Track Visualisation of Charged Particles in a Dipole Magnetic Field.

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Abstract: This paper presents results on the visualisation of tracks of charged particles in a non-uniform magnetic field. The field modelled is that generated by a coil driven by DC current. The model was generated in 2D axial geometry in order to conserve computing resources. Visualisation of the track was done using the Lorentz force model. The gravity force was ignored, even though it would be simple to add it. The motion of typical particles, such as electrons, ions and multiply-charged heavy particles has been simulated.

The motion is initially assumed to be in vacuum, so that collisions with neutral particles can be ignored. This could simulate for example the motion of auroral particles in the higher atmosphere.

Results are also presented for ambient atmospheric pressure conditions by introducing the weakly compressible Navier-Stokes flow equations. This simulates particle flows in man-made devices such as ion generators.

Keywords: Charged particle tracks, magnetic fields, Lorentz force, aurora, ion generators.

1. Introduction

The subject of the motion of charged particles in magnetic fields is a fascinating one. It occurs in nature e.g. in the aurorae and in man-made machines such as ion thrusters. It results in fascinating spiral trajectories which can be luminous resulting in stunning displays.

COMSOL has a very useful post-processing facility which allows the study of particle trajectories in a particular field configuration. This would be very difficult if not impossible to do "directly" in view of the fact that (a) there is usually a very large dimensional difference between the main model and the particles and (b) it is not necessary to study in detail the conditions around the particles – in terms of subdomains and boundary conditions. Further more, it is possible to simulate "massless" particles, which map the field lines and also launch a large "bundle" of particles, which gives good insight into the shape of streamlines, vortices, etc.

The paper describes fairly simple physical problems that illustrate the power of COMSOL and are highly educational in nature.

The magnetic field model is that generated by a solenoid driven by DC current. Stylised lines of force are shown in the following 2D sketch.
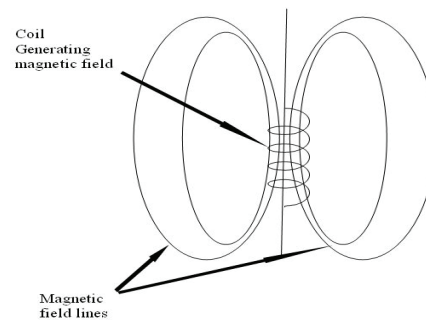

Fig.1. 2D sketch of the magnetic field generated by a coil

The lines of force are intended to give a rough idea of the geometry and are not an accurate depiction of the actual field. This depends on the dimensions of the coil or magnetic dipole that generates it and is affected by the boundary conditions e.g. shape and size of bounding box, as will be seen later.

Two scenarios are considered, in relation to the generated models.

(1) Motion of charged particles in vacuum, Magnetostatics physics only, and
(2) Motion of charged particles in a flowing gas. Magnetostatics + Weakly compressible Navier-Stokes physics.
Electric fields are ignored in this study.

2. Governing Equations

2.1 Magnetic field generation

In both models the magnetic field is generated by selecting the Physics (application environment) AC/DC module, Quasi-statics, magnetic / Azimuthal Induction currents vector potential. The model of the coil field is derived from a COMSOL application [ref. 1]. There is good description of this model there and will not be repeated here. The coil was simulated as an entity, rather than as a collection of individual turns.

Simulation was done in 2D axial symmetry and therefore the coil appears as a line (see Fig. 2). This, if revolved by 360 degrees around the vertical axis of symmetry, would become a cylindrical surface in 3D space.
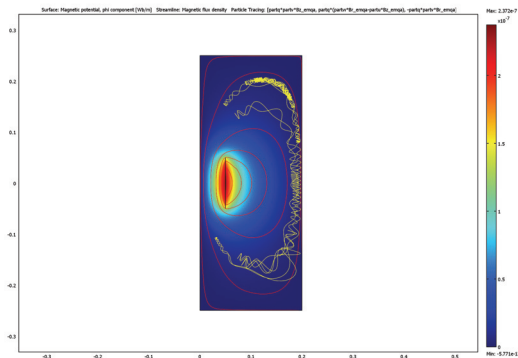

Fig. 2 Surface plot of the magnetic potential's φ component, in Wb/m. Streamlines show the magnetic flux density (B). The particle tracing (in yellow) shows the trajectory of an electron

Since the plot labels are too small to read, here are the details: X-axis and Y-axis 0.1 m/ div. Box dimensions X: (0 - 0.2), Y: (-.0.25 - + 0.25) m. False colour scale: Dark blue: 0, Dark red: $2.37 \cdot 10^{-7}$ Wb/m.

