MAGNETIC NANOPARTICLE SIMULATION

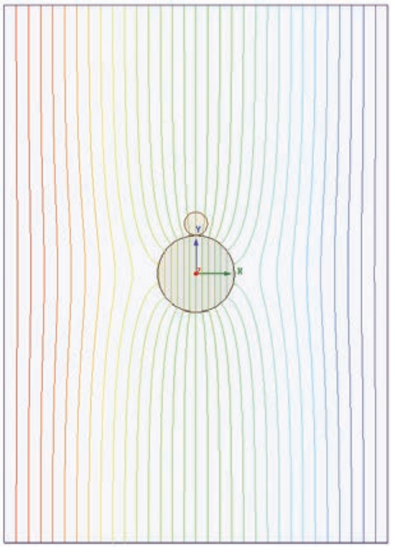
Research using simulation will help to develop biomagnetic beads for disease treatment.

By John R. Brauer, Adjunct Professor, Electrical Engineering and Computer Science
Milwaukee School of Engineering, U.S.A.

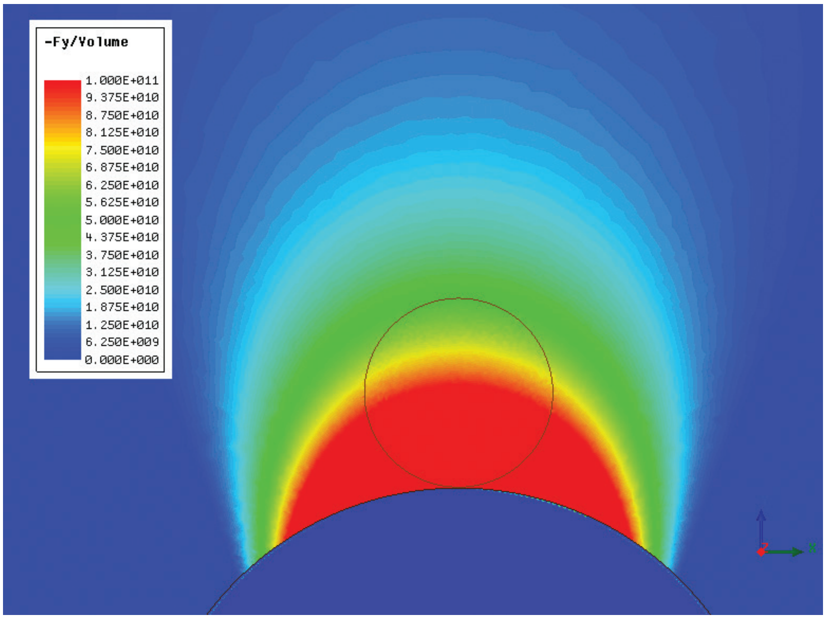
Courtesy Dexter Magnetic Technologies.

Magnetic separators are used to extract magnetic parts and particles from nonmagnetic materials. For example, recycling centers use magnetic separators to remove steel objects from other metals and nonmetals. The magnetic permeability of steel and iron is much higher than that of other materials and air, and this high permeability interacts with the magnetic field of the separator to produce a magnetic force attracting the iron or steel parts or particles. Magnetic nanoparticles are particles containing iron or iron compounds that range in size from a micrometer to nanometers.

Organizations perform extensive research applying biomagnetic beads and magnetic separators to a variety of healthcare challenges.



Magnetic separator analyzed by Oberteuffer containing a steel wire. The applied vertical magnetic field has flux lines that are distorted near the wire and particle.



Display of force density distribution on particle above the wire in separator

HEALTHCARE APPLICATIONS

Biomagnetic beads are special magnetic nanoparticles that have been developed recently for use in biomedical screening and other healthcare applications. They are spheres made of iron compounds that have a strong magnetic permeability surrounded by a thin coating made of a polymer and biological molecules. Each variety of coating will bind to a specific biomolecule so each type of bead can be used to magnetically separate a specific type of biomolecule. Biomagnetic beads can be used to screen DNA, RNA, various proteins or genes, and possibly even detect cancer cells. Several large healthcare companies and other high-technology organizations are performing extensive research applying biomagnetic beads and magnetic separators to a variety of healthcare challenges.

