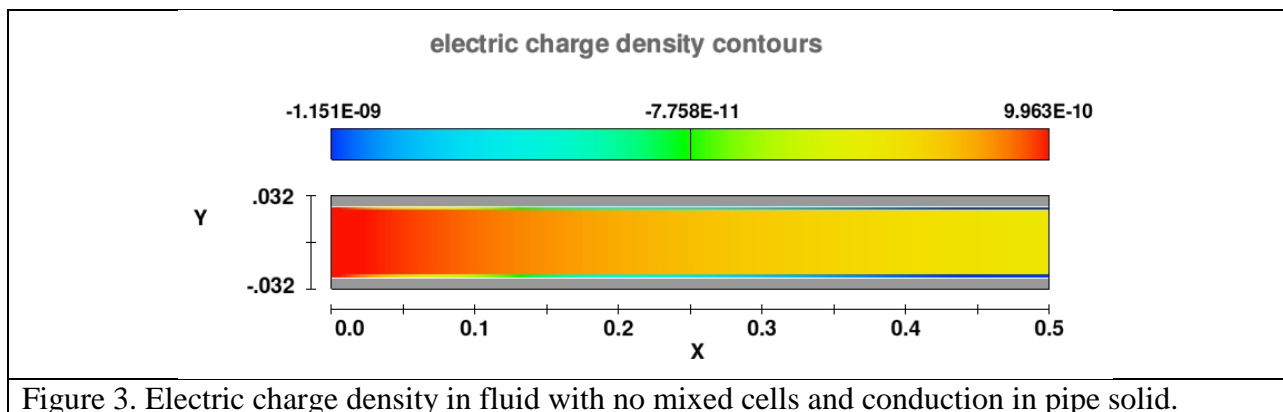
The color shading in these plots represents the fluid charge density. The potential is shown in Fig. 2b.



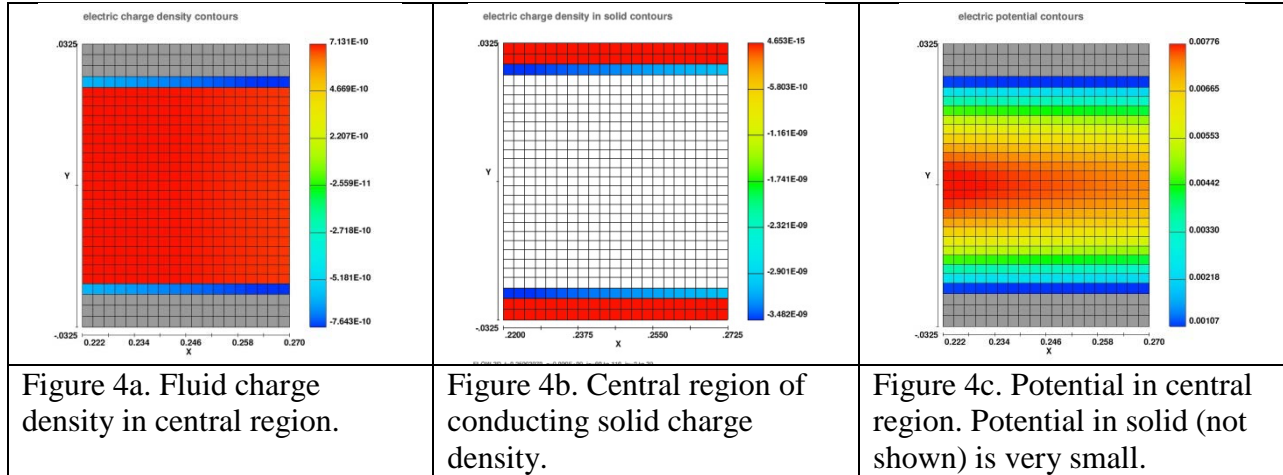
It will be seen that the fluid cell adjacent to the pipe wall has a low, but not zero potential. The charge density in the fluid is essentially constant vertically between the pipe walls, but varies some along the pipe from the inlet at the left to the outlet at the right. The charge decreases because of conduction into the zero-potential pipe.

Because the pipe wall has been treated as a constant potential region it has no surface charge or potential variations in its interior. This is to be contrasted to the next simulation in which the pipe is treated as a conducting solid with conductivity=1.0e-5 and dielectric constant 2.0. The conductivity is five orders of magnitude larger than the conductivity of the fluid (the original value of 10.0 could have been used, but was changed because of an apparent convergence problem that later turned out to not be a problem).

Figure 3 shows the electric charge density in the fluid at t=0.25s. This figure is to be compared to the case shown in Fig. 1, which has a nearly constant fluid charge density perpendicular to the pipe walls while decreasing down the pipe. At the outlet, and centered between the top and bottom wall, the charge density in Fig. 3 is 4.718e-10, the same as the outlet value in Figure 1.



