A Modified Computer Model of a Hyperbolic Energy Analyzer to Determining Its Potential for Operating as a Mass Spectrometer

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Abstract *— Conventional energy analyzers are used as a plasma diagnostic tool for the determination of ion and electron energy spectra and temperature, having applications in a broad range of disciplines, including molecular spectroscopy, electron microscopy, and plasma physics. In addition, in specific commercial applications in which plasma characteristics such as high density and high temperature may affect the optimization of a process, the hyperbolic energy analyzer (HEA) was developed. The HEA consists of three components: a plane parallel disc with interchangeable diameter orifices for rejection of electrons and collimation of the ion beam; a dual hyperbolic lens for particle energy selection and beam focusing; and a Faraday cup as the collector. If a potential V_R is imposed on the hyperbolic lenses, then only paraxial ions with energy greater than qV_R can pass through the lenses and into the Faraday cup, while the remainder of the ions are discriminated against. Furthermore, while traveling through the instrument, charged particles are exposed to both magnetic and electric fields, giving a hyperbolic energy analyzer the potential for operating as a mass spectrometer, making this characteristic the objective of this research. Results from computer simulations have indicated that both the standard and the modified hyperbolic energy analyzer models can discriminate different charged particles against energy as well as separate them from a beam according to mass-to-charge values.*

Key Terms — *Concentric Faraday Cup, Equipotential Surfaces, Hyperbolic Energy Analyzer, Hyperbolic Lenses, Mass Spectrometer.*

INTRODUCTION

Conventional energy analyzers are used as a plasma diagnostic tool for the determination of ion and electron energy spectra and temperature, having applications in a broad range of disciplines, including molecular spectroscopy, electron microscopy, and plasma physics, as demonstrated in [1], [2], and [3]. In addition, in specific commercial applications in which plasma characteristics such as high density and high temperature may affect the optimization of a process, the hyperbolic energy analyzer was developed, according to [1], [2], and [3]. The HEA consists of three components: a plane parallel disc with interchangeable diameter orifices for rejection of electrons and collimation of the ion beam; a dual hyperbolic lens for particle energy selection and beam focusing (Fig. 1); and a Faraday cup as the collector, according to [1], [2], and [3]. If a potential V_R is imposed on the hyperbolic lenses, then only paraxial ions with energy greater than qV_R can pass through the lenses and into the Faraday cup, while the remainder of the ions are discriminated against, according to [1], [2], and [3]. Furthermore, while traveling through this plasma diagnostic instrument, charged particles are exposed to both magnetic and electric fields, and by taking advantage of this fact, the objective of this research is to determine the potential of a hyperbolic energy analyzer for operating as a mass spectrometer as well as discriminating charged particles against energy.

Mass spectrometry (MS) is a technique for creating gas phase ions from molecules or atoms in a sample, separating the ions according to their mass-to-charge ratio $\left(\frac{m}{z}\right)$ and measuring the abundance of the ions formed, according to [4]. Also, it is an analytical technique that provides qualitative information, including the mass of molecules and atoms in samples, as well as the molecular structure of organic and inorganic compounds, according to [4]. All mass

