INDEX to Displayed SHEETS:-

CONSIDERATIONS OF THE SUBJECT OF "INDUCED (Magnetic) FIELDS", IN PARTICULAR THE CALCULATION OF ITS VALUE AT A GIVEN SITE, HAS BEEN POSSIBLE TILL NOW BECAUSE OF THE SIMPLE SUMMATION PROCEDURE WHICH COULD BE EVEOLVED INSTEAD OF THE CONVENTIONALLY ESTABLISHED METHOD OF SETTING UP INTEGRALS WHICH INVARIABLY TURN OUT TO BE MORE INVOLVED MATHEMATICALLY FOR EVALUATION.

This simple summation procedure provides for the access to arrive at the induced field contributions in several contexts which were not as easy by the earlier established methods. This method had to be verified for reliability by reproducing the already known table of demagnetization factors. Since this mathematical approach was simpler and more than that appealed to the chemical intuitions much better, several associated questions and contexts which were unthinkable earlier could be raised and it was also possible to get answers to the queries consistent with the conjectures possible till then.

AS IT SHOULD BE OBVIOUS, IT HAS ALL BEEN WITH THE SPECIMEN WHICH ARE HOMOGENEOUSLY MAGNETIZED IN THE MAGNETIC FIELD; BUT, LEAVING OPEN THE POSSIBILITIES TO ADDRESS THE CASE OF SPECIMEN WITH INHOMOGENEOUS MAGNETIZATION.

The conspicuous and simplifying feature is that the Demagnetizing factors depend on the shape and not on the actual size of the sample specimen. Also only specific shapes result in homogeneous magnetization but not others even if they are describable by regular analytical equations for the boundary surfaces. Since the present procedure is simple to apply, an effort seemed possible to study the trends for shapes which were exceptional earlier.

The value for INDUCED FIELD at a specific site in the specimen (usually, in most cases, the center of the specimen is typical of the points within homogeneously magnetized specimen) is a single number. In this procedure this singular numerical value can be obtained by summing the contributions from all parts of the sample and it is possible to record the details of the break up of contributions from different part while summing for the final single numerical value. It turns out that by this procedure one can discern that certain large magnitudes of contribution are built up during the process eventually becoming large magnitudes of equal value and opposite in sign, thus at the end resulting in a cancellation to arrive at (near) zero induced fields. As long as it is the case of HOMOGENEOUSLY magnetized material, to arrive at the final value for demagnetized factors it is only necessary to ensure that, in spite of the fact that the result is cancellation of two large values of equal magnitude and opposite in sign, the results can be reproduced with good accuracy and higher significance factors. Since this reproducibility seemed to be assured then it is necessary to study the trends of this break-up contribution if it is a question of handling the inhomogeneous magnetization. In the case of the sample material which is homogeneous, but gets in-homogeneously magnetized because of the regularly describable shapes other than the ellipsoids of revolution, various shapes like the spindle and cylinder (with the symmetry of revolution as for the ellipsoids) are considered and compared with the spherically shaped specimen of the same material. The perspectives for such trend-studies are described in the next two introductory Sheets.

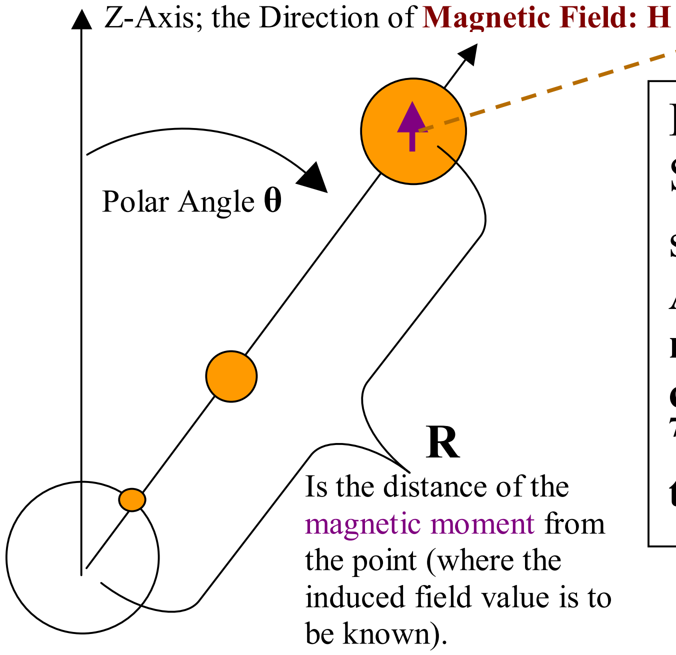
These perspectives make a beginning in this presentation from where it was left deferred in the earlier presentation materials at the 4th Alpine Conference on SSNMR at Chamonix Mont Blanc, France in Sept. 2005. These materials can be viewed from the Website URL: http://nehuacin.tripod.com/id3.html

The case of proportionately same (similar) shape for outer surface and the inner cavity resulting in zero induced fields within an ellipsoid has been given a more general outlook in this presentation. For example, the shapes of a Spindle and Cylinder (the case for inhomogeneous categories) for the specimen are considered with similar shaped cavities as well as with spherical cavities (Lorentz type) and the trends of the break up, the total are recorded for inference and arriving at more general criteria for the shape dependences. Particularly, A radial vector (R.V.) with a polar angle is considered and along the vector the distances from the central site to the cavity surface (R-small) and to the specimen boundary surface (R-Big) are plotted as a function of polar angle which reflects the respective shapes considered. Along the vector (the difference Vector "Rbig – Rsmall") the number of closely packed spheres are calculated and plotted which also reflects consistently the shapes involved. Finally, the sum of contributions for each polar angle is also plotted for the trends.

A display of the detailed break ups and the possibility thus to access for the characteristics of the break-up contributions (in terms of the patterns reflected in the graphs) could further confirm the following (i) for homogeneous magnetizations, even for non-spherical shapes (ellipsoids), the field inside the cavity is zero if the cavity is similar in shape to that of the macroscopic specimen itself. (ii) Even in the case of specimen shapes with inhomogeneous magnetization if the cavity is of similar shape (SHEET-10) as the outer shape of the specimen, the induced field inside the cavity (at the center) is zero. (iii) In the case of homogeneous magnetization, the value at the center of the specimen can be typical of any other point in the specimen; but, for inhomogeneous magnetization, the zero field situation as at the center of the specimen would not be typical if the same cavity is located in any other part of the specimen (SHEET-18 & 19) (iv) but, when the cavity is placed in the specimen off from the center, then a site can be found within that cavity in that location where the induced field is zero but the site may not be at the center of the cavity, if the cavity is not at the center of the specimen. All these specific aspects have been well established by the trends displayed in these poster sheets. This gives the possibility to look for the Line-shape studies in detail so that it would be possible to distinguish the line positions and the line shape changes which seem to apparently shift the line peaks which are truly due to line shapes described at the off-the-peak line positions.

Susceptibility is ISOTROPIC

Commensurate with the Susceptibility the magnetic moment **M** would be in accordance with the equation $\mathbf{M} = \chi_v \times \mathbf{H}$



Is the distance of the magnetic moment from the point (where the induced field value is to be known).
The distance is along the radial Vector specified by its Polar angle

