FSI-00-TN52(Rev3/01)

SELF-CONSISTENT ELECTRIC FIELDS AND ELECTRIC FORCES ON CHARGED PARTICLES

Flow Science, Inc.
January, 2000

SCOPE

A recent addition to the computational fluid dynamics program ***FLOW-3D***® is a capability for modeling discrete mass particles moving through a continuum. This model implicitly couples the particles and continuum so that they may exchange momentum in a conservative way.

This report addresses how that model has been extended to account for mass particles having an electric charge and moving in an electric field. The extension is self-consistent in the sense that the particle charges contribute to the electric field. For this reason the field is time dependent and must be recomputed for each time step of a numerical simulation.

In addition to the charged particles, solid objects (obstacles) located within the computational region may be assigned arbitrary, but constant in time, potentials. Each obstacle may have a fixed potential value consistent with the obstacle being a conductor. A zero potential value is the default value if not otherwise specified. It should be noted that an electric potential can be computed even when there are no charged particles, although this field will have no effect on flow processes unless the user adds some kind of additional interaction to the model.

Mesh boundaries that are rigid walls may be assigned non-zero potential values. All other boundaries are treated as symmetry boundaries with respect to the potential. Furthermore, no insulated obstacles are allowed in this model. It is also assumed that if there are free fluid surfaces or fluid-fluid interfaces then the dielectric constants (i.e., ratios of material permittivities to that of vacuum) of the different materials must be the same, otherwise additional development will be needed to solve for the electric potential. In general, this is not correct because the dielectric constant does vary with material type; for example, water has a dielectric constant about 81 times that for air.

NEW DEVELOPMENT SUMMARY

A capability for calculating a self-consistent electric potential has been added to ***FLOW-3D***® according to the governing equations:

$$\vec{F}_i = e_i \vec{E}$$

$$\vec{E} = -\nabla f$$

$$\nabla^2 f = -\frac{4pr}{e}$$

The first equation gives the electric force acting on particle "i" having an electric charge of e_i as the product of the charge times the electric field intensity. This field can be computed as the gradient of a scalar potential ϕ (second equation). Finally, the potential is obtained from the solution of a Poisson equation having a source term proportional to the electric charge density ρ (i.e., electric charge per unit volume) divided by the permittivity constant ε for the continuous medium (last equation). For the present development it has been assumed that every mass particle will have the same total electric charge. This could be changed in the future to either make the charge proportional to mass, or to add a new property to mass particles that would allow for any charge amount.

The boundary conditions for the potential are symmetry conditions at all boundaries of the computational region unless the boundary is a rigid wall, in which case the potential can be set to a non-zero value. Obstacles within the computational region can be given specified values for the electric potential. The default potential for obstacles is zero.

Adding an electric potential to ***FLOW-3D***$^{®}$ has been done using the basic scalar-variable capability existing in the program. The electric potential is assigned to the scalar having index ***iepot***, which is set in the input file to whatever number is the next available scalar index. Actually, there are two arrays used in the program for each scalar variable, one corresponding to the new time-level values and the other to old time-level values. The two levels are used for the general scalar case in which it is necessary to keep old values available for computing advection and diffusion effects.

For the electric potential there is no advection or diffusion, and this fact simplified the development because the new time-level array could then be used for the potential and the old time-level array for storing the electric charge density (i.e., the density of charged particles).

An alternating-direction scheme is used for the solution of the Poisson equation defining the potential. The convergence level of the iteration method is controlled by the input parameter ***epsele***, which has a default value of 0.01. Convergence is achieved when the maximum change in the potential during an iteration is less than ***epsele****RES, where RES is the maximum cell residual computed during the first iteration pass.

A new routine has been added to the program to compute the electric potential. This routine, ***epot.for***, consists of three parts. First, values for the potential are assigned to every mesh cell that contains an obstacle or any piece of an obstacle. These are the "boundary" values for conducting obstacles. The value assigned to the cell is the value input for the obstacle residing in that cell, ***oepot***. This value may be time dependent.

Second, charge densities associated with each computational grid cell are evaluated. For convenience, what is stored in the old time-level scalar array is what is needed for the source in the Poisson equation, namely the product of the electric charge density times 4π divided by the permittivity constant, ***diele***.