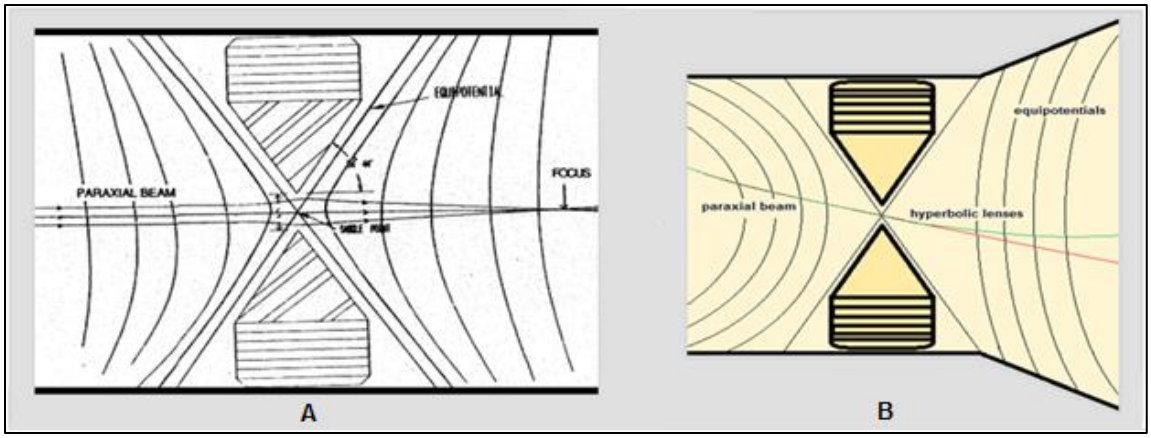

Figure 1

Two-Dimensional Views of Paraxial Beam Paths and Equipotential Surfaces near Hyperbolic Lenses for a Standard HEA Model (A) and a Modified HEA Model (B). By gradually increasing the diameter of the cylindrical wall from the hyperbolic lenses to the Faraday cup, the separation between charged particles can be either maintained or increased.

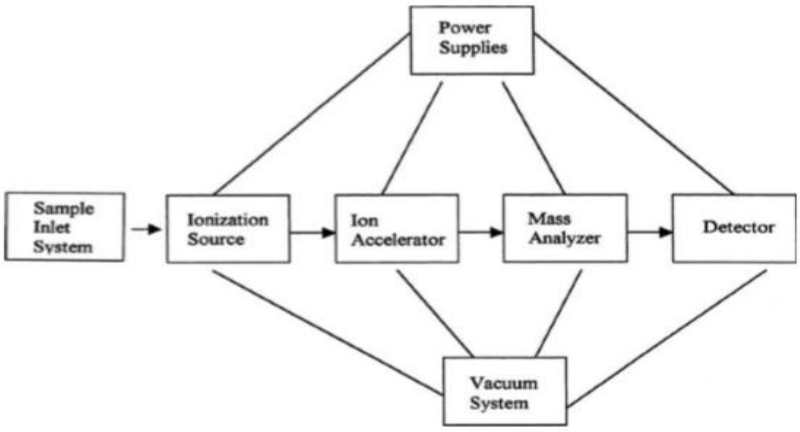

Figure 2

Block Diagram of a Typical Mass Spectrometer, as Demonstrated in [4]

spectrometers require a sample input system, an ionization source, a mass analyzer, and a detector, as shown in [4]. All of these components, with the exception of some sample input systems or ion source volumes, are under vacuum, according to [4]. A block diagram of a typical mass spectrometer is shown in Fig. 2.

The mass analyzer is at the core of the mass spectrometer. Its function is to differentiate among ions according to their mass-to-charge ratio $\left(\frac{m}{z}\right)$. Although there are a variety of mass analyzer designs, for this research, a current HEA computer model was modelled after a magnetic sector mass spectrometer, which is a single-focus mass spectrometer. In a magnetic sector mass spectrometer, the gas phase molecules in a sample inlet are ionized by a beam of high energy electrons passing closely among them, according to [4]. The rapidly changing electric field can both eject electrons from the atom or the molecule (ionization) and transfer sufficient energy to the molecule to cause its bonds to rupture (fragmentation), according to [4]. The ions are then accelerated in an electric field at a voltage V, according to [4]. In a hyperbolic energy analyzer, atoms and molecules are already ionized when they enter the instrument as a result of existing in a plasma state.

The energy of each ion is equal to the charge z times the accelerating voltage (zV), and this energy acquired by an ion on acceleration is kinetic energy. It is important to note that the kinetic energy of an ion accelerated through a voltage V depends only on

the charge of the ion and the voltage, and not on the mass of the ion [4]; the translation component of the kinetic energy is equal to $\frac{1}{2}mv^2$ [4]. As m varies, the velocity v changes such that the kinetic energy remains a constant, according to [4]. The velocity of an ion depends on its mass, and it is inversely proportional to the square root of the mass of the ion, according to [4]. In a hyperbolic energy analyzer, ions are accelerated when they are exposed to a potential field that exists between an orifice through which they enter the instrument and the segmented, concentric Faraday collector (SCFC).