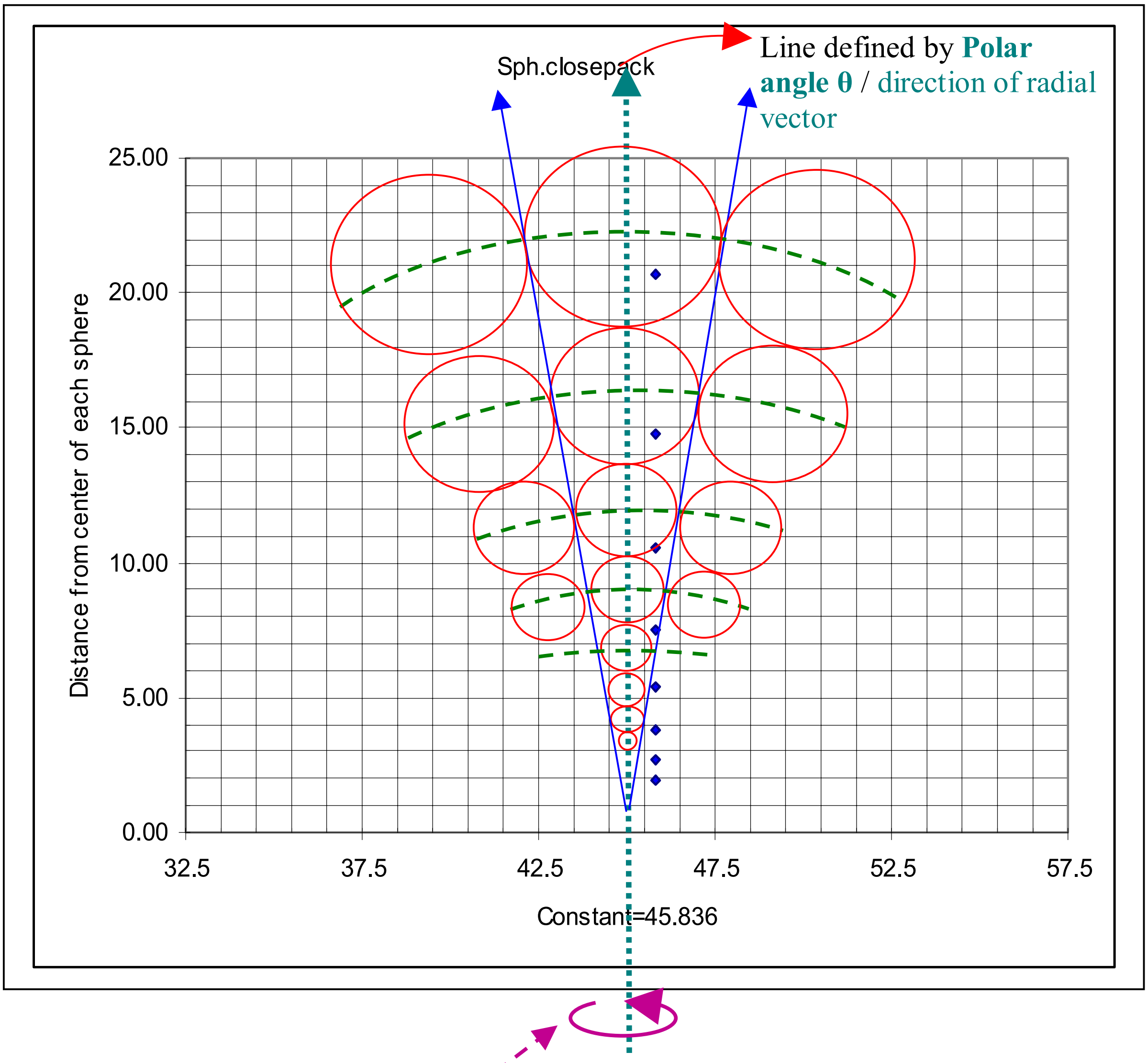
In these calculations VOLUME Susceptibiltiy is used. That is specified as $\chi\ \mathrm{cm}^3$
A typical value for Organic molecules (Diamagnetic) can be a convenient value and -2.855×10^{-7} units can be typical per cc. of the material

r is the radius of the **spherical magnetized material** specifically demarcated.
$(4/3)\ \pi\ r^3$ will be the spherical volume of the material at a distance **R** contributing at the point of origin in the illustration on the left

The equation for induced field on the basis of a dipolar model would then be

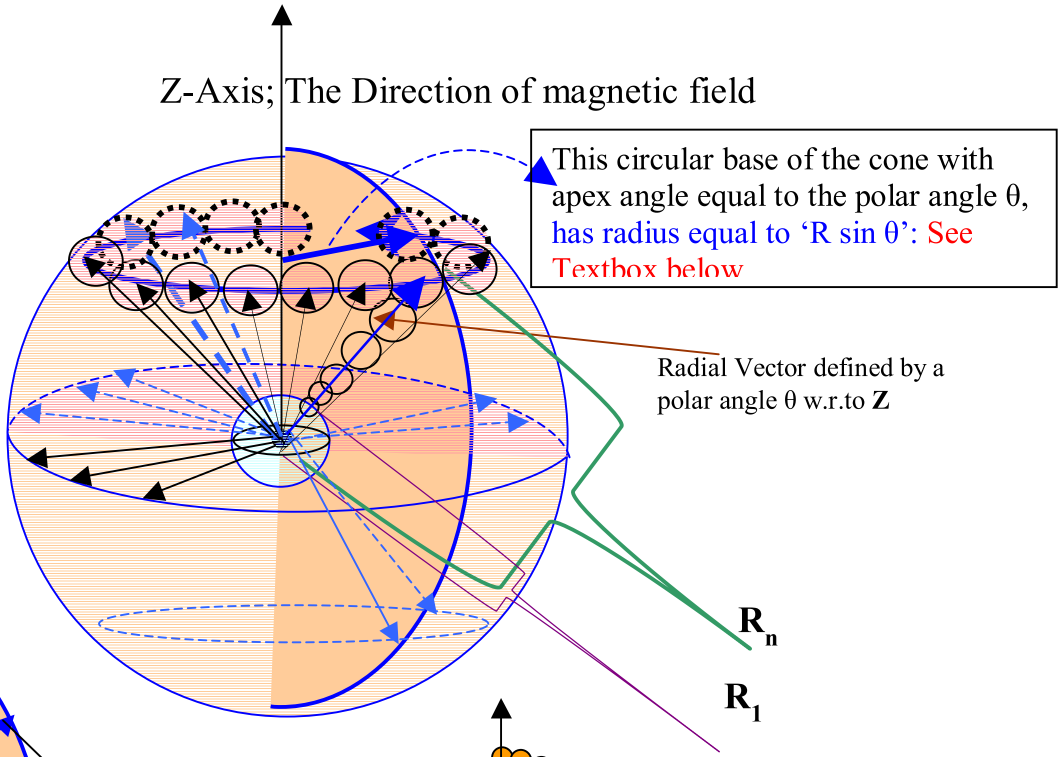
$$\sigma = -2.855 \times 10^{-7} \times [(4/3)\ \pi\ r^3]\ \chi_v \times (1-3\cos^2\theta) / R^3$$

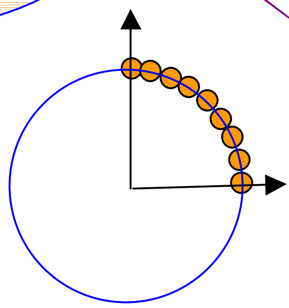
From the above equation it is obvious that along this radial vector with the specified polar angle if spherical volume elements of the material are placed such that they all have the ‘radius- r’ to ‘distance- R’ ratio the same, then every one of such sphere would contribute the same induced field at the specified point.

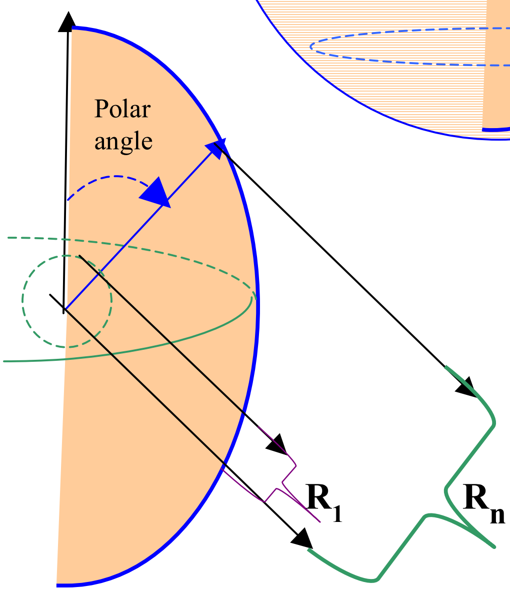


Quantitative ILLUSTRATION of Close packing with the constraint r_i / R_i = Constant

A Rotation by 360° results in a cone in conformity with the filling above and the cone is filled with the spheres closely packed. This is cone is a section of the full sphere and the sphere can be well envisaged with the closely filled spheres. The specimen then is left with the voids due to the regions not filled by the spheres. Hence the material, in the actual specimen, corresponding to the amount filling the void must be taken into account; and, also its contribution to induced field at the point.







With "C= **Ri / ri , i=1,n"**
For a sphere of radius =0.25 units, and the polar angle changes at intervals of 2 .5°
There will be 144 intervals. Circumference= 2π/4 so that the diameter of each sphere on the circumference = 0.0109028; radius = 0.0054514
C = R/r = 0.25 / 0.0054514 = 45.859779
[46.859779/44.859779] = 1.04458334
Log (1.0445834) = 0.0189431 $(r/R)^3$=1.0368218e-5 =0.000010368218

Equation for calculating the number of spheres, the dipole moments, along the radial vector is as given below:

$$n = 1 + \frac{\log \frac{R_n}{R_1}}{\log \frac{C+1}{C-1}}$$

Using above equation 'n' along the vector length is calculated, for the direction with polar angle θ. Which is ' σ' per spherical magnetic moment x number of such spheres 'n'.

$\sigma_\theta = \sigma \times n$. At the tip of the vector, there is circle along which magnetic moment have to be calculated. This circle has radius equal to 'R sinθ'. The number of dipoles along the length of the circumaference = 2 π R sinθ/2.r = π R/ r sinθ. Again R/ r is a constant by earlier criteria.

Along each of the radial vector direction of polar angle θ, spheres can be closely packed with the specified constraint. It is this constraint which brings in the simplicity that, every one of the spheres along a radial vector contributes the same induced filed at the specified point (site) within the material. Thus if the value for one sphere is known, and the number of closely packed spheres are calculated (as given by the equation stated earlier), then, the total contribution from that direction can be obtained by multiplying by the number 'n' of such spheres.