Finally, the last and largest part of the new subroutine consists of the ADI Poisson solver that computes the potential in all grid cells that contain no obstacles, i.e., in VF=1.0 cells. No provision has been made to make ADI sweeps in only one or two directions, as is done for fluid pressures. This could be added at a later time, as could an SOR solver, if it appears that such options would be useful.

Once the potential has been computed, the remainder of the computational time cycle proceeds without change, except for the inclusion of electric forces on the mass particles. These are evaluated whenever the particle charge, ***echrg***, is not zero. The force is computed as the product of the charge times the gradient of the electric potential at the center of the cell containing the particle.

In order to account for the presence of solid boundaries and/or baffles across which potential gradients should not be computed, the cell-centered potential gradient is computed as an area-weighted average of the boundary gradients, e.g., in the x-direction this gradient is evaluated as,

$$\left(\frac{\partial f}{\partial x}\right)_i = \left[Ax_{i+1/2}\left(\frac{f_{i+1}-f_i}{dx_{i+1/2}}\right) + Ax_{i-1/2}\left(\frac{f_i-f_{i-1}}{dx_{i-1/2}}\right)\right] \Big/ \left(Ax_{i+1/2} + Ax_{i-1/2}\right)$$

Area weighting has the effect that if one of cell boundaries is closed off (i.e., has a zero area fraction, Ax=0), then the gradient in the cell is the value computed at the other side of the cell.

USING THE ELECTRIC POTENTIAL MODEL

To make use of an electric potential, the user must input in Namelist SCALAR an index , ***iepot***, for the scalar function to be used for the potential. A non-zero index is the flag used to activate the computation of the potential.

It is also possible to define in the same SCALAR Namelist the material permittivity constant, ***diele*** (value depends on selection of units and material in), and the convergence criteria for the potential Poisson equation solver, ***epsele*** (default value 0.01).

Potential values can be set for rigid wall mesh boundaries (i.e., for type 2 boundaries) using the scalar boundary condition values, SCLRB(m,n), located in Namelist BCDATA. Potentials can be defined for each obstacle within the grid using the parameters ***oepot***(t,m) for obstacle number m at time point t. Obstacle potentials are set in Namelist OBS. The default potential for obstacles and wall boundaries is zero.

Finally, if charged particles are present that alter the potential and are affected by the electric field, this is indicated in Namelist PARTS by setting the particle electric charge, ***echrg***, to a non-zero value (either negative or positive). Of course, if the particles affect the surrounding flow, it is also necessary to set the implicit fluid-particle coupling flag, ***impprt***=1. In any case, charged particles will affect, and be affected by, a potential whether or not they are coupled to the surrounding fluid.

If charged particles enter a computational grid cell containing an obstacle, they are neutralized because obstacles are conductors. Neutralized paticles do not contribute to the potential.

Output for a computed electric potential can be viewed (or plotted) as the scalar function that was selected by ***iepot***. Also, the number of iteration passes required to solve for the electric potential is designated by "itpot" and is printed with short prints in the summary file, hd3out.dat.

A WORD ABOUT UNITS

Most people use the MKS system of units for electrostatic and electromagnetic problems. In this system the standard unit of charge is the coulomb and the unit of potential is the volt. Electric field intensities are measured in newton/coulomb in the MKS system. When using the CGS system of units, it is customary to express charge and potential in the "electrostatic" units of statvolt and statcoulomb, where

$$1 \text{ coulomb} = 2.998 \cdot 10^{9} \text{ statcoulomb}$$

$$1 \text{ volt} = 3.336 \cdot 10^{-8} \text{ statvolt.}$$

Electric forces are then,

$$1 \text{ newton} = 1 \text{ coulomb* volt/m} = 10^{5}\text{dyne}$$

$$1 \text{ dyne} = 1 \text{ statcoulomb*statvolt/cm} = 10^{-5}\text{newton.}$$

To connect the units of charge with other physical quantities it is necessary to assign the proper value to the vacuum permittivity ε_0,

$$\varepsilon_0 = 8.854\ 10^{-12} \text{ coul}^2/\text{joule} \cdot \text{m in MKS units}$$

$$\varepsilon_0 = 7.958\ 10^{-3} \text{ statcoul}^2/\text{erg} \cdot \text{cm in CGS units.}$$

SAMPLE ILLUSTRATIVE PROBLEMS

In this section we present some very simple problems that illustrate the basic features of the new model.