In magnetic sector mass spectrometers, after an applied voltage has accelerated the ions, they enter a curved section of a magnet of homogeneous magnetic field B and a fixed radius of curvature, according to [4]. This magnetic field acts on the ions, making them move in a circle. The attractive force of the magnet equals Bzv, and the centrifugal force on the ion is equal to $\frac{mv^2}{r}$, where the radius r is the radius of the circular path traveled by the ion, according to [4]. If the ion path is to follow the radius of curvature of the magnet, these two forces must be equal, according to [4]. That is, the radius of the circular path of an ion depends on the accelerating voltage V, the magnetic field B, and the ratio $\frac{m}{z}$. When V and B are kept constant, the radius of the circular path depends on the $\frac{m}{z}$ value of the ionized molecule, according to [4]. Ions of different $\frac{m}{z}$ travel in circles with different radii; this is the basis of the separation by $\frac{m}{z,}$, according to [4]. Ions with different paths are shown as the dotted in Fig. 3, and only one particular $\frac{m}{z}$ has the right r to pass through the mass spectrometer under given magnitudes for V and B, according to [4]. The others follow paths that cause them to hit the sides of the instrument and be lost, according to [4]. By varying V or B, one can select which $\frac{m}{z}$ will pass through the system, according to [4].

In a hyperbolic energy analyzer, ions traveling through the instrument are exposed to an external magnetic field that is used to confine the plasma. This magnetic field, along with the electric field, makes ions travel in a circular path, resulting in the separation of the charged particles from a beam according to mass-to-charge values, and by gradually increasing the diameter of the cylindrical wall from the hyperbolic lenses to the Faraday cup, the separation among charged particles can be either maintained or increased, potentially.

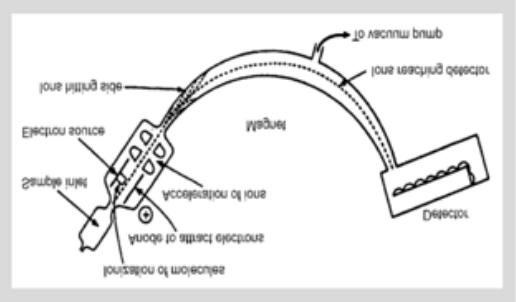

Figure 3
Schematic of Magnetic Sector Mass Spectrometer, which is a Single-Focus, as Demonstrated in [4]

In all modern magnetic sector mass spectrometers, the applied magnetic field B of the electromagnet is varied while the accelerating voltage V is held constant [4]. The radius of curvature of the magnetic sector of a given instrument is constant, so only ions with trajectory of radius r pass through [4]. Then, for a particular magnetic field strength, only ions with a $\frac{m}{z}$ value that satisfies $\frac{B^2r^2}{2V}$ will exit the chamber [4]. Consequently, for different values of B, ions with different mass-to-charge ratios will pass through the instrument to the detector, and by varying B, one can scan the range of $\frac{m}{z}$ ratios of the sample ions and measure their abundance with a detector which either counts and sums individual ions or measures a current produced by their impact on the detector [4]. To increase the detection efficiency of different charged particles in a hyperbolic energy analyzer, a segmented, concentric Faraday collector will be used (Fig. 4): once separated from a single beam as a result of both electric and magnetic fields acting on them, each one of the charged particles will travel to a specific segment of the concentric Faraday collector to be counted.

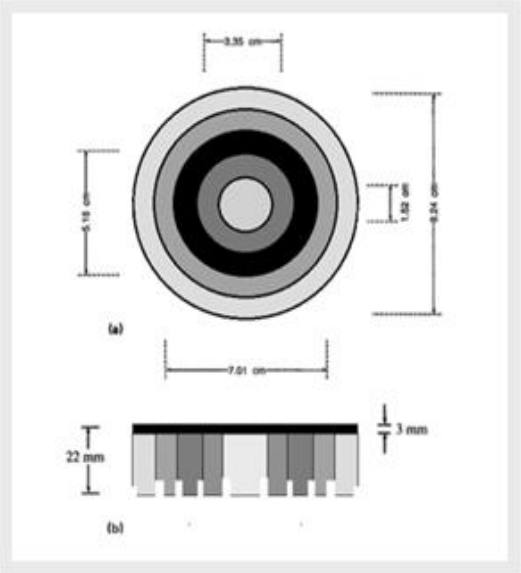

Figure 4
Schematic Diagram of a Concentric Faraday Collector, as shown in [5]. (a) Top view of a five-element segmented concentric Faraday collector (SCFC) and (b) Cross-sectional view of a SCFC, as shown in [5].