Let the contribution of (one) i-th sphere along the vector direction θ be = $\sigma^{i,\theta}_{\varphi}$

Then the contribution from 'n' spheres would be $= n \times \sigma^{i,\theta}_{\varphi} = \sigma^{\theta}_{\varphi}$

This is only along the line of a radial vector which is for a fixed φ. The φ dependent contributions for a given polar angle, θ can be obtained by recognizing the rotational symmetry around the magnetic field direction and this above value of σ^{θ} would be the same for all radial vectors on the surface of rotational cone with apex angle θ. If the circle described by the base of the cone is considered its radius would be, '$R \sin\theta$' where R is the radial distance to the surface of the sphere from the site. By calculating the circumference of the circle described by the base, (to be $2 \times \pi \times R \sin\theta$) and dividing the circumference length by the diameter of the Sphere in that base layer, which is $2 \times r$, the number of such closely packed spheres on the circumference can be known. This number $[(2 \times \pi \times R \sin\theta) / 2 \times r]$ would be the number of radial vectors with the same polar angle θ and all the radial vectors would contribute each the same as calculated for one of vector . Thus the final value for the given polar angle would be

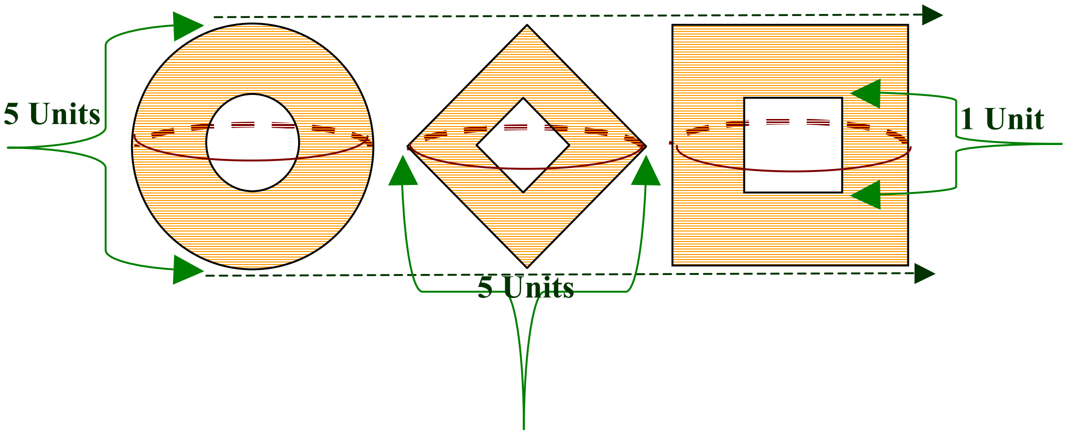
$\sigma_{\theta} = [(2 \times \pi \times R \sin\theta) / 2 \times r] \times \sigma^{\theta}_{\varphi}$. This procedure is repeated for all values of θ discretely at known (specified before) interval and sum over the polar angles would give the total contribution from the entire specimen. R/r value would be the same as the value set as constraint.

For one sphere = $\sigma^{i,\theta}_{\varphi}$ For 'n' spheres = $n \times \sigma^{i,\theta}_{\varphi} = \sigma^{\theta}_{\varphi}$

Summed for all azimuthal angle values for the given polar angle = σ_{θ} .

Summing Over all polar angles thus gives final total contribution from the specimen material corresponding to spherical filling = $\boldsymbol{\sigma}$. Since the spheres at their respective points can be replaced by cubes with the side equal to the diameter of that sphere, there can be no further void to account for. This step increases the magnetic moment at each point by the ratio of the cube to sphere volume. i.e.,

$(8 \times r^3) / (4/3 \times \pi \times r^3)$ = **1.909859** . Final value = **1.909859** $\times\ \boldsymbol{\sigma}$

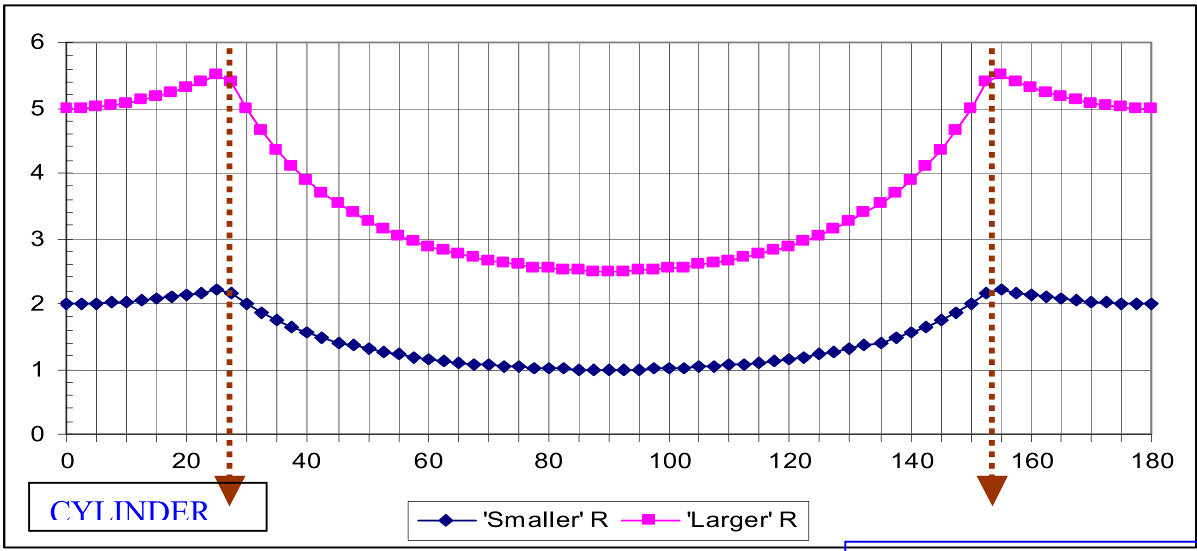


SPHsph = Total Induced filed at Centre: **0.222579E-08**
Along each polar directiona radial vector 49.37 close packed spheres

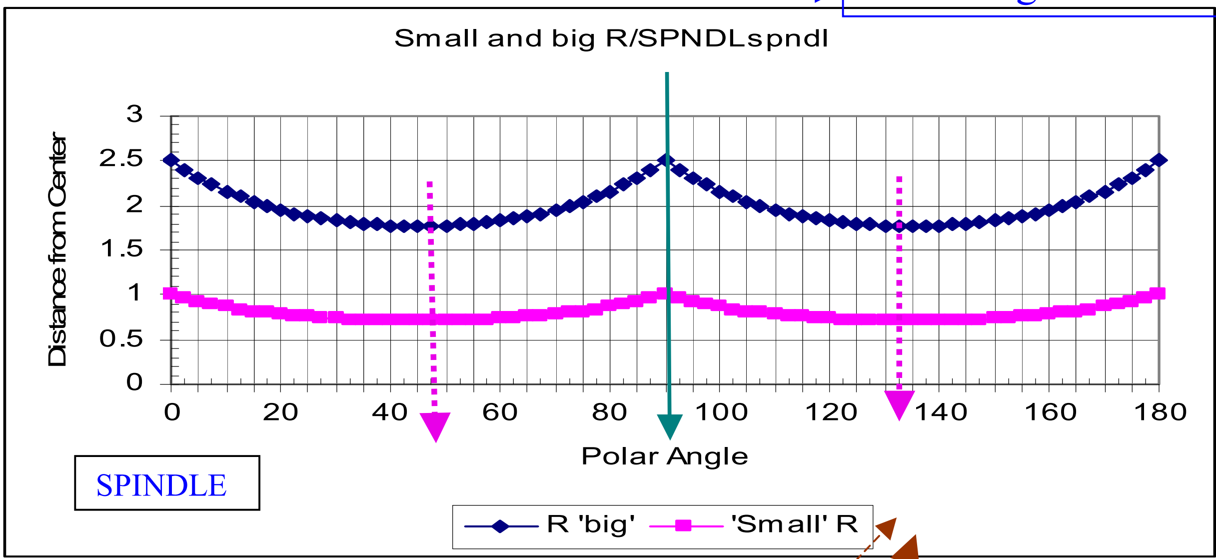
SPNDLspndl = Total Induced filed at Centre: **0.22256730E-08**
Along each polar directiona radial vector 49.37 close packed spheres

CYLcyl = Total Induced filed at Centre**:** **0.2226E-08**
Along each polar directiona radial vector 49.37 close packed spheres