Potential between an Obstacle and Boundaries

A circular cylinder is placed at the center of a square cross-sectioned channel. Walls of the channel are grounded and, therefore, given a zero potential. The cylinder is assigned a potential value of 50. Figure 1 shows the potential contours generated. There are no particles in this computation and no flow develops. The contours are consistent with the specified boundary potential and the geometry.

Charged Particles inside Grounded Channel

The same grounded, two-dimensional channel used above forms a container for a block of charged mass particles. That is, the cylindrical obstacle has been removed and replaced by a rectangular block of mass particles. The particles are assumed to be in a vacuum so there is no surrounding fluid to interact with. There are 400 particles in the block each with a negative unit charge (the sign of the charge only changes the sign of the potential with respect to the zero potential walls).

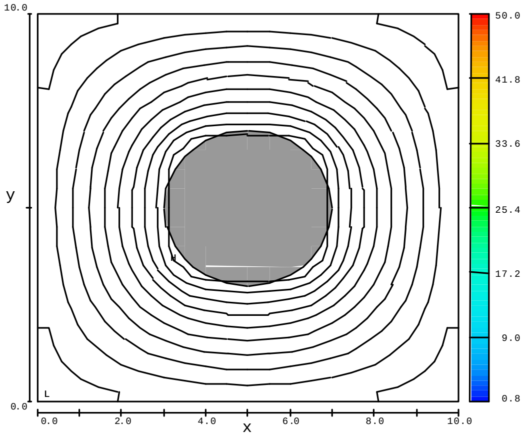

Figure 1. Contours of electric potential between a cylinder and grounded walls.

Figure 2 shows four frames of the evolution of the particles as they fly out onto the channel walls and are neutralized. Color shading indicates the electric potential.

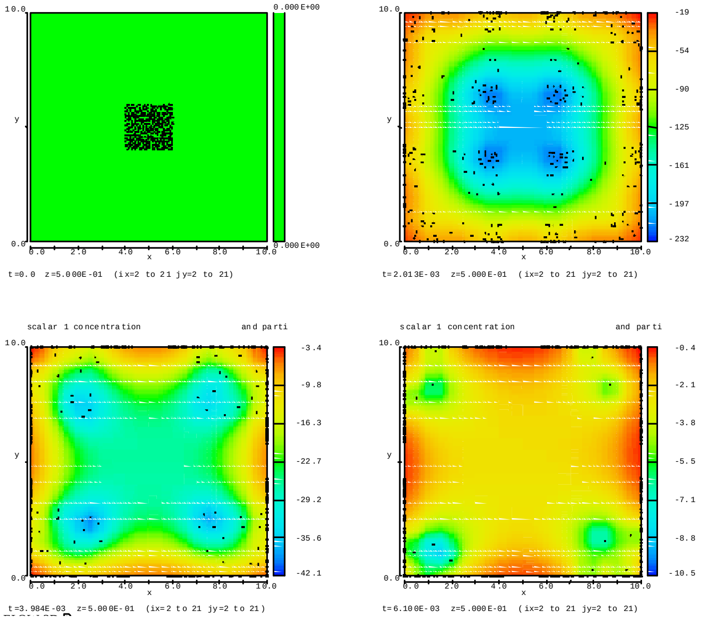

Figure 2. Charged mass particles inside of a grounded, square channel. Particles are neutralized when they hit and stick on the channel wall.

There is some grouping of particles seen in the second frame because of grid effects. The grid is 20 by 20 and there are no fluid drag or diffusion effects to smooth out the cell-to-cell repulsive forces between particles. This is a good reminder that it is not individual particles that repel one another but the electric forces generated by the net charge densities in cells.