The coil is driven with 1 A dc current and has a "surface current density" = 10 A/m.

This plot shows a simulation of the motion of an electron with the following parameters:
Mass: partm = 9.1E-31 kg, charge: q = 1.6E-19 C. This is launched from an initial position (r,z) = (0.1, 0.2) m and an initial velocity (partu, partv, partw) = (0,0,-1) m/s.
Due to the rather low (default) relative tolerance, the "width" of the spiral (Larmor diameter) is exaggerated, in order to improve the viewing

clarity. Several reflections of the spiral path near the two "poles" can be seen. The electron keeps oscillating between the two poles of the magnetic field in a yo-yo like fashion.

The reason for the reflection of the spiralling trajectories is simple. Where the magnetic field lines converge, there is an "inwards" radial magnetic component. This interacts with the current element of the orbit to generate a decelerating force. This gradually reduces the drift velocity of the guiding centre of the helical tracks until it become zero and then changes direction. This process continuous at every field convergence node, giving rise to the oscillatory nature of the trajectory.

Note: The axis of symmetry in Fig 2 is the vertical axis. This in mathematical convention is assumed to be z-axis. However, in COMSOL this is assumed to be the y-axis. This can easily lead to confusion and wrong equations! The modeller is urged to be very conscious of this unusual convention. There is some indication that COMSOL might change this in future to conform to universal mathematical conventions. The strength of the field is specified via the current density flowing through the coil structure. The simulation is static, for simplicity, and therefore skin effects are ignored.

The governing equations for the magnetic field can be seen by inspecting the subdomains in the COMSOL environment.
This is:

$$(j\omega\sigma - \omega^2\varepsilon_o\varepsilon_r)A_\phi + \nabla\times(\mu_o^{-1}\mu_r^{-1}\nabla\times A_\phi)$$

$$-\sigma v\times(\nabla\times A_\phi) = \frac{\sigma V_{loop}}{2\pi r} + J_\phi^e$$

This equation can be derived from Ampere's law subject to certain conditions [see Ref. 2, §4.5].

2.2 Lorentz Force

The motion of a charged particle was modelled by specifying the Lorentz force in the particle tracing post-processing equations.
The force equations normally appear automatically but they have been checked against theory to ensure that they are OK for the assumptions made here viz. that no electrostatic field is present and that no meridional currents

are flowing. The latter condition makes the azimuthal magnetic field Bφ =0; this is a direct consequence of the Biot-Savart law (Ref. 2) and allows considerable simplification of the force equations.

The general vector equation for the Lorentz force exerted onto a particle in a magnetic + electric field is:

$$\underline{F} = q\underline{v} \times \underline{B} + q\underline{E}$$

This equation is further simplified because of the assumption E=0. The vector cross product can be expanded in Cartesian coordinates to yield:

$$\underline{v} \times \underline{B} = \underline{i}(v_y B_z - v_z B_y) - \underline{j}(v_x B_z - v_z B_x) + \underline{k}(v_x B_y - v_y B_x)$$

Where i,j,k are the unit vectors in the x,y,z directions. In our case we deal in the cylindrical polar coordinates r,φ,z. These 3 axes are still orthogonal and therefore the same equations can be used but we have to observe the following substitutions, in order to move to the cylindrical polar co-ordinates. Also we have to make the new variable names compatible with the COMSOL nomenclature.

NOTE: COMSOL uses the prefix "part" to indicate particle variables and u,v,w for the r,φ,z velocity components. Thus partq ≡ q, partu ≡ v_r , partv ≡ $v_φ$, and partw ≡ v_z .

Also COMSOL uses the suffix "_emqa" to indicate the "physics" (Electro Magnetic Quasi(static) Azimuthal…) used in here to analyse the model. The suffix will be different for the Navier-Stokes physics environment, as will be seen later.

Thus Br_emqa ≡ B_r and similarly for the other B components.

Thus, the radial polar components of the force in COMSOL notation, and for Bφ_emqa = 0 become:

Fr = partq*partv*Bz_emqa
Fphi = partq*(partw*Br_emqa-partu*Bz_emqa)
Fz = -partq*partv*Br_emqa

These are, thankfully, identical to the equations appearing in the Particle Tracing, Equation of Motion, Force component text boxes, with the exception of the E term which was assumed to be 0 and therefore is absent.