ELECTROMECHANICAL SYSTEM SIMULATION — BUILDING THE FUTURE
ansys.com/91nano

FORCES ON A HIGH-PERMEABILITY PARTICLE IN A SEPARATOR

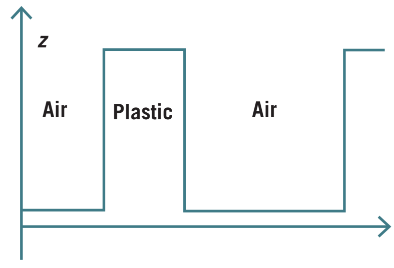
A classic magnetic separator consists of cylindrical steel wires placed in a uniform direct-current magnetic field. A classic formula by Oberteuffer has been historically used to compute the forces for both cylindrical and spherical particles. [1] To investigate the accuracy of the Oberteuffer formula, the researcher used ANSYS Maxwell electromagnetic field simulation software to compute the magnetic flux lines and magnetic force for magnetic particles with diameters of 0.1, 1.0, 2.0 and 3.0 µm (micrometers).

The permeability of both wire and particle is assumed to be 1,000 times that of air, which is typical for steel or iron. The ANSYS Maxwell analysis is a 2-D planar analysis, in which the particle — like the wire — is assumed to be a cylinder normal to the plane. As expected, the flux pattern is not symmetric above and below the wire because the particle alters the field. Unfortunately, Oberteuffer's formula does not account for such alteration by the particle; it includes only the alteration of the field by the wire itself. Additionally, the formula assumes that the magnetic flux density at the center of the particle acts on the entire particle.

To compare Oberteuffer's formula for force per unit volume with ANSYS Maxwell computations, the researcher examined the wire separator with an applied vertical magnetic flux density of 1 tesla. Various particles were considered, but all particles were assumed to be located at a radius 13.3 µm from the center of the wire. The approximate formula yields a force per unit volume in the vertical direction of -105.75×10^9 N/m^3. The negative value indicates a downward force on the particle above the wire.

The researcher carried out finite element force computations using ANSYS Maxwell. He computed the magnetic flux density without modeling the high-permeability particle and developed a fields calculator expression for ANSYS Maxwell to compute and display the force density in color.

ANSYS Maxwell's field calculator can be used to carry out volume integrals to determine the total magnetic force acting on any particular magnetic particle.



Simulation model with nearby well

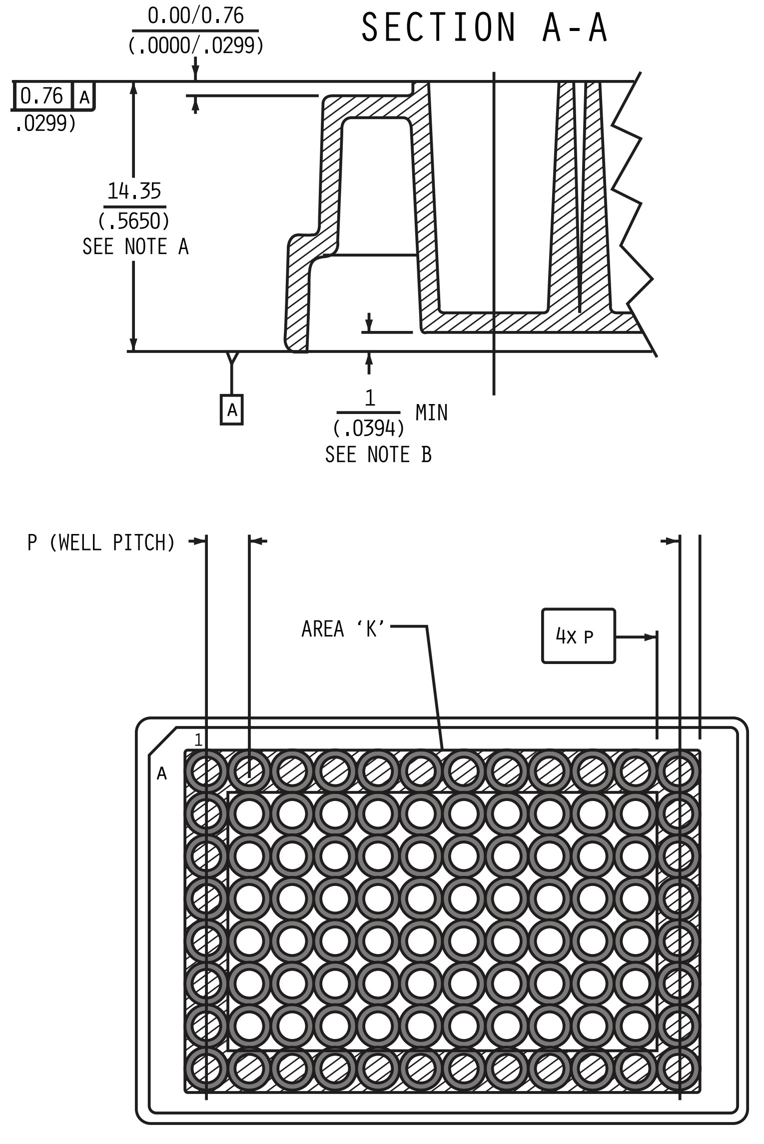


Diagram of microplate for separation of biomagnetic beads (96 wells with well pitch p = 9 mm) (top), cross section with dimensions in mm (bottom)

