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Addition of Dielectric Phenomena to *FLOW-3D*ò

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Overview

There are situations where it would be helpful to account for the interaction of electric fields with liquid and solid materials. For example, electrostatic air cleaners rely on the ability to attract small particles in flowing air to a surface where they can be collected and removed from the air. In this case the primary attractive force arises from dielectric polarization of the particles.

Spraying liquid drops onto a surface, as in spray painting, is often improved by electrifying the drops so that they repel one another and produce a more uniform distribution. Also, electrified drops can be driven to overcome air resistance by suitable electric fields.

In many types of micro-electrical-mechanical-systems (MEMS) fluids are caused to move by the application of electric potentials. Usually this behavior is induced by electric forces acting on dielectric polarization charges generated at free fluid surfaces or at the interfaces between two fluids.

In some situations the effects of both dielectrically induced charges as well as free electric charges in a fluid must be considered. For these cases the fluid has some non-zero conductivity that must be accounted for by tracking charge densities and adding additional body forces to the fluid. The range of possibilities when conduction is present includes bound and free charges, recombination, ionization, currents without net charge densities, etc. As described next, we shall limit the present development to a useful subset of the many possibilities.

In this note we describe a set of program developments that give ***FLOW-3D*ò** the capability to model fluid and particulate flows involving both free and induced charge densities. In the current released version of ***FLOW-3D*®** (Ver. 7.7) both particles and fluid can contain a fixed charge density, but there is no provision for dielectric materials. Here we describe the addition of dielectric properties for particles, fluids, and solids. In addition, linear polarization forces acting on particles and fluids by electrostatic fields are added to the momentum equations for fluid and particles.

Developments

The developments have been separated into several parts.

Part I – Adding Dielectric Effects

For electrostatic problems in regions other than free space it is necessary to define the dielectric properties of the region. When the region is homogeneous the appropriate permittivity can be input using *elperm*. For more general situations it is necessary to define the permittivity distribution, or what is equivalent the dielectric constant distribution, for all regions in a computation model. For this purpose the dielectric constants are stored in a new scalar array having index *idiel*, which is a new input parameter. A positive, non-zero value of *idiel* is the flag that indicates non-uniform dielectric properties.

Associated with variable dielectrics there may be polarization forces. We assume that polarization is always linear and proportional to the electric field. This makes the resulting forces proportional to the gradient of the square of the electric field,

$$\vec{F} \propto \nabla E^2$$

To facilitate the evaluation of these forces we compute the square of the field strength at the same time the electric potential is evaluated and store it in an available scalar array. No new scalar arrays are needed because there are already two scalar values (old and new) that are kept for each scalar quantity. Thus, we can make use of the old-time array associated with the dielectric constant.

Part II – Adding Dielectric Forces to Mass Particles

We assume that the polarization of a particle is linearly proportional to the strength of the electric field, and can be described with a dielectric constant for the material of the particle, κ_p. The net force on the particle then reduces to a value that is proportional to the gradient of the square of the electric field strength as mentioned earlier.

This force must account for the dielectric constant of the material constituting the particle, κ_p, and whether it is larger or smaller than the dielectric constant of the surrounding medium, κ. The force on a particle assuming that the particle does not significantly affect the electric field is (see H. Pohl, "Dielectrophoresis", Cambridge University Press, Cambridge, 1978),

$$\vec{f} = 3V_p e_0 \left(\frac{k\left(k_p - k\right)}{2k + k_p} \right) \frac{1}{2} \nabla E^2$$

Here V_p is the particle volume and ε_0 is the permittivity of free space (vacuum). It should be observed that there is no force when the dielectric constant of the particle equals that of the surrounding medium. Also, the force changes sign depending on whether the particle dielectric constant is larger than or smaller than that of the surrounding medium.

The flag indicating that dielectric forces are to be included is a positive (non-zero) value for the dielectric scalar *idiel.* The input value for κ_p will be *dielpr*, which will have a default value of unity.