1.3 Khan-Richardson Force

The Khan and Richardson force model [ref.3] is used in the COMSOL Navier-Stokes Physics to model the force on a particle under viscous conditions and a large dynamic range of Reynolds numbers (several orders of magnitude).

The Physical equation in compact form is:

$$F = \pi r_p^2 \rho (v - v_p)^2 [1.849(\text{Re}_p)^{-0.31} + 0.293(\text{Re}_p)^{0.06}]$$

This is translated in the COMSOL nomenclature in the following 3 cylindrical polar components:

Fr=sign(u-partu)*pi*partr^2*rho_chns*(u-partu)^2*(1.84*(abs(u-partu)*2*partr*rho_chns /eta_chns)^(-0.31)+0.293*(abs(u-partu)*2*partr *rho_chns/eta_chns)^0.06)^3.45

Fphi=sign(w-partv)*pi*partr^2*rho_chns*(w-partv)^2*(1.84*(abs(w-partv)*2*partr*rho_chns /eta_chns)^(-0.31)+0.293*(abs(w-partv)*2*partr *rho_chns/eta_chns)^0.06)^3.45

Fz=sign(v-partw)*pi*partr^2*rho_chns*(v-partw)^2*(1.84*(abs(v-partw)*2*partr*rho_chns /eta_chns)^(-0.31)+0.293*(abs(v-partw)*2*partr *rho_chns/eta_chns)^0.06)^3.45

Notice that in the Fphi and Fz force components the velocities for the particle and the flowing fluid have been mixed up e.g. (v-partw) term. This is because of the confusion between the y and z axes of rotation which led to a bug in the embedded code. The only way to get correct results (until this is corrected in the next release) is to commute the velocities as shown in the above equations

3. Model Results

3.1 Vacuum case

In the vacuum case the only force on the charged particle is the Lorentz force, as detailed in § 2.2. Three types of particles are studied:
  (a) An electron. Charge q = e = 1.6·10⁻¹⁹ C and mass m = 9.1·10⁻³¹ kg

(b) An ion of molecular mass M=56 (Fe ion) triply charged (+3e). Charge q = $4.8 \cdot 10^{-19}$ C , mass m = $9.4 \cdot 10^{-26}$ kg

(c) A large particle with radius r = $5 \cdot 10^{-6}$ m, charge q = $1.6 \cdot 10^{-16}$ C and mass m = $5 \cdot 10^{-13}$ kg

3.1.1 Electron trajectory

The results for the electron trajectory are shown on Fig. 3. This is similar to Fig.2 except that it has been rotated by 90° anticlockwise and cropped, in order to maximize viewing clarity.
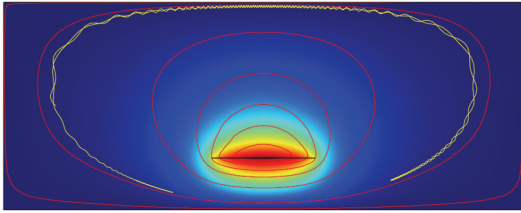

Fig.3. Electron trajectory in vacuum. Pattern rotated for clarity. The N pole original on the top of the picture is now on the LHS

There are several differences between Fig. 2 and 3 apart from the rotation. These are:

(a) The relative tolerance has been decreased from the default value (0.001) to 0.0001. This has two effects (i) to reduce the "width" of the helical trajectory – the coarse tolerance artificially increases this width. This was done intentionally in Fig. 2, in order to improve clarity and (ii) to reduce the total length of the simulated track, since each simulation step is reduced proportionately in size.

(b) the max number of steps was increased from the default value (1000) to 2000 in order to counteract the above effect
(c) the electron initial velocity and direction was changed to particle velocities (u,v,w) = (50,0,50).This was in order to counteract effect a(i) and get a reasonable helix width.
With the above parameters, the particle track starts at (r,z) = (0.1, 0.2) which lies at mid LHS of Fig 3, travels ClockWise (CW), spiralling around an invisible line of force, gets reflected back when it reaches the S pole where the field density is high travels back the N pole in a CCW direction and gets reflected again and starts

travelling CW for a short length; there the simulation stops.

3.1.2 Ion trajectory

Trajectories for triply charged Fe ions have been computed with m = $4.8 \cdot 10^{-26}$ and q = $4.8 \cdot 10^{-19}$.