METHODOLOGY

The methodology for achieving the objective of this research is as follows: After values are chosen for the potential of the cylinder wall, the hyperbolic lenses, the orifice (pinhole lens), and the concentric Faraday cup, as well as values are chosen for the geometric dimensions of both the standard HEA model and the modified HEA model themselves, their potential distributions are determined by using the finite-difference method, which is built into the computer codes of the HEA models. Once the potential distributions are determined, computer simulations are performed to determine whether or not different charged particles can be separated from a beam and travel to different locations on a concentric Faraday collector and to determine whether or not different charged particles can be discriminated against energy while the HEA is operating as a mass spectrometer.

In addition, it was observed that the performance of the standard HEA model, when operating as a mass spectrometer, is maximized when it is given the potential values for the components of the modified HEA model that generate straight-line shaped equipotential surfaces near the hyperbolic lenses. However, it needs to be noted that these potential values will not generate straight-line shaped equipotential surfaces near the hyperbolic lenses of a standard HEA.

To determine the conditions at which the modified HEA model can operate as a mass spectrometer as well as discriminate charged particles against energy, the following computer simulations are performed: using the modified HEA model, singly positively charged particles are positioned away from the longitudinal axis of the instrument and given initial velocities in both the z- and the x-direction; using the modified HEA model, singly positively charged particles are positioned away from the longitudinal axis of the instrument and given an initial velocity in the z-direction; using the modified HEA model, singly positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in both the z- and the x-direction; using the modified HEA model, singly positively charged particles are positioned on the
longitudinal axis of the instrument and given an initial velocity in the z-direction; using the modified HEA model, double positively charged particles are positioned away from the longitudinal axis of the instrument and given initial velocities in both the z- and the x-direction; using the modified HEA model, double positively charged particles are positioned away from the longitudinal axis of the instrument and given an initial velocity in the z-direction; using the modified HEA model, double positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in both the z- and the x-direction; and using the modified HEA model, double positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in the z-direction.

Similarly, to determine the conditions at which the standard HEA can operate as a mass spectrometer as well as discriminate charged particles against energy, the following computer simulations are performed: using the standard HEA model, singly positively charged particles are

positioned away from the longitudinal axis of the instrument and given initial velocities in both the z- and the x-direction; using the standard HEA model, singly positively charged particles are positioned away from the longitudinal axis of the instrument and given an initial velocity in the z-direction; using the standard HEA model, singly positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in both the z- and the x-direction; using the standard HEA model, singly positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in the z-direction; using the standard HEA model, double positively charged particles are positioned away from the longitudinal axis of the instrument and given initial velocities in both the z- and the x-direction; using the standard HEA model, double positively charged particles are positioned away from the longitudinal axis of the instrument and given an initial velocity in the z-direction; using the standard HEA model, double positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in both the z- and the x-direction; and using the standard HEA model, double positively charged particles are positioned on the longitudinal axis of the instrument and given an initial velocity in the z-direction. After analyzing the results from the computer simulations, the performance of the modified HEA model is compared with the performance of the standard HEA model.

RESULTS

The following results were obtained from the computer runs:

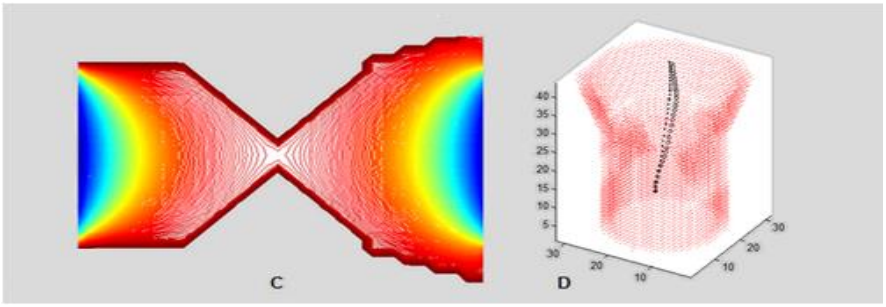

Figure 5

(C) A modified HEA computer model output indicates a potential distribution that is not generating straight-line shaped equipotential surfaces near the hyperbolic lenses. (D) Although the electric field from the potential distribution and the magnetic field manage to separate the trajectories of the different charged particles briefly, they eventually combine.