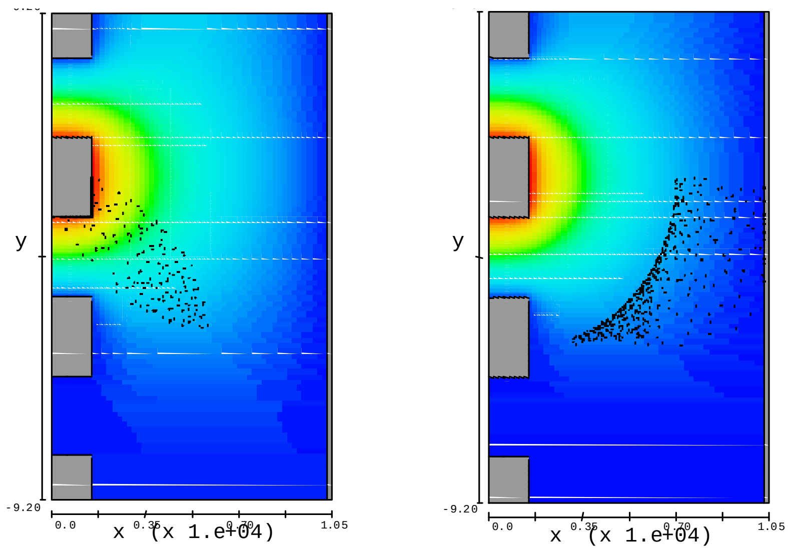

Figure 1. Two cases of dielectric forces acting on mass particles. Only the dielectric constant of the particles has been changed between the two cases.

Figure 1 illustrates this capability for a two-dimensional array of particles. On the left of each plot are electrodes all having a zero potential except for the third one from the bottom, which is at 100 volts. At the right side is a conducting layer at zero potential. The computational region is 105µm wide and 184µm high. Initially, the particles are in a rectangular array in the middle of the flow region. After a short time the particles will either move away from or toward the charged electrode depending on whether the particle dielectric constant is larger or smaller than the dielectric constant of the surrounding fluid. The plots in Fig.1 show an example of each case.

Part III – Adding Non-Uniform Dielectric Constants

For liquids with free surfaces that have dielectric constants different from that of air, or for two liquids having different dielectric constants, the evaluation of electric potential currently in ***FLOW-3D®*** is not correct. Non-uniform dielectric properties require a change in the potential equation, but the basic solution strategy remains unchanged.

We introduce new input values for the dielectric constants for each fluid in one and two fluid cases. The values within each fluid are constant and denoted by *dielf1, dielf2.* The although that restriction could be relaxed at a later time. The reference permittivity constant for void (or vacuum) regions is denoted by the parameter ε_0 (input as *elperm* formerly denoted by *diele*).

The potential equation that accounts for spatially changing dielectric constants κ is,

$$\nabla \bullet (k \nabla f) = -\frac{r_c}{e_0}.$$

The electric field is still the gradient of the potential, **E**=-∇ϕ.

In the numerical scheme, where potential gradients are evaluated at the faces of control elements, it is necessary to have a local value for the dielectric constant. Generally, this value is computed as the reciprocal average of the dielectric values in the elements on either side of the face.

At the surface of a conductor we use the average dielectric constant for the element in contact with the conductor at this surface. This is consistent with the current practice of assigning potential values to conductors and using them as fixed boundary values.

If the dielectric fluids can be polarized by an electric field they are subject to forces that must be included in the fluid momentum equations. If the fluids are linearly polarized as characterized by a dielectric constant $\kappa=\varepsilon/\varepsilon_0$, where ε is the permittivity of the fluid, the polarization density vector **P** is given by

$$\vec{P} = e_0 (k - 1)\vec{E}$$

The corresponding force density generated by polarization is then,

$$\vec{F} = \frac{1}{2} e_0 (k - 1) \nabla E^2$$

An example of variable dielectric properties is given by the dielectrophoresis of a drop of one fluid immersed in another fluid in the presence of an electric field. For illustration purposes only a two-dimensional example is considered. The arrangement is the same as for Fig. 1 except there is a drop (cylinder) of fluid with dielectric constant 80 (water)