Charged Particles Coupled with Surrounding Fluid

The next example is a repeat of the previous one except that the particles are placed in a fluid and coupled to it. In this case the particle charge was reduced to 0.1 and the fluid was water so that the 0.02cm diameter particles would experience enough drag to lengthen the time scale to a few milliseconds. With more charge, or less drag, the particles fly to the walls of the channel (10 cm square) extremely quickly.

Figure 3 is a snapshot at t=10ms that shows the particles spreading out more uniformly because of their interaction with the water. The water velocities appear a little mixed, but a closer look indicates that they are quite reasonable. Perfect symmetry is not achieved because the initial particle distribution contains some random placement. The basic flow pattern has fluid moving outward with the particles toward the corners of the channel. Because water is incompressible, there are return flows to the center coming from the midpoints of the sidewalls. The color shading in the plot is the electric potential.

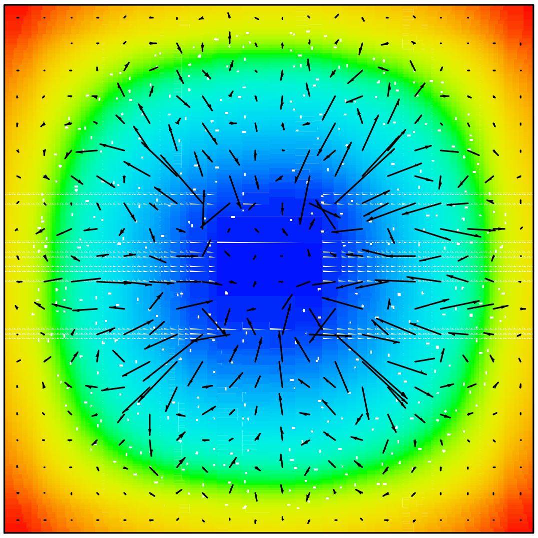

Figure 3. Charged particles moving in water with grounded side walls.

An Electrostatic Scrubber

As a final example we have chosen to model an electrostatic scrubber consisting of two parallel plates 50 cm long and spaced (face to face) 6 cm apart. One plate is grounded and the other is at 100 volts. An air flow of 100 cm/s external to the plates is applied as a boundary condition. Between the plates the average flow speed is somewhat higher at 135cm/s because of the blockage of the flow channel by the plates.

A source of charged mass particles was placed at the left of the computational region. Four sizes of particles having diameters between 0.02cm and 0.08cm were generated and all were given an initial velocity of 135cm/s, so that they had little relative velocity with respect to the airflow. The particles had the same electric charge of 0.001coul. This is rather large, but we have also used a rather low voltage between the plates for this sample problem that is only intended to illustrate the possibilities of the new model.

In Fig. 4, which shows computed results after 1.0s of simulation time, we can clearly see how the four particle sizes have been separated and collected on the grounded (top) plate. The largest of the particles are not all collected. Some of them escape out the right side of the computational region.

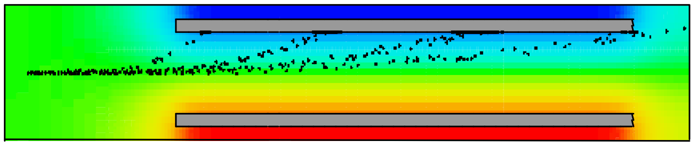

Figure 4. Example of an electrostatic collector. Four sizes of particles are flowing from left to right. All but the largest are trapped on the top plate. Some of the largest particles escape at the right side.

SUMMARY

A new addition to ***FLOW-3D***® has been described that permits the computation of an electrostatic field. This field is defined by the potentials of obstacles and/or mesh boundaries. Additionally, the field includes effects of having charged particles in the computation. These particles are subject to an electric force arising from the self-consistent electric field. Particles may be coupled with the surrounding fluid or not.

When using charged particles there is one important point to remember. Particles are inherently three-dimensional point objects. If a two-dimensional or axisymmetric problem is defined, the grid dimension in the third direction is important because it is used to compute the charge density and will therefore affect the electric-potential magnitude.

The principal limitation of the model is that only one dielectric constant can be input, so that this model is not correct for situations involving more than one type of open region. For example, it would not be proper for a case having both liquid and void regions. An extension to permit such cases is anticipated for the future.