In order to get similar track "widths", it is necessary to roughly match the Larmor radius. This is given by:

$$r_g = \frac{mv_p}{qB}$$

Where r_g is the Larmor radius (radius of gyration), m and q are the mass and charge of the particle, v_p is the velocity component perpendicular to the magnetic field vector B.

Thus in order to get similar spiral tracks to those obtained with the electrons the initial velocity was dropped to ~ 0.05 m/s
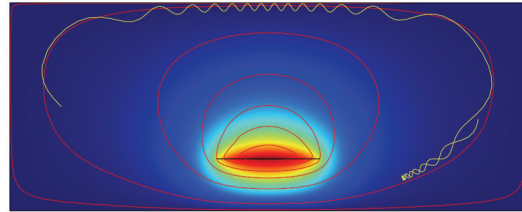The results are shown in Fig 4 below.

Fig.4 Ion trajectory in vacuum. Pattern rotated in a similar way as Fig. 3.

The parameters for this plot are: initial velocity components (u,v,w) = (0.05,0,0.05). Rel. tolerance = 0.00001 and max number of steps = 250. This allows just one CW oscillation. The reflection can be clearly seen near the S pole and then the CCW spiral overlaps the CW one.

3.1.3 Dust particle trajectory

Trajectories for a dust particle with m = $5 \; 10^{-13}$ kg and q = $1.6 \cdot 10^{16}$ C have been obtained and are shown below.
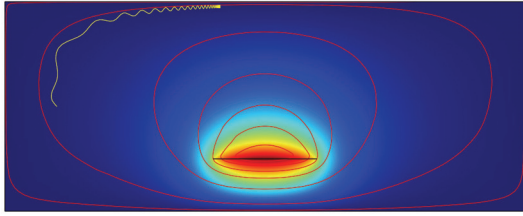
Fig. 5 Dust particle trajectory in vacuum. Axes are rotated as before.

Again, it is necessary to scale the initial velocity, in order to get approximately the same Larmor radius and hence about the same width of helical track. Because of the large dust particle mass this implies exceptionally small particle velocities viz. ~10^{-13} m/s. This implies essentially a static particle! The results are shown in Fig. 5 above. The relevant plot parameters are:
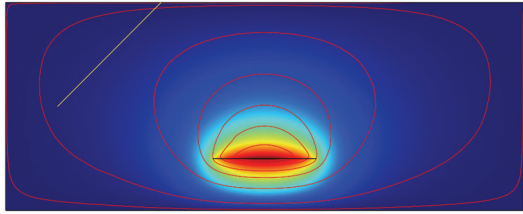$(u,v,w) = (10^{-13}, 0, 10^{-13})$, Rel. tolerance = 0.00001 and max number of steps = 250.

Fig. 6 Dust particle trajectory in vacuum. Using a more realistic velocity of ~ 0.005 m/s.

A plot is also made for a plausible velocity.
Fig. 6 shows the resulting trajectory for a velocity of ~ 0.005 m/s. Note that under these conditions the track is a straight line i.e. the magnetic field has a negligible effect.
The relevant plot parameters are:
$(u,v,w) = (0.005, 0, -0.005)$; the z component was made negative in order to get a longer track (going in a SE direction - else it would exit the plot boundary almost immediately and result in a very short track). Rel. tolerance = 0.00001 and max number of steps = 250.

The implication of the above results is the massive particles have high values of kinetic energy even at very low speeds and therefore are not appreciable affected by magnetic fields.

3.2 Ambient pressure case

This case assumes that the particles move under ambient air conditions i.e. $p \sim 1\text{Atm} \sim 10^5$ Pa.
Under this assumption, there are frequent collisions between the test particle and the air molecules. The way that collisional interactions can be modelled, depends on the size of the particle relative to the size of the air molecules and also relative to the mean free path (the average distance between intermolecular collisions). For large particles, like the dust particle that we considered above with a typical radius r ~ $5 \cdot 10^{-6}$ m, the effect of collisions can be best described, macroscopically, as a viscous force. This is because r is much larger than the typical molecular diameter (d ~ $3 \cdot 10^{-10}$ m) and also much larger than the mean free path (λ ~ $6 \cdot 10^{-8}$ m).
As discussed in § 1.3, the viscous force can be modelled under these conditions, fairly accurately, via the Khan and Richardson force equation.
In the case of the ion as the test particle the dimensions are of the same order as those of the air but it is considerably smaller that the mean free path. In the case of the electron, this is much smaller than both the air molecules and the mean free path.
The Khan and Richardson equation is not valid for the calculation of viscous forces on such particles. They can be treated macroscopically via the diffusion equations and assigned a drift velocity proportional to the strength of the driving field (be it magnetic or electric) and described via a mobility constant. These calculations are beyond the scope of this paper and will not be presented here. Suffice to say that the drift velocity depends critically on the type of particle (r, q, and m), the pressure of the air and its state of ionisation (density of neutrals, electrons, negative and positive ions). The mobility constants are very difficult to predict theoretically and rely on experimental measurements under specific conditions. Calculations are therefore very specific to the prevailing conditions.
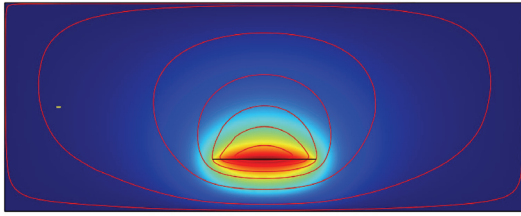
3.2.1 Dust particle trajectory