ANSYS Maxwell's fields calculator can be used to carry out volume integrals to determine the total magnetic force acting on any particular magnetic particle. The total magnetic forces for various particles with radii in the micrometer and nanometer range are easily calculated for the wire separator. By dividing the forces by the volumes of the cylindrical and spherical particles, the researcher obtained computed average force densities and plotted them versus particle radii. The computations using ANSYS Maxwell agreed reasonably well with Oberteuffer's formula, but the theoretical densities were all slightly smaller, within –8.46 percent to –0.12 percent, which can be explained in part by the more accurate field representation from the finite element solution. [2]

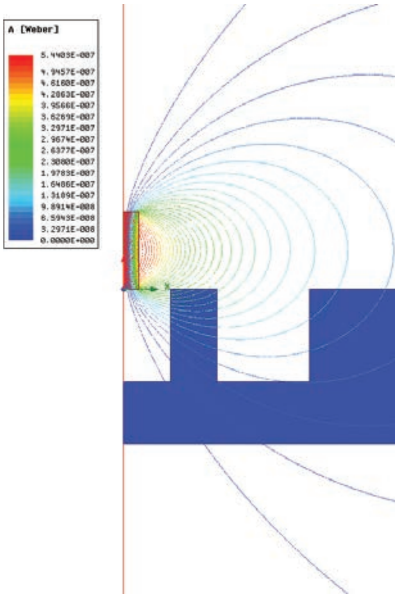
FORCE DENSITY OF A PERMANENT MAGNET SEPARATOR ON A MICROPLATE

In addition to iron separation using magnetic field gradients, a rapidly growing area of magnetic separation involves medical devices and biomolecular screening such as DNA testing. For example, high-field gradient separation is used to separate red blood cells from whole blood and to separate cancer cells from bone marrow. Other biomedical magnetic separators are being investigated to target drug delivery and to remove toxins. Permanent magnets (as opposed to electromagnets) are often used as a field source for magnetic separators; these are being investigated for biomolecular screening using standard biomolecular testing apparatus.

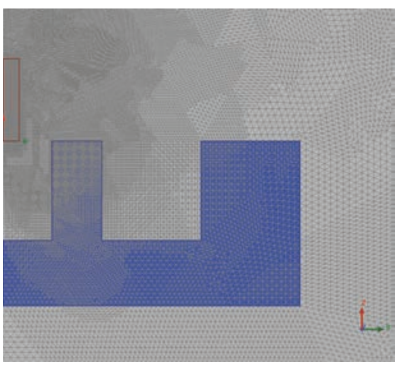
A microplate, which typically contains 96 wells, is regularly used in drug discovery, DNA/RNA testing, detection of proteins/antigens/genes and other types of biomolecular screening. A solution with suspended biomagnetic beads is placed in each well of the microplate. Biomolecular screening is possible by coating the beads with different proteins or other biological molecules so that the nanoparticles can serve as magnetic sensors. Bead diameters are often in the range of 1 μm to 4 μm, but may be in the nanometer range.

The researcher used ANSYS Maxwell to analyze magnetic force density acting on such nanoparticles in one of the wells with a permanent magnet separator immediately above it. Since permanent magnets can be made of different materials, the analysis first included a permanent magnet made of ceramic 5 ferrite and next a permanent magnet made of neodymium iron boron (NdFeB). [2]

The specific gravity of magnetic beads placed in the solution in microplate wells is less than that of iron because such particles are made of iron oxide mixed with polymers. This reduces the permeability of the nanoparticles compared to iron. Biomagnetic nanoparticle specific gravity and permeability are either unknown or proprietary and, thus, cannot be reported here. For comparison purposes, both



Cylindrical permanent magnet added to axisymmetric ANSYS Maxwell microplate model



Adaptively refined mesh

forces were computed using the properties of iron.

For a permanent magnet separator to function properly, the magnetic force density in the primary well must exceed downward force density. The downward force density is the vector sum of gravitational, buoyancy, viscous and surface tension force densities. Here the gravitational force is assumed to dominate. Since gravitational force density is of magnitude 7,644 N/m^3, magnetic force density is displayed in the range from 0 to 10,000 N/m^3.