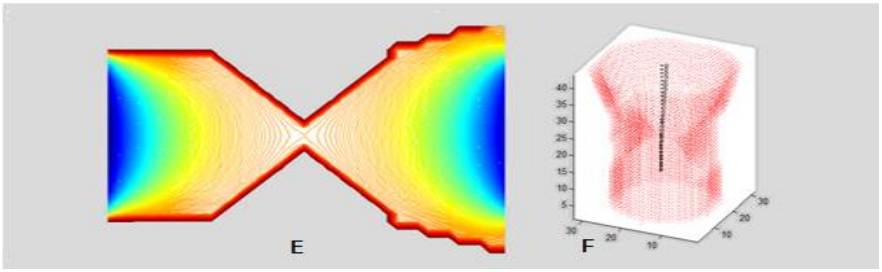

Figure 6

(E) A modified HEA computer model output indicates a potential distribution that is generating straight-line shaped equipotential surfaces near the hyperbolic lenses. (F) The electric field from the potential distribution and the magnetic field successfully separate the trajectories of the different charged particles permanently.

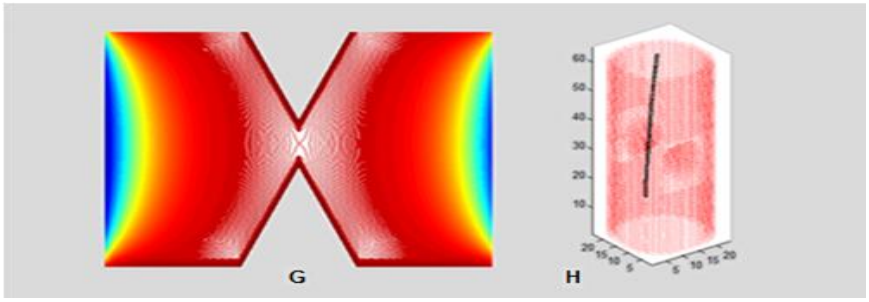

Figure 7

(G) A standard HEA computer model output indicates a potential distribution that is generating straight-line shaped equipotential surfaces near the hyperbolic lenses. (H) The electric field from the potential distribution and the magnetic field fail to separate the trajectories of the different charged particles.

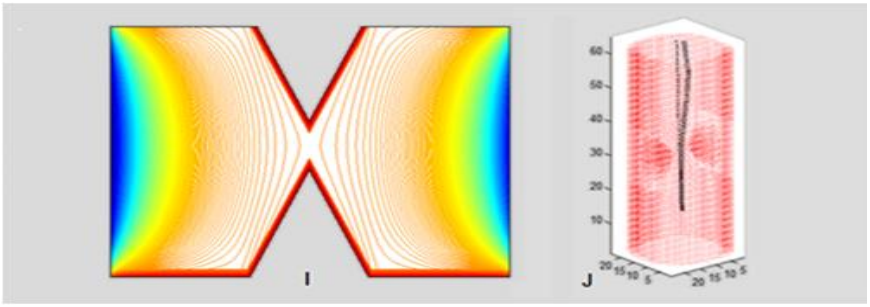

Figure 8

(I) A standard HEA computer model output indicates a potential distribution that is not generating **straight-line shaped equipotential surfaces near the hyperbolic lenses. (J) The electric field from the potential distribution and the magnetic field successfully separate the trajectories of the different charged particles. The potential distribution is equal to the potential distribution for a modified HEA model.**