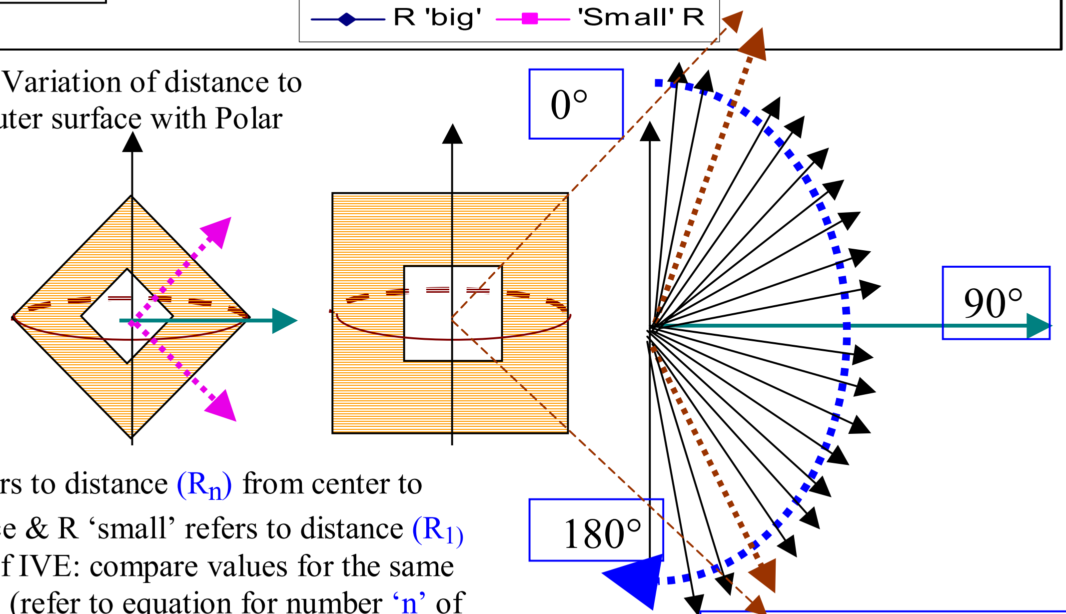
With reference to NMR Chemical shifts, note that these values are 2.2 x 10^{-3} ppm and is considered here close to zero. The variation in this small residual value from this calculation procedure can be attributed to known effects of non-cancellations of large +ve and equal –ve values. In this procedure, the summation would have to result equal but large +ve and –ve values which will cancel due to symmetry considerations (essential geometrical consequence as the shape is important). Such situations are encountered in several calculations of parameters and on the same footing these can also be explained. But these details are deferred to a later occasion. **This consequence of zero induced field at the centre for Ellipsoids with ellipsoidal IVE can be argued out using the table of Demagnetization factor values. S.Aravamudhan, Indian Journal of Physics, Vol.79(9), p 985-989 (2005)**



Polar Angle 0° - 180°

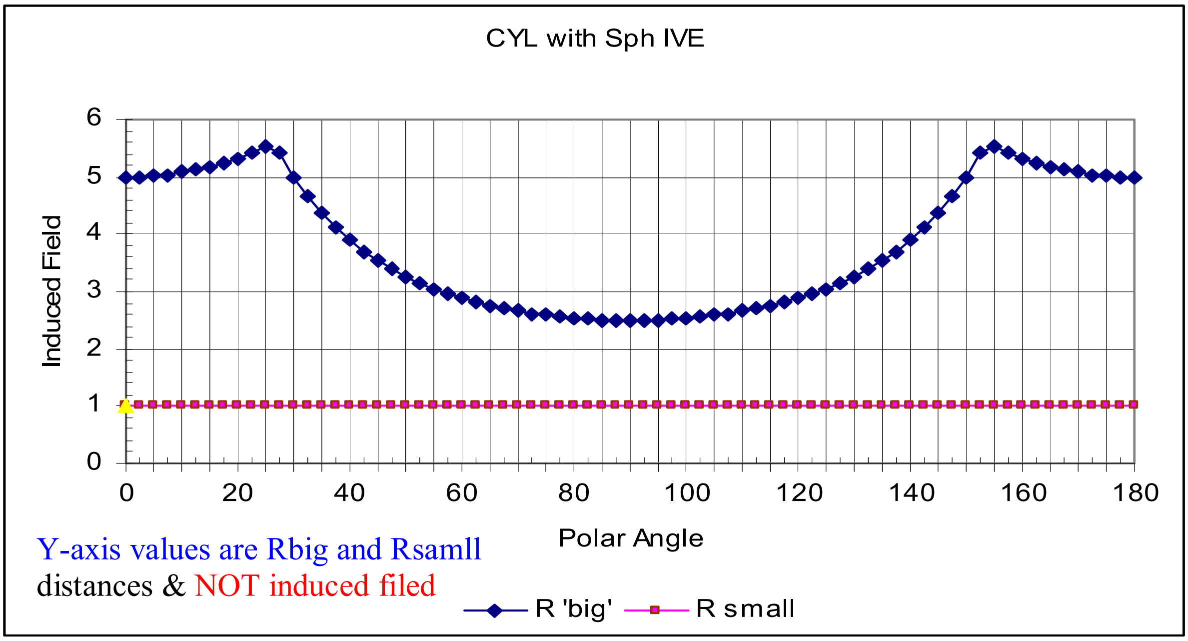


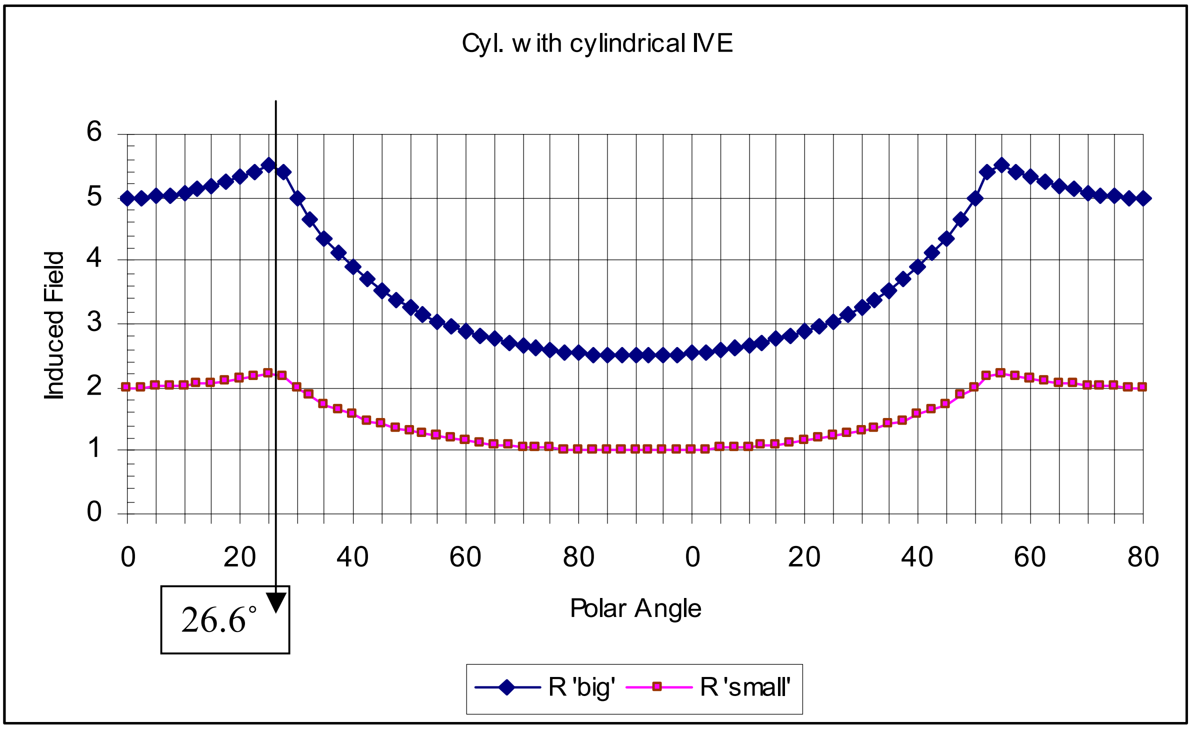
PLOTS of Variation of distance to IVE and outer surface with Polar angle

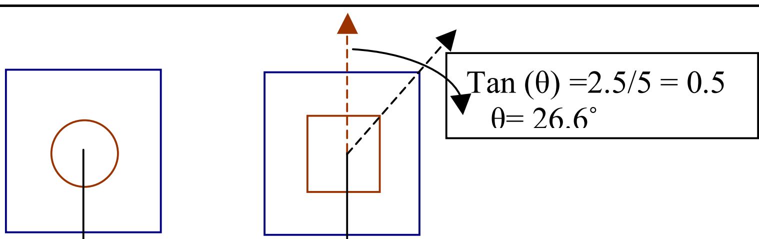


R 'big' refers to distance (R_n) from center to outer surface & R 'small' refers to distance (R_1) to surface of IVE: compare values for the same polar angle. (refer to equation for number 'n' of closely packed spheres