Figures 4a-c show a close up of the central region with the grid overlaid of the fluid charge, the solid charge and the potential.



The principal difference between the plots in Fig. 1 and Fig. 3 is the value of the fluid charge density at the surface of the pipe wall, which is roughly the negative of the value in the center of the fluid, Fig. 4a. In the first cell of the solid, Fig. 4b, the charge density is about five times more negative. Together, the fluid and solid charges at the boundary between the fluid and solid are accounting for the requirement that there must be a surface charge on the conducting solid and the electric field in the solid must be zero. The two-cell distribution of the negative charge is the best the finite volume representation can muster.

The key to the observed difference is the value of the conductivity used at the boundary between the fluid and solid. On the one hand, when the solid is specified as a pure conductor at a given potential, the value of the conductivity at the boundary with fluid is taken to be equal to that of just the fluid. On the other hand, when the solid conductor is given a finite conductivity and computations are performed in its interior, the boundary conductivity is taken to be a reciprocal average of the fluid and solid values. For a high value of conductivity in the solid with respect to that in the fluid, the reciprocal average is about twice the fluid value. Thus, in the fluid element next to a conducting solid there is more current leaving the fluid and entering the solid than is coming into the fluid element from its fluid neighbors. In the present case this causes a negative charge to appear in the fluid at the solid boundary.

Aside from the local details in charge at the fluid/solid boundary the two simulations give nearly the same results for the remainder of the fluid region. Both of these cases have the boundary coincident with a mesh grid line and it was only the treatment of the solid conductor that differed between them.

Next, the boundary of the solid is moved outwards by one half of a grid width so that the volume fraction of solid (and fluid) in the inner most grid element containing solid is one half. This element is a mixture of fluid and solid. Mixed cells are treated in the same way as ordinary fluid cells. Even though they may contain some solid that is specified as a constant potential the remaining region of a mixed cell needs to be computed to insure a proper treatment of free charge densities and potentials. Simulation results for the case where the solid is a perfect conductor are shown in Fig. 5

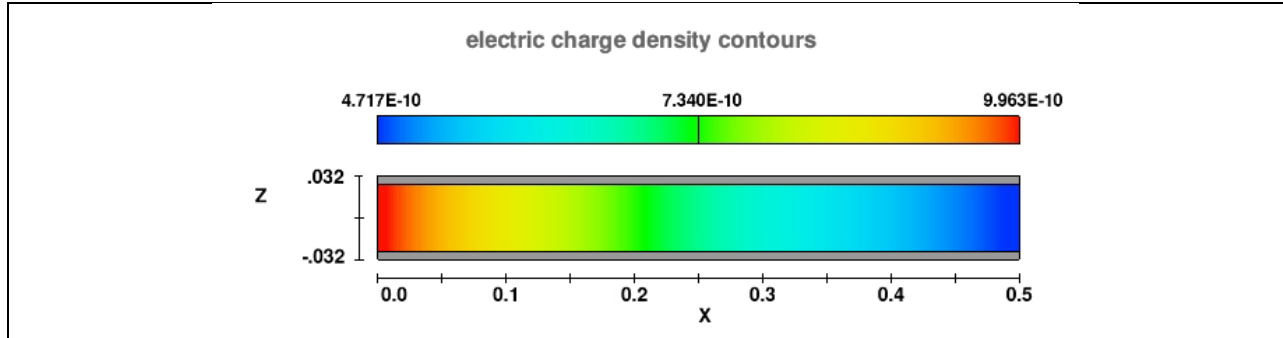


Figure 5. Fluid charge density with mixed cell boundaries and a constant potential solid.

This result looks nearly identical to those in Fig. 1. Figures 6a-b show close ups of the central region. The charge density in Fig. 6a is uniform across the pipe in the fluid region and only varies slowly along the pipe axis. The central values are nearly those (within about 1%) shown in Fig.2a, although the scale change makes this difficult to see.