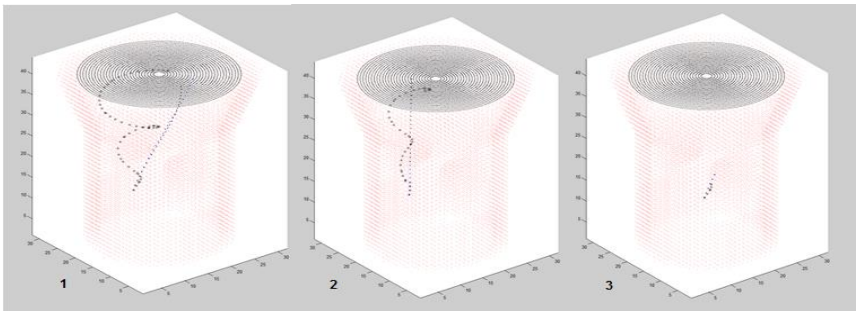

Figure 9

Computer outputs of a modified HEA model are illustrated in this figure. (1) When singly (positively) charged particles, of specified initial conditions, enter the instrument at an angle and through an orifice away from the longitudinal axis, trajectories successfully separate. (2) However, when the same singly (positively) charged particles enter through an orifice on the longitudinal axis, trajectories partially separate. (3) When the same singly (positively) charged particles enter through an orifice on the longitudinal axis, trajectories completely fail to separate.

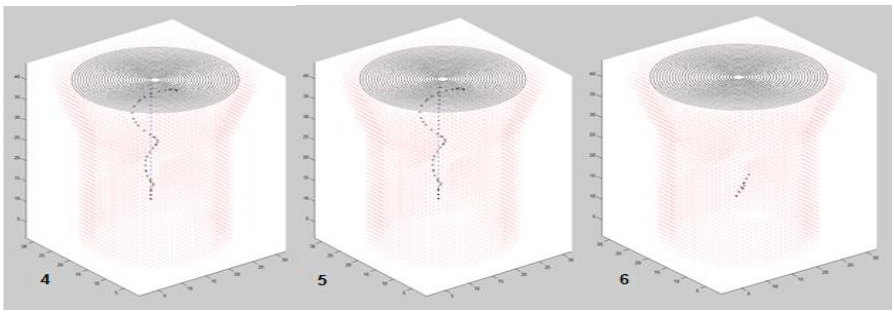

Figure 10

Computer outputs of a modified HEA model are illustrated in this figure. (4) When singly (positively) charged particles, of specified initial conditions, enter through an orifice on the longitudinal axis, trajectories partially separate. (5) However, when double (positively) charged particles, with the same initial energy, enter through an orifice on the longitudinal axis, trajectories partially separate. (6) And, when the same double (positively) charged particles enter through an orifice at an angle, trajectories completely fail to separate.

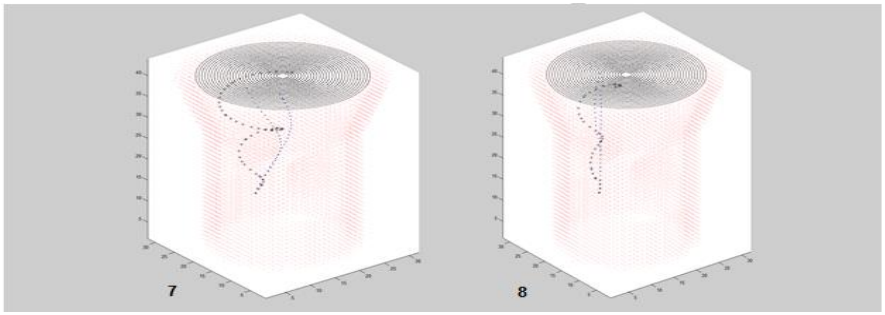

Figure 11

Computer outputs of a modified HEA model are illustrated in this figure. (7) When double (positively) charged particles, of specified initial conditions, enter the instrument at an angle and through an orifice away from the longitudinal axis, trajectories successfully separate. (8) However, when the same double (positively) charged particles, enter the instrument through an orifice away from the longitudinal axis, trajectories successfully separate, but not to the same extent as in (7).