CERAMIC 5 FERRITE VERSUS NEODYMIUM IRON BORON

First, the investigator assumed that the permanent magnet is made of ceramic 5 ferrite with a coercive field intensity H_c = 1.91 × 10^5 A/m and a permeability 1.08 times that of air. The simulation of the vertical magnetic force density shows that the 10,000 N/m^3 zone is much smaller than the primary well. Thus, over most of the well, the magnetic force density is insufficient to overcome the gravitational force density.

Next, the researcher assumed that the permanent magnet is made of neodymium iron boron with H_c = 8.9 × 10^5 A/m and a permeability 1.1 times that of air. The vertical magnetic force density simulation now has a 10,000 N/m^3 zone that is large enough to encompass most of the primary well top without affecting the adjacent well. Thus the magnetic force density overcomes gravitational force density in most of the primary well while not interfering with adjacent wells, resulting in proper magnetic separation of the microplate [2].

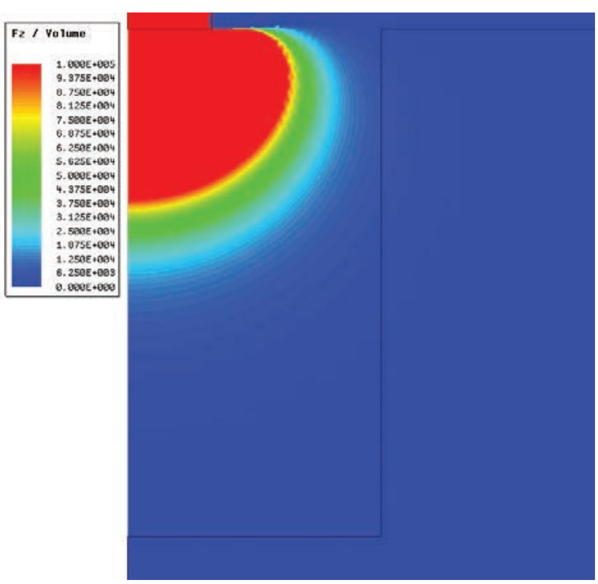
In actual microplate magnetic separation, it is accepted that neodymium iron boron magnets are needed so the force density displays agree qualitatively with observed behavior. ANSYS Maxwell computations can readily analyze many other designs of magnetic bead separators made of permanent magnets, steel and other materials.

The applications of biomagnetic beads are widely varied and rapidly growing. In addition to separation of various cell types, research into DNA extraction and genetic exploration is underway. Exosome analysis, bioassays for determining the efficacy of drugs, and regeneration of tissues such as heart muscle with the help of cell separation are among many exciting areas of research using magnetic nanoparticles.

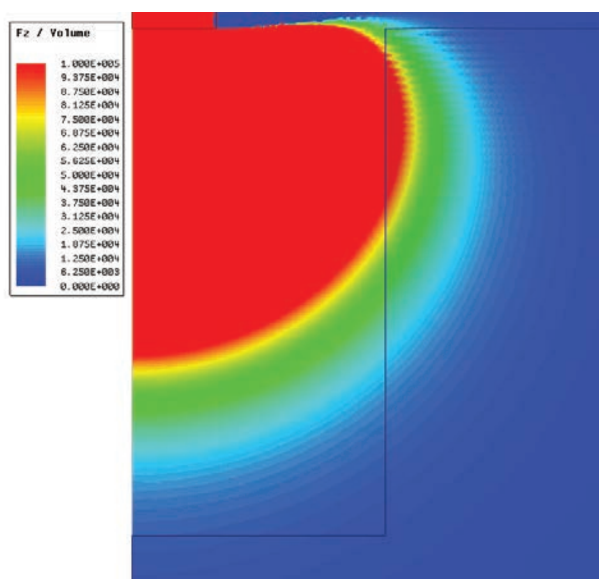
References

[1] Oberteuffer, J.A. Magnetic Separation: A Review of Principles, Devices and Applications. *IEEE Trans. Magn.* **1974**. Vol. MAG-10, No. 2, pp. 223–238.

[2] Brauer, J. R. *Magnetic Actuators and Sensors*, 2nd Ed., Wiley IEEE Press, **2014**.



ANSYS Maxwell-computed force density for ferrite magnet (H_c=1.91 × 10^5 A/m)



Computed force density for NdFeB magnet (H_c=8.9 × 10^5 A/m)