Fig.7. Dust particle trajectory in ambient atmospheric pressure. This is the small dash on the LHS of the picture, due to the quick stopping by the air molecules viscous force.

The dust particles lose their energy quickly in ambient air pressure due to the collisions with air molecules. This is described macroscopically as a viscous force. The equation for this was given in §1.3 and is knows as the Khan-Richardson equation. For a dust particle with initial velocity $(u,v,w) = (0, 0, -1)$ the track is only a few mm long and appears as a short track on the middle LHS of Fig.7. This velocity is too high in order to see any spiralling by the Lorentz force. If the velocity is reduced the track becomes so short that it is essentially invisible. It the velocity is increased, the track length increases but the spiralling effect is further reduced. Therefore it is impossible to see any spiral trajectories with this scenario (initial particle energy not replenished).

It would be possible to introduce a flow and allow the dust particle to drift with the flow. Then it would be possible to see manifestation of the Lorentz force in the particle trajectory. This is however beyond the scope of the present study.

4. Conclusions

From the above presentation, and my general experience with the COMSOL software suite, the following salient conclusions can be drawn.

1) COMSOL is a user-friendly software package. It has a good GUI and enables a professional Scientist / Engineer to formulate a complex physical problem quickly and efficiently and generate reports and stunning colour graphics in 1D, 2D and 3D.

2) COMSOL is not really suitable for the non-professional. The user has to understand the limitations of the model that he wishes to adopt and ensure that it satisfies all his requirements, else the results will be invalid. Ideally, he should be able to derive, at least confirm, all the equations utilized by the program. This will allow positive confirmation of the validity of the model and the solution. It will also ensure directly or indirectly that there are no minor (or major!) bugs, errors or omissions. COMSOL is a major software suite as such it has not been fully debugged. There is a continuous improvements process which relies heavily on user feedback.

3) The postprocessing routine of "particle tracing" is a very useful tool in not only studying the movement of various types of particles in complex fields but also in helping to visualize such field by injecting test particles. Unfortunately, it still needs a fair amount of "polishing" and debugging but it can yield excellent results as is. The predefined equations are particularly useful for quick development but the user must exercise caution, for the reasons mentioned above.

4) The 2D axial geometry is a very useful mode. It allows reduction of the mesh points and calculation nodes. This speeds up computations and allows the entry and solution of more complex models, assuming that they posses cylindrical symmetry. It also allows much easier to understand and display output graphics. Unfortunately, it has some bugs and confusing traits with the rotational conventions (confusion between the y and z axes). These hopefully will be corrected in the next release.

5) Regarding the simulation of charged particles in magnetic fields studied here, COMSOL copes very well in the vacuum case where the problem is purely electromagnetic. In the case of ambient atmospheric conditions the problem can be solved for large particles by adding the Navier-Stokes

Physics environment. In between cases e.g., the simulation of an Aurora with a variety of particles and varying pressures along the particle trajectories from near vacuum to ~ 1Atm is a very complex problem which would require special procedures – I expect it might be possible to attack this problem by writing MATLAB scripts (MATLAB - COMSOL coupling) to vary the equations as the pressure changes; also it would require different equations for different particles!

6) The present simulations show all the features in nature e.g. spiral tracks gyrating around the magnetic liens of force, drifting along the lines of force and reflections where the field becomes strongly non-uniform. As such it is a very useful educational tool even if exact quantification may be difficult for a complete simulation of, say, an Aurora.

5. References

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6. Acknowledgements