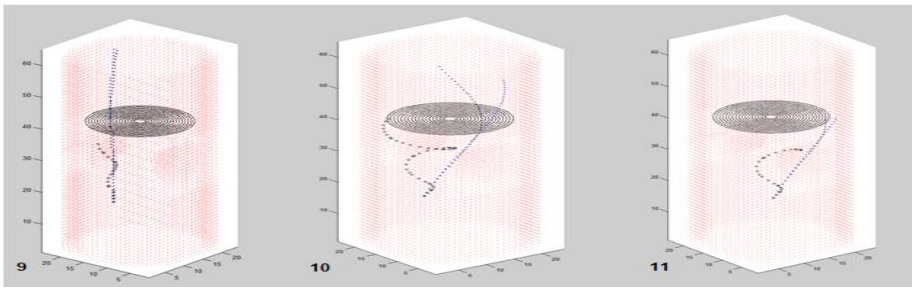

Figure 12

Computer outputs of a standard HEA model are illustrated in this figure. (9) When singly (positively) charged particles, of specified initial conditions, enter the instrument through an orifice away from the longitudinal axis, trajectories successfully separate, but not all of the charged particles make it into the concentric Faraday cup. (10) However, when the same singly (positively) charged particles enter the instrument at an angle and through an orifice away from the longitudinal axis, trajectories successfully separate and all of the charged particles make it into the concentric Faraday cup. (11) And, when the same singly (positively) charged particles enter at an angle and through an orifice on the longitudinal axis, trajectories successfully separate, but not all of the charged particles make it into the concentric Faraday cup.

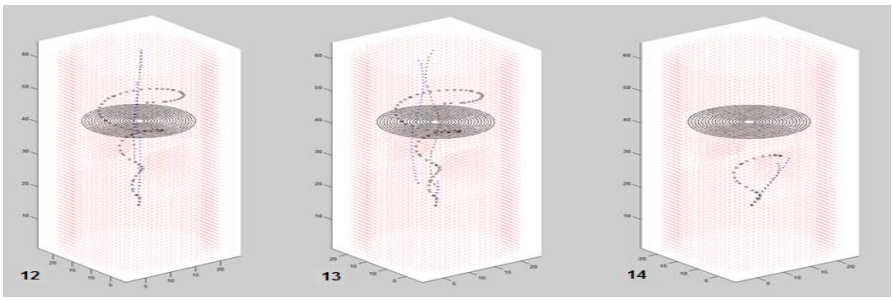

Figure13

Computer outputs of a standard HEA model are illustrated in this figure. (12) When singly (positively) charged particles, of specified initial conditions, enter the instrument through an orifice on the longitudinal axis, trajectories successfully separate. (13) However, when double (positively) charged particles, with the same initial energy, enter the instrument through an orifice on the longitudinal axis, trajectories successfully separate, but to an extent better than in (12). (14) However, when the same double (positively) charged particles enter at an angle and through an orifice on the longitudinal axis, trajectories not only fail to separate, but also are discriminated against.

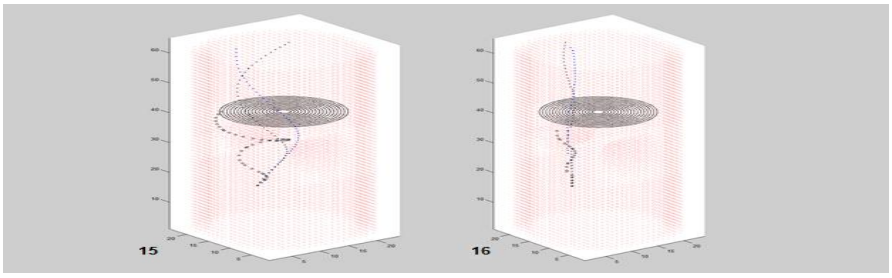

Figure 14

Computer outputs of a standard HEA model are illustrated in this figure. (15) When double (positively) charged particles, of specified initial conditions, enter the instrument at an angle and through an orifice away from the longitudinal axis, trajectories successfully separate. (16) When the same double (positively) charged particles enter the instrument through an orifice away from the longitudinal axis, trajectories successfully separate, but not all of the charged particles make it into the concentric Faraday cup.

DISCUSSION

Although the standard HEA model is capable of separating charged particles according to mass-to-charge ratios, its performance is maximized as a mass spectrometer when the potential values for its components are equal to the given potential values for the components of the modified HEA model. The standard HEA model has an inherent tendency to focus charged particles into a Faraday collector, and this tendency is maximized when the potential values given to its components generate straight-line shaped equipotential surfaces near the hyperbolic lenses, causing the loss of any separation gained among the charged particles along the way (Fig. 7). However, when the potential values for the components of the modified HEA model are given to the standard HEA, this tendency to focus charged particles is no longer maximized, allowing charged particles of different mass-to-charged ratios to enter different positions in the concentric Faraday collector (Fig. 8). On the other hand, to maximize the performance of the modified HEA model as a mass spectrometer, the potential values given for its components must generate straight-line shaped equipotential surfaces near the hyperbolic lenses (Figs. 5-6).