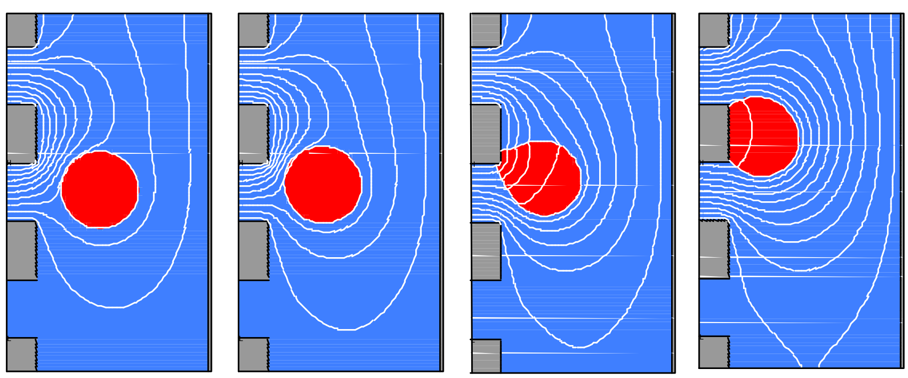

Figure 2. Dielectrophoresis: Drop is attracted to charged electrode.

surrounded by a carrier fluid having dielectric constant 4. Dielectric forces move the drop to the charged electrode. It can be observed that the drop also influences the potential distribution.

Part IV – Adding Dielectric Obstacles

To compute electric potentials (and fields) in obstacles it is necessary to devise a test to separate solid conductors from solid dielectrics. For this purpose we use a zero dielectric value in conductors. This provides a simple quantity to test on to avoid the computation of the electric potentials in conductors. Since a zero value is non-physical it further emphasizes that the value is meant to be a flag and not a real value. The graphical display of potentials in obstacles and fluids will eventually require some changes in the ***FLOW-3D***® plotting options because solid and fluid regions are usually mutually exclusive when it comes to plotting. For the time being, users can manually turn off "blanking variables" to make plots of the potential in both obstacle and fluid regions.

Figure 3. Electric field in the presence of dielectric solid (covering electrodes) and two dielectric fluids.

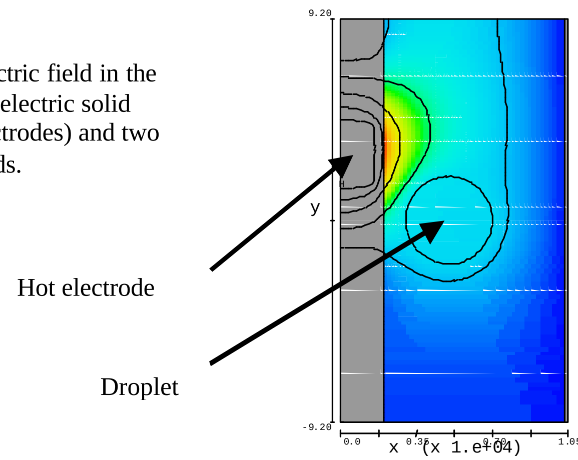

Figure 3 shows and example having a dielectric solid. In this case the solid covers the electrodes, which are not visible in the plot. Otherwise the arrangement is the same as in Fig. 2.

Part V – Conductivity in Liquids

To model situations involving perfectly conducting liquids that remain at fixed potentials, such as in the Taylor Cone experiment, we propose that users simply use a large dielectric constant. This will produce a nearly constant potential within the fluid and has the advantage that when the liquid is in contact with a solid conductor it will assume the same potential as the conductor.

Summary

A variety of program extensions have been described that give ***FLOW-3D***® many new capabilities. It is anticipated that these extensions will find wide use in the rapidly expanding area of MEMS devices, which often make use of electric fields to move and control small amounts of liquid.

A guideline used for many of these developments was the text "Fundamentals of Applied Electrostatics," by Joseph M. Crowley, Laplacian Press, CA 1999.