Polar Angle 0° - 180°





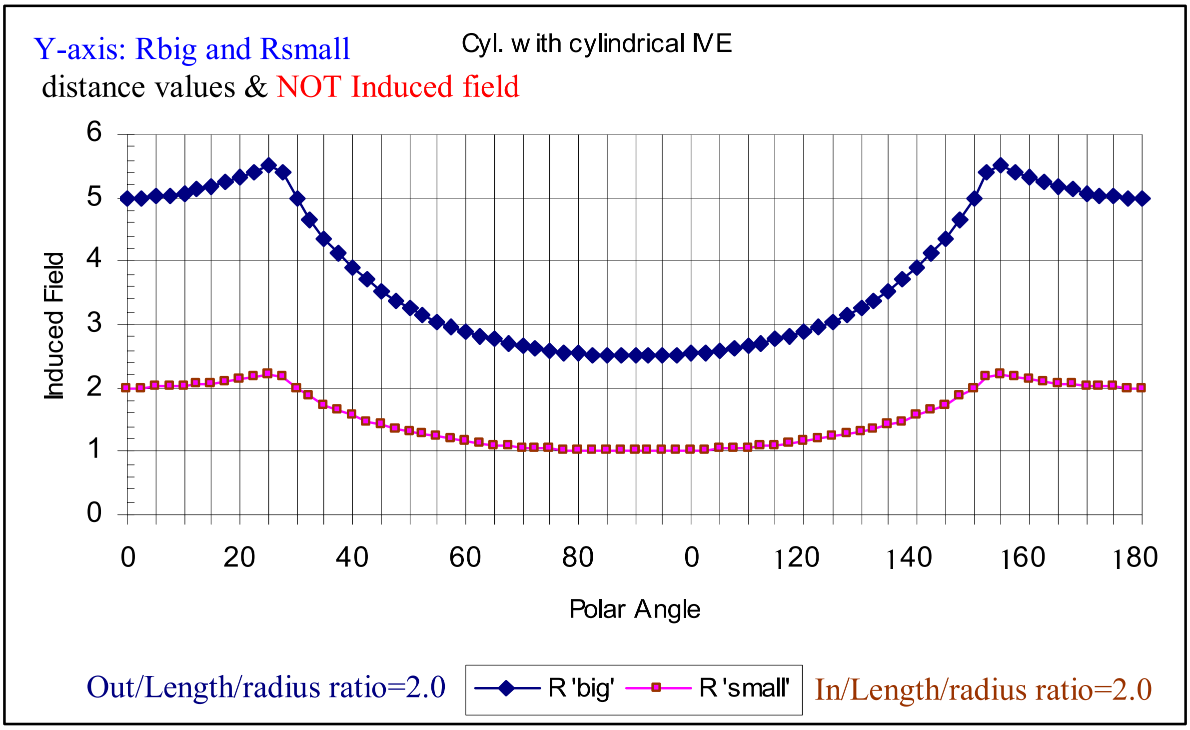


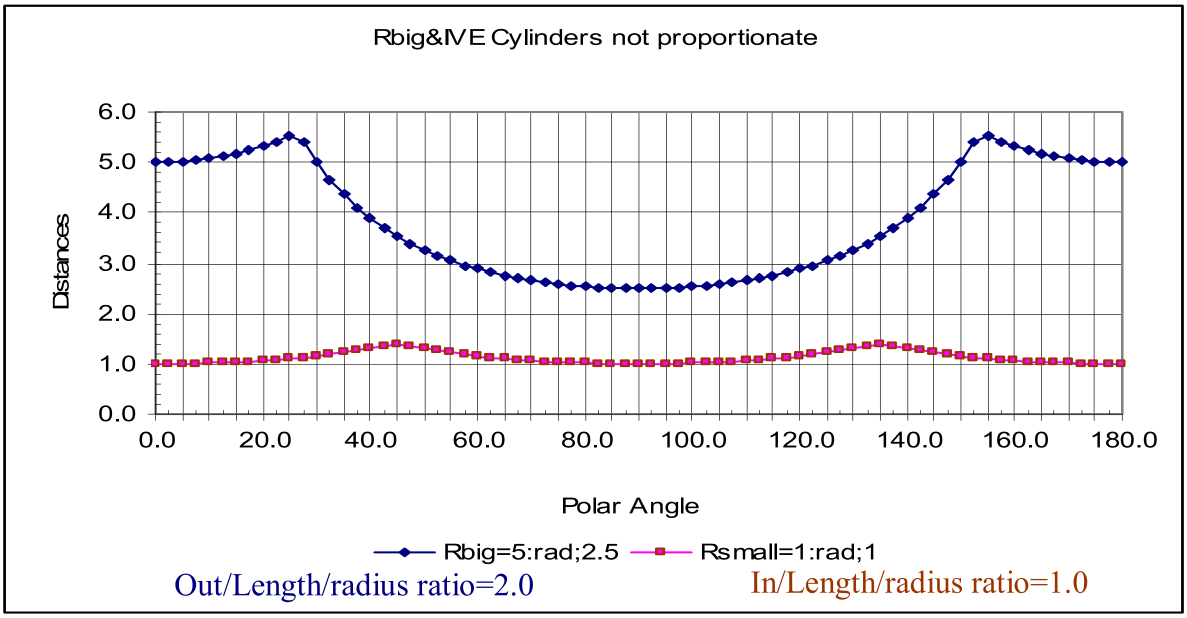
L-outercylinder Leng= 5. Rad= 2.5
IVE Sphere. Rad= 1.

L-outercylinder Leng= 5. Rad= 2.5
S-innercylinder Leng= 2. Rad= 1

Induced Field at Centre:

0.18833158E-05 >> 0.2226E-08

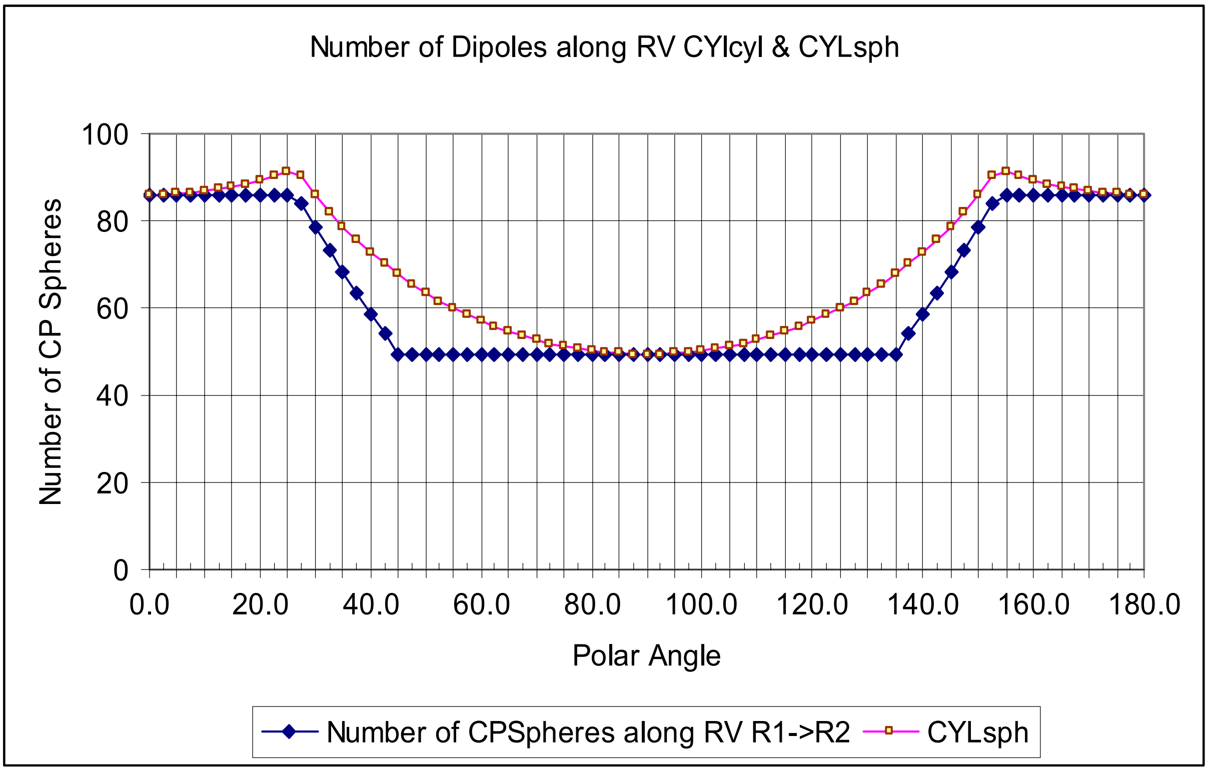




Induced Field at Centre:

For proportionate as in upper graph: 0.2226E-08

For out of proportion as in Lower graph: 0.1549E-05

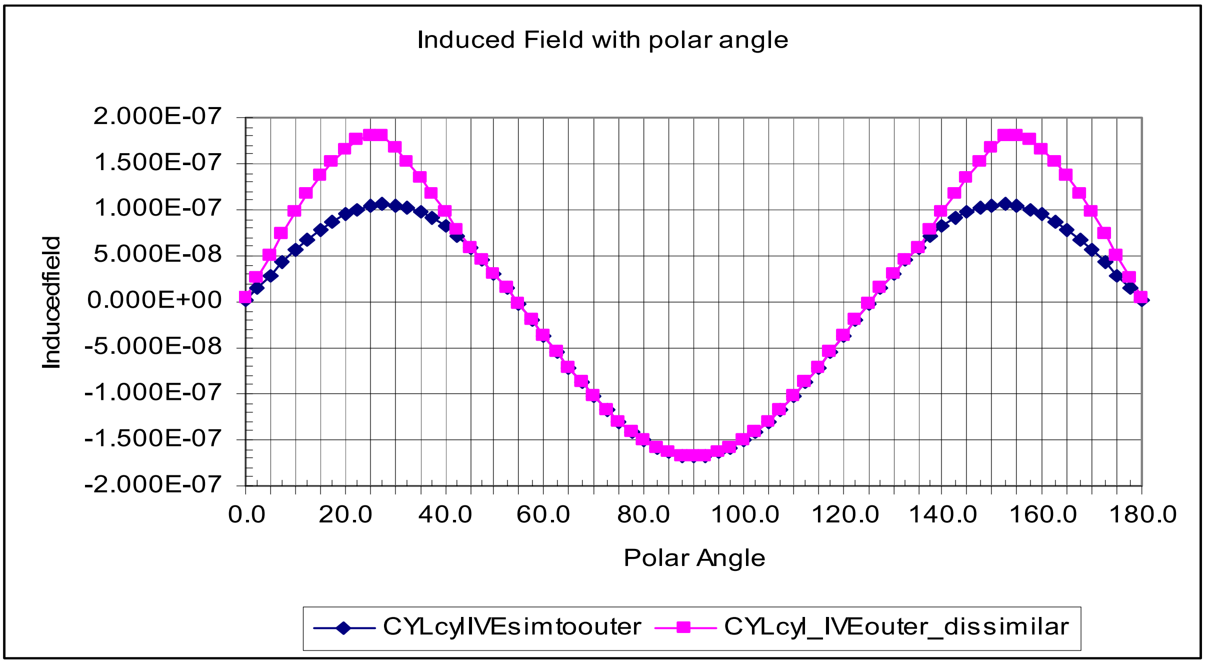


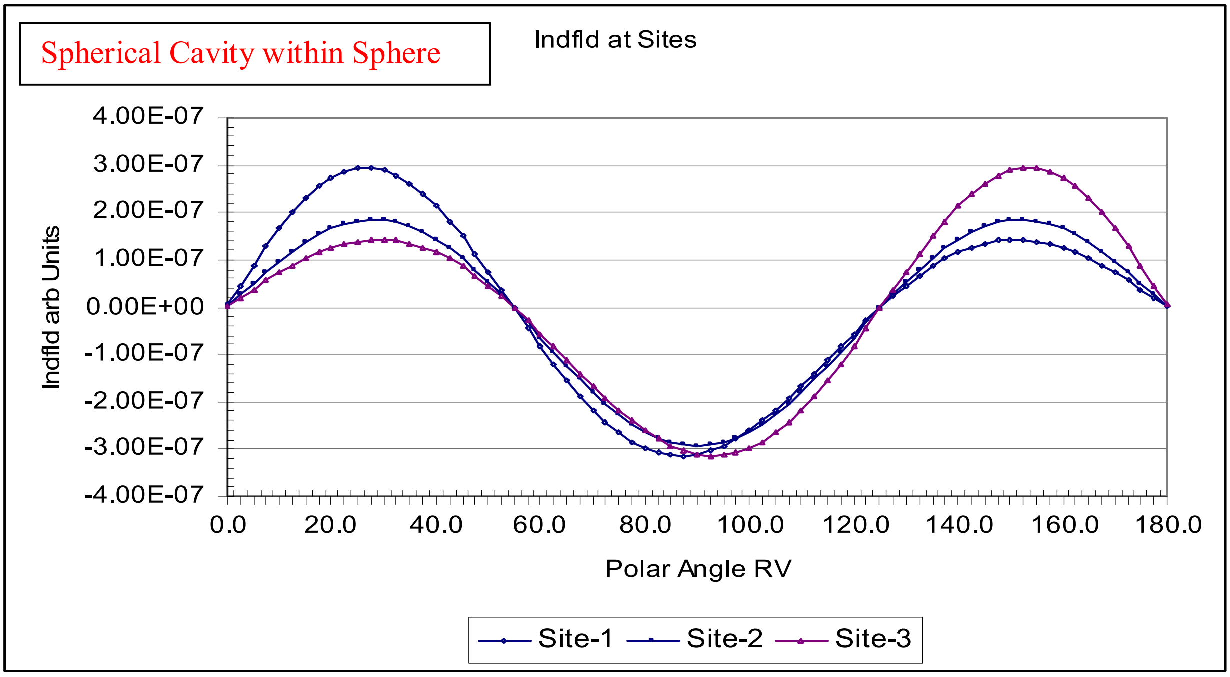
For CYLsph Induced field at the Centre **1.883316E-06**

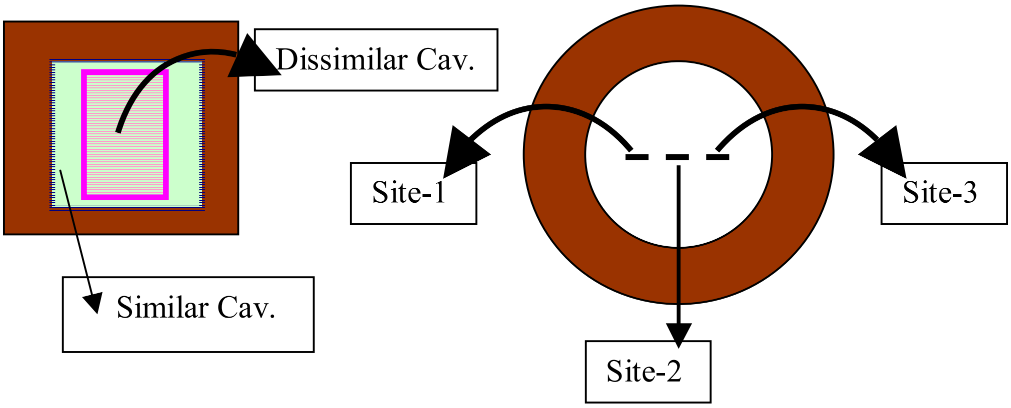
The Plot on top indicates the Spherical shape inside

For CYLcyl Induced Field at Center **1.549000E-06**

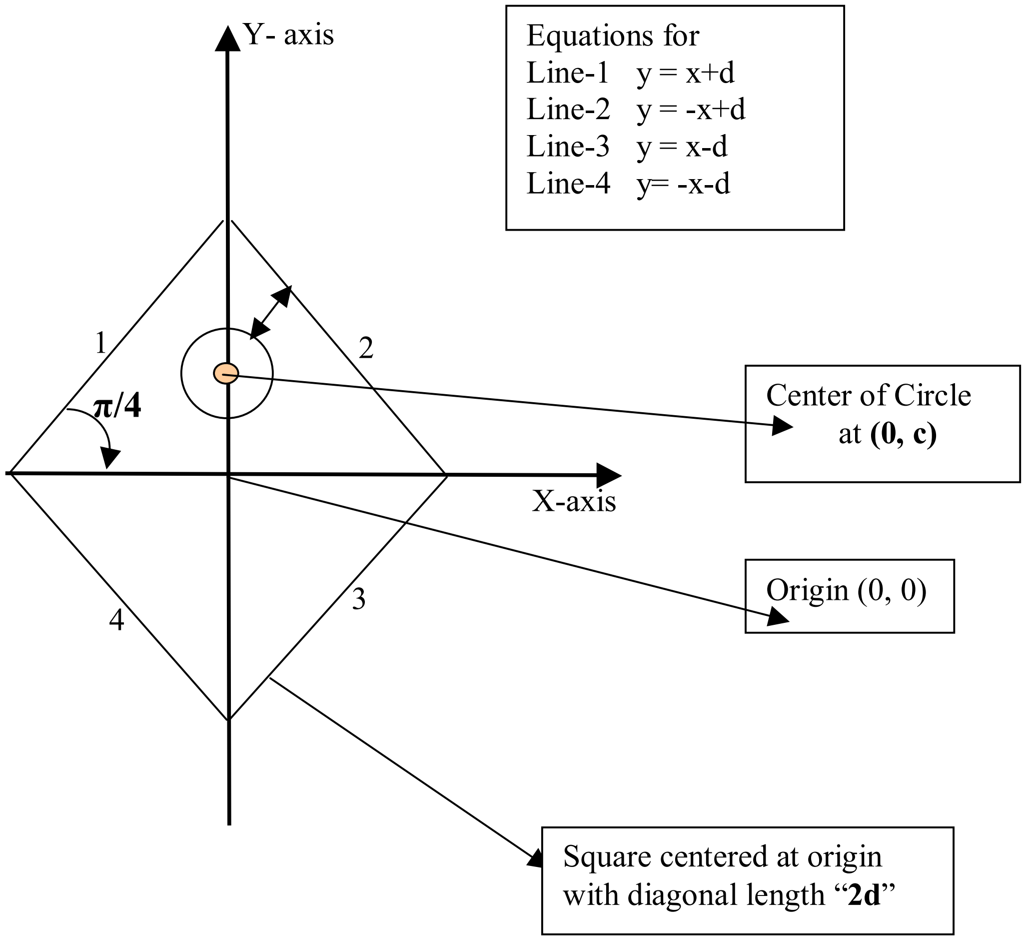
Plot below is CYLINDER (cavity) inside a Cylinder
Inner Cylinder is of same shape but not of same proportion as the outer Cylinder