In addition, for both the modified and the standard HEA models, computer simulations have indicated that the best separations, according to mass-to-charged ratios, are achieved when the charged particles enter the instrument at an angle to and at a position that is away from the longitudinal axis, as shown in Figs. 9(1), 11(7), 12(10), and

14(15): when traveling through the electric and magnetic fields inside the instrument, charged particles with the same kinetic energy but of different mass-to-charge ratios will follow circular paths with different radii. (For the computer simulations, only a magnetic field along the longitudinal axis of the instrument is modelled.) It can also be noted that separations of charged particles according to mass-to-charge ratios depend on the starting position in the instrument as well, as indicated in Figs 10(4), 13(14), and 12(11); even when entering the instrument at an angle to the longitudinal axis, charged particles may fail to separate altogether or may be discriminated against energy.

Furthermore, separation efficiency may be increased by taking advantage of the fact that computer simulations have consistently indicated that charged particles have different translational components of kinetic energy when traveling through the instrument; the separation among charged particles may be increased by extending the length of some sections of the instrument, creating a "field-free drift tube" effect.

Finally, for the given initial conditions and the given geometric dimensions for both HEA models, so far the standard HEA model indicates strong tendencies to discriminating charged particles against energy and to focusing charged particles into a segmented, concentric Faraday collector, degrading its performance as a mass spectrometer. However, this flaw may be offset by changing the initial conditions of the charged particles and by adjusting the location of the segmented, concentric Faraday collector.

CONCLUSION

Results from computer simulations have indicated the following: (1) For both modified and standard hyperbolic energy analyzers, a beam of charged particles that enters the instrument at an angle to and from a location that is away from the longitudinal axis has the highest probability of breaking down into separate trajectories corresponding to each of the charged particles making up the original beam; (2) by gradually increasing the diameter of the cylindrical wall from the hyperbolic lenses to the concentric Faraday collector, as in the case of the modified hyperbolic energy analyzer, the separation between charged particles can be maintained or even increased; (3) although the standard hyperbolic energy analyzer indicates an acceptable performance as a mass spectrometer, the inherent tendency of the instrument for focusing charged particles into a concentric Faraday collector degrades its efficiency; (4) since, consistently, there are differences among the translational components of the kinetic energies of the charged particles, the separation efficiency could be improved by extending the length of some sections of the HEA, creating a "field-free drift tube" effect, according to [4]; and (5) both the standard and the modified hyperbolic energy analyzers can discriminate charged particles against energy as well as separate different charged particles from a beam according to mass-to-charge ratios.

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REFERENCES

[1] E. Leal-Quiros, "Novel Probes and Analyzers for RF and Micowave Heated Plasmas for Controlled Fusion Research: The Hyperbolic energy analyzer, The Magnetic Moment Analyzer, The Double Energy Analyzer, and The Variable Energy Analyzer," Ph.D. Dissertation, Dept. Nucl. Eng.; Univ. of Missouri, Columbia, MO, 1989.

[2] E. Leal-Quiros *et al.*, "Hyperbolic energy analyzer." *Rev. Sci. Instrum.* vol. 61(6), pp. 1708−1712, Oct. 1990.

[3] E. Leal-Quiros *et al*., "Electron Populations in the hot-electron ring regions of mirrors and cusps, measured by hyperbolic energy analyzer," *Rev. Sci. Instrum.* vol. 61(10), pp. 3304−3305, Oct. 1990.

[4] J. W. Robinson *et al.*, *Undergraduate Instrumental Analysis 6th ed.*New York, NY: Marcel Dekker, 2005.

[5] T. A Peyser *et al.*, "A segmented concentric Faraday cup for measurement of time-dependent relativistic electron beam profiles," *Rev. Sci. Instrum.* 62 (12), pp. 2895-2903, Dec. 1991.