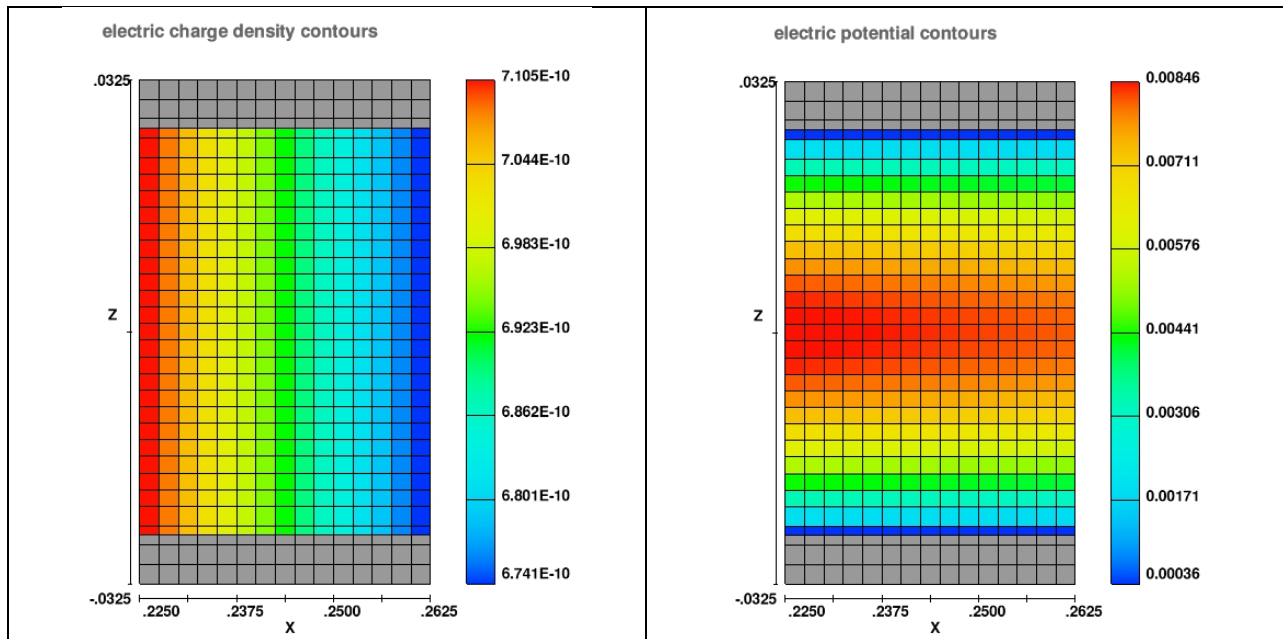


Figure 6a. Fluid charge density in central region. Note split cells at boundaries.

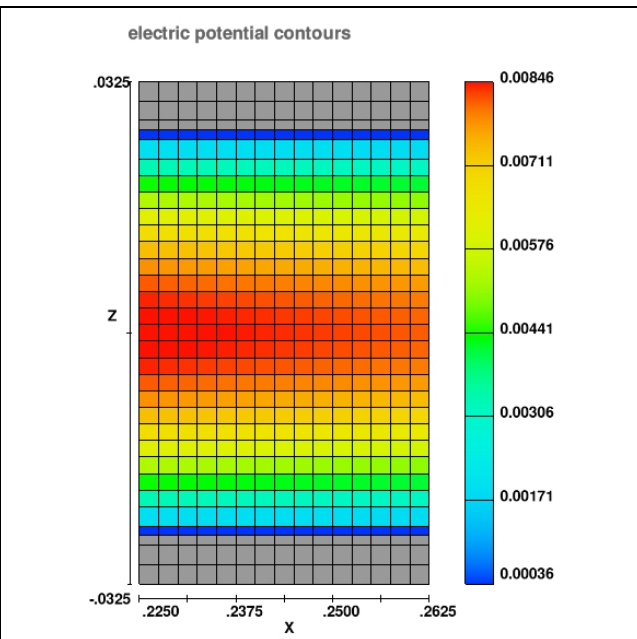


Figure 6b. Potential in the central region.

The potential shown in Fig. 6b is close to that in Fig.2b. For instance, the potential in the last full fluid cell (adjacent to the solid) in Fig.2b has a potential value of 0.00153. In Fig. 6b the potential in the mixed cell (hence, adjacent to the solid) is smaller at 0.00054, while in the last full fluid cell the potential is a little larger at 0.0025. This is what would be expected since the fluid in the mixed cell is closer to the zero potential solid.

For a last comparison using mixed cells the solid pipe is given a finite conductivity ($1.0e-5$) so that computations are carried out in the mixed cell as well as the neighboring fully solid cells. Figure 7 displays the full pipe section at the end of the simulation ($t=0.25s$) and is colored with the fluid charge density.