Induced Field with polar angle
Inducedfield
2.000E-07
1.500E-07
1.000E-07
5.000E-08
0.000E+00
-5.000E-08
-1.000E-07
-1.500E-07
-2.000E-07
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
Polar Angle
CYLcylIVEsimtoouter
CYLcyl_IVEouter_dissimilar


Spherical Cavity within Sphere
Indfld at Sites
Indfld arb Units
4.00E-07
3.00E-07
2.00E-07
1.00E-07
0.00E+00
-1.00E-07
-2.00E-07
-3.00E-07
-4.00E-07
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
Polar Angle RV
Site-1
Site-2
Site-3


Dissimilar Cav.
Similar Cav.
Site-1
Site-3
Site-2

Equation of the Circle = $x^2 + (y-c)^2 = r^2$



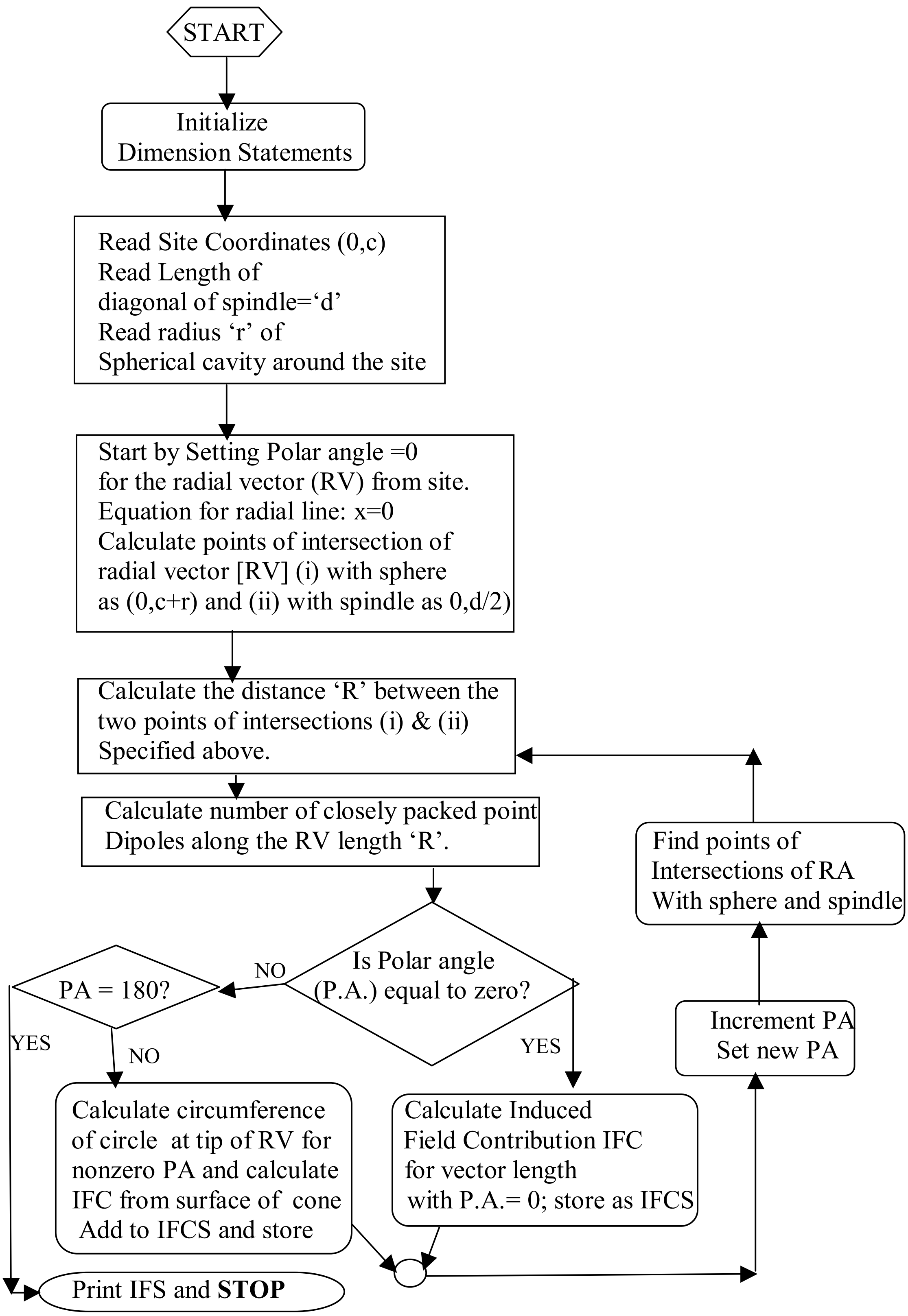
$$n = 1 + \frac{\log \dfrac{R_n}{R_1}}{\log \dfrac{C+1}{C-1}}$$

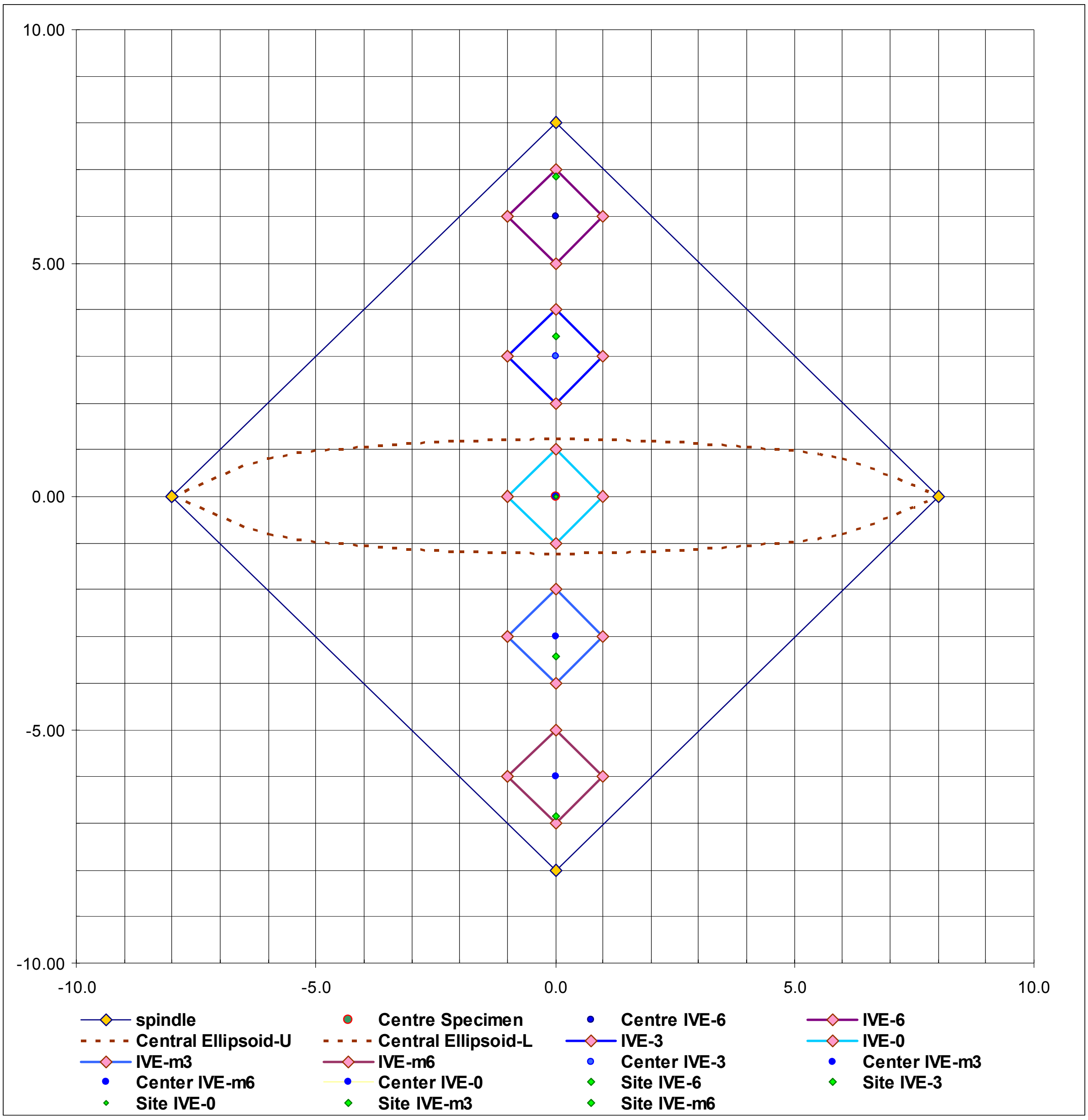
With "C= **Ri / ri , i=1,n**"