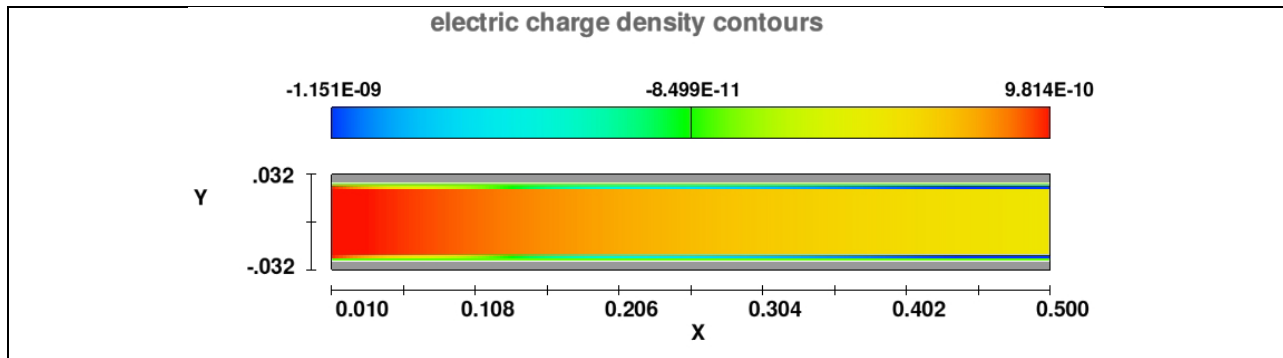


Figure 7. Fluid charge density with mixed cell boundaries and a conducting solid.

This plot is to be compared with Fig. 3 in which there were no mixed cells and the pipe was a finite conducting solid. The comparison is quite good in that the maximum and minimum charge densities are nearly identical. Both plots also show a layer of negative charge at the fluid/solid boundary and this charge is in the same grid elements. A larger negative charge is in the solid portion of the mixed cell.

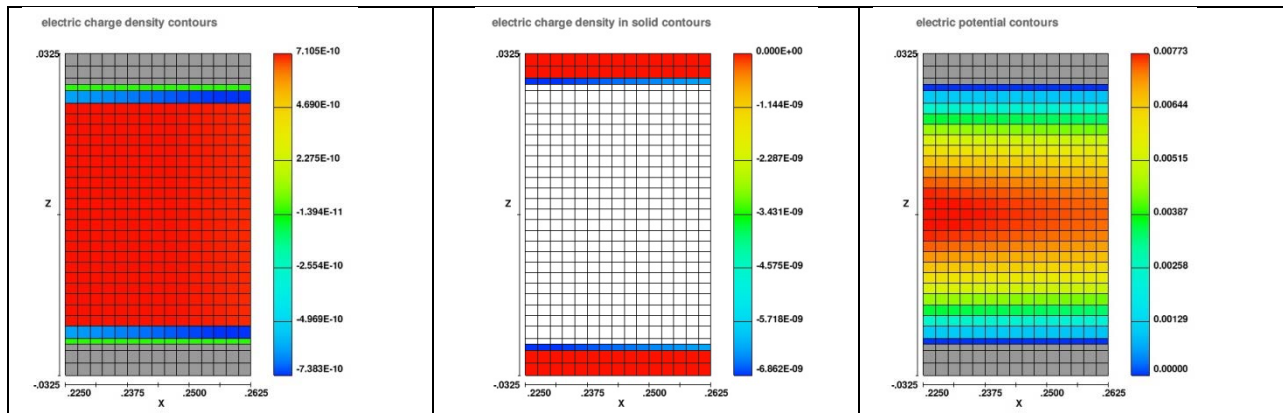


Figure 7a. Fluid charge density in central region of pipe.

Figure 7b. Solid charge density in central region of pipe.

Figure 7c. Potential in central region of pipe. Grey regions are solid having essentially zero potential.

Figures 7a-c show regions in the center of the pipe with the grid overlaid to help identify the mixed cells along the fluid/solid boundaries. These plots can be compared to those in Fig. 4a-c. It will be seen that they are quite similar to one another. The solid charge density in Fig. 7b is twice that in Fig. 4b because the solid fraction in the mixed cell is half that in the first full solid cell in Fig. 4b. This is a reflection that the negative charge at the boundary represents a *surface* charge.

Moving the interface from a grid boundary partway into a neighboring cell has not resulted in any major changes in the computed flow and electric charge and field distributions when the solid is treated as having a large but finite conductivity.

Conclusion

The comparisons of simulations described in this note show that the presence or absence of a mixed cell containing a boundary between fluid and solid does not alter the computational results in any significant way.

Comparisons between simulations using a solid with a specified potential and a solid having a large conductivity does produce some differences at the boundary. In particular, when the solid is treated as a finite conductor and has not been given a specified potential then a surface charge is computed at the boundary as required by the governing equations. This charge layer is spread over the two grid elements spanning the boundary. The remaining conductor, away from the interface has a near zero potential and zero charge density consistent with its large conductivity.

Conversely, when the conductor is specified to have a fixed potential there is no surface charge computed since none is required to adjust the field within the conductor. Computationally, this is treated by assigning the conductivity at a boundary to be equal to that of the fluid region and to not perform computations of electrical properties in any grid element filled with a fixed potential solid. In a mixed cell, one containing both a conducting fluid and some part of a fixed potential solid, the solid conductivity and potential are ignored and only the fluid (or void) portion is used in computations.

The last comment amounts to a change in the program; in previous versions mixed cells containing some fraction of a fixed potential solid were held at the potential of the solid and fluid in the cell could not then be properly taken into account.