For a sphere of radius =0.25 units, and the polar angle changes at intervals of 2.5°
There will be 144 intervals. Circumference= 2π/4 so that the diameter of each sphere on the circumference = 0.0109028; radius = 0.0054514

C = R/r = 0.25 / 0.0054514 = 45.859779 [46.859779/44.859779] = 1.04458334

Log (1.0445834) = 0.0189431 $(r/R)^3$=1.0368218e-5 =0.000010368218


START
Initialize
Dimension Statements
Read Site Coordinates (0,c)
Read Length of
diagonal of spindle=‘d’
Read radius ‘r’ of
Spherical cavity around the site
Start by Setting Polar angle =0
for the radial vector (RV) from site.
Equation for radial line: x=0
Calculate points of intersection of
radial vector [RV] (i) with sphere
as (0,c+r) and (ii) with spindle as 0,d/2)
Calculate the distance ‘R’ between the
two points of intersections (i) & (ii)
Specified above.
Calculate number of closely packed point
Dipoles along the RV length ‘R’.
Find points of
Intersections of RA
With sphere and spindle
Is Polar angle
(P.A.) equal to zero?
NO
PA = 180?
YES
NO
YES
Increment PA
Set new PA
Calculate circumference
of circle at tip of RV for
nonzero PA and calculate
IFC from surface of cone
Add to IFCS and store
Calculate Induced
Field Contribution IFC
for vector length
with P.A.= 0; store as IFCS
Print IFS and STOP



0.00	6.00	6.857
0.00	5.00	5.714
0.00	4.00	4.571
0.00	3.00	3.429
0.00	2.00	2.286
0.00	1.00	1.143
0.00	0.00	0
0.00	-1.00	-1.143
0.00	-2.00	-2.286
0.00	-3.00	-3.429
0.00	-4.00	-4.571
0.00	-5.00	-5.714

1	2	3	4	5	6	7

S.No	Center of inner Cavity	Series 1	Series 2	Coordinate of SITE	Series 3	Series-4
1	6.00	-3.600761	-5.379115	6.857	-5.674923	-9.158108E-03
2	5.00	-2.207148	-3.152036	5.714	-4.218981	-9.157889E-03
3	4.00	-1.173087	-1.728898	4.571	-2.968869	-9.157839E-03
4	3.00	-0.384413	-0.695102	3.429	-1.888949	-9.159081E-03
5	2.00	0.184228	0.043739	2.286	-0.876701	-9.157531E-03
6	1.00	0.534325	0.497607	1.143	-0.213899	-9.158962E-03
7	0.00	0.653988	0.653988	0.000	-0.009159	-9.159081E-03
8	-1.00	0.534322	0.497600	-1.143	-0.213903	-9.159088E-03
9	-2.00	0.184220	0.043727	-2.286	-0.876709	-9.158664E-03
10	-3.00	-0.384428	-0.695118	-3.429	-1.888960	-9.158962E-03
11	-4.00	-1.173105	-1.728915	-4.571	-2.968877	-9.157813E-03
12	-5.00	-2.207167	-3.152055	-5.714	-4.218988	-9.157280E-03
13	-6.00	-3.600782	-5.379138	-6.857	-5.674924	-9.159162E-03

Series-1: Calculated for Spindle shaped specimen with spherical Inner Volume (CAVITY) Element around the site. But the site coordinates are NOT THE SAME as that of the CENTER (Col.2) of the INNER SPHERE. The site coordinates are inside the IVE with recalculated coordinate values (Col.5) for the site location inside the IVE.

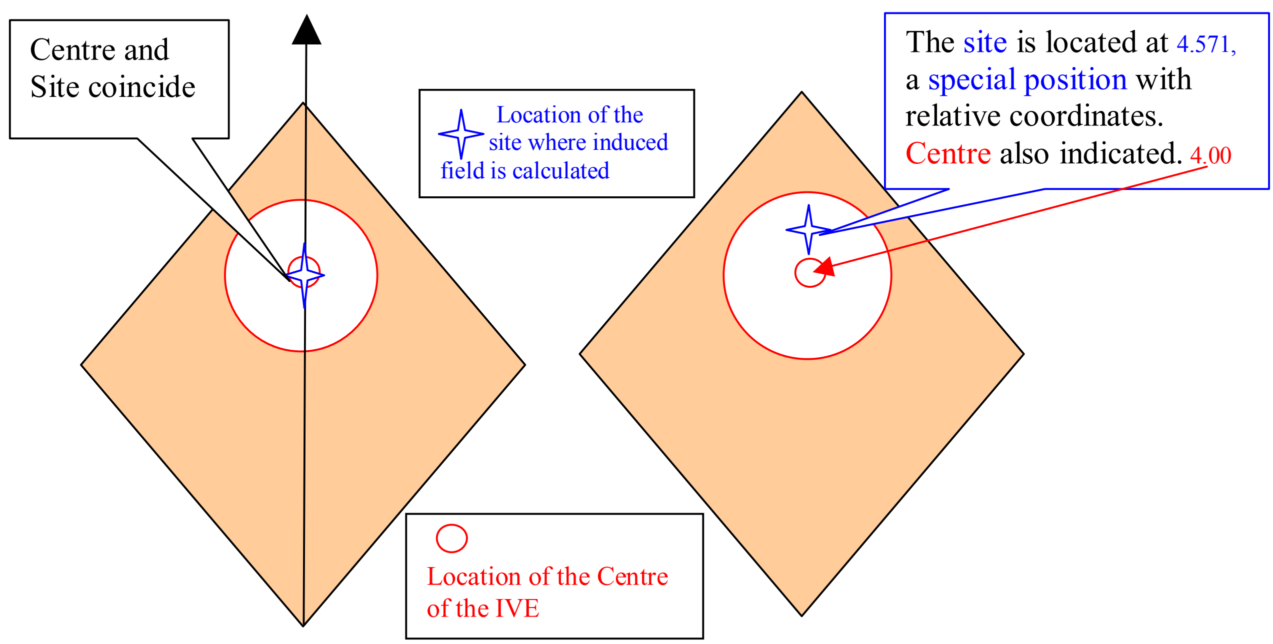
Series-2: The same case above but the site locations are at the same coordinate values as that of the center of the Spherical IVE.

In Column 6 and 7 of the Table, the calculated values are for the spindle shaped specimen with correspondingly similar spindle shaped cavity inside as the INNER VOLUME ELEMENT

Series-3: Calculated for the spindle shaped IVE at a site coinciding with center of IVE.

In column 7 the calculations are same as for Col.6 but the site is located inside IVE at a specially recalculated value.

The last column values are all the same for induced fields as if it is a homogeneously magnetized specimen (homogeneity indicated for Homogeneous specimen of spindle shape)



In the case of Inhomogeneous Magnetization due to shape dependences in homogeneous specimen (Uniform Magnetic Susceptibility) within the cavity, (the IVE), it seems possible to find at least one point where the induced field is zero which may be off-centre when the IVE has similar shape to that of the macroscopic specimen.

The possibility of carving out an cavity, an IVE is only hypothetical and depends on whether it would be possible to discretely sum the intermolecular (neighborhood molecules) contributions within the IVE and take into account separately from the macroscopic continuum contribution. This depends upon whether such a discrete sum within the IVE would converge to be able demarcate an IVE with the off center point as the site. Hence the considerations of the type held upto now on this must be repeated with the view on off-center point situations in the IVE.

But the calculations carried out till now with this procedure indicates that this is also within the reach for study and investigations might reveal interesting patterns to be discerned indicative of the nature of the magnetized material and the field distributions which arise.

Line shape and line width analysis concomitantly carried out with the hypothetical IVE and the field within them might provide much better grasp of the filed distribution patterns and pave the way for better approximations to molecular shielding tensor values in single crystals by HR PMR results besides providing leading information to the situation of IVE in a liquid sample and the time averages with varying correlation times of motions in liquids to be compared with a hypothetical rigid structure (a frozen state for example) where the discrete sum would be possible even with random and arbitrary orientations of molecules like a powder pattern.

From such studies and corresponding experimental observations with HR PMR techniques, a lot more can be inferred for the Magnetic materials with large internal fields.