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Geometric Modeling of Electrospun Micro-/Nano-Fiber System for Simulation of Physical Properties

Prasoon Kumar[1], Rishav Kumar[2]

[1]Department of Mechanical Engineering, Indian Institute of technology, Mumbai, India 400076

[2]International institute of Information Technology, Hyderabad, A.P, India

Abstract: ***Polymeric micro-/nano-fibers have potential for a variety of applications e.g. tissue engineering, filter media, biosensors, textiles etc. Many of these applications depend onporosity and pore size distribution of thesemicro-/nano-fiber meshes, that need to be characterized before any application. Therefore, in the current work, we aimed at understanding the interplay of structural and physical properties of micro-/nanofiber meshes by generating an insilico geometric model of these meshes through a novel algorithm. A new algorithm for fiber mesh generation was developed which generated fiber meshes with controlled structural parameters such as fiber diameter, length, alignment, angle of bend and fusion, thereby enabling study of physical properties. Furthermore, the surface mesh model generated by our algorithm may enablecomputational study of mechanical properties, transport phenomenon before landing upon an actual fabrication and application. This will not only save numerous attempt of trial and error method of parameter optimization during fabrication of micro-/nanofibrous materials but also save time, energy and resources.***

Keyword: Geometric modeling, solid volume fraction, micro-/nanofibers, electrospinning

1. Introduction

Fibrous materials are ubiquitous in nature having their basic units as fibers. These fibers by virtue of their assembly (random or oriented) and dimension (extremely high length to diameter ratio) impart physical and mechanical properties to these fibrous materials, which are hardly observed in any other materials. Due to such diverse properties, these polymeric fibrous materials have flexed their arms in a wide variety of applications like filters, insulators, tissue engineering scaffolds, biomedical devices, drug delivery agents, fuel cells and cosmetic/hygiene products, apart from their traditionally known usage in textiles [1-2]. The above listed applications of any fibrous materials are attributed to their high strength, toughness, ease of processibility, properties tailor ability and durability[3]. In spite of the promise posed by fibrous materials majorly micro-nanofibrous materials in the above applications, their commercial exploitation has still not achieved to an appreciable extent. The major problem lies in the fabrication of desired micro-nanofibrous materials and subsequentlytheir physical-mechanical characterization. Therefore, for any application, it is quite important to simulate mechanical or transport phenomenon of the fibrous structure before final application or fabrication. Thus, there is a need to develop a robust geometric model which can mimic the three dimensional fibrous structure of a real system.

The generation of insilico fibrous structures have been practiced since 1983, when Ghani and Davis demonstrated the fibrous mesh by straight lines in two dimension for filtration simulation[4]. Further, H Kim *et al* represented three dimensional nanofibrous mesh model by connected spherical beads[5]. A step further, B. Pourdeyhimi et al generated simulated fibrous mesh by random network of three dimensional cylinders lying over each other[6]. However, it's being much realistic model; it could not capture bending of fibers at the cross-over which is observed in a real system. Thus, Benoit Maze *et al* used square cross-sectioned long rods lying over each other and bent at the cross-over but, the essence of a cylindrical fiber was lost[7]. Therefore, 2012Kunal et al generated a fiber mesh model with cylindrical fibers bent at the cross-over[8]. Although, computational simulation of fiber mesh model have realistic model but there is stillroom for further development and assessments of physical properties by manipulation of structural properties.

Therefore, these simulated fiber mesh models not only provide a tool to access such properties but also help us to further gain insight about their properties, refine the fabrication process and finally cut down expenses on the repeated trials of experimentation.In the current work, we have developed an algorithm for generation of 3-D fibrous meshes (random and aligned) with a capability to maneuver their structural properties like diameter of fibers, pore size distribution of mesh, degree of cross-over, alignment and others. We have used the above geometric model to simulate and predict solid volume fraction (SVF). Further, we have developed surface mesh model to be used for any mechanical simulation studies.

2. Method

2.1.1Geometric Modeling algorithm

Electrospinning results in a continuous generation of micro-/nano-fibers, which get deposited on a collector randomly, forming a non-woven fibrous mesh. During the development of algorithms for the geometric model of nanofibrous structures, fibers were assumed to be falling on each other and bending at a cross-over, thereby forming layer- by-layer deposition as observed in an actual electrospinning process.

2.1.2 Assumptions

Fibers in a mesh are cylindrical with uniform diameter throughout their length. 2) Bending of a fiber occurs mainly in z- direction only. 3) Bending of a fiber occurs only at a cross-over of another fiber; it occurs only once for that fiber, if it encounters any cross-over. 4) Maximum angle of rotation is based on the fiber rigidity and length to diameter ratio of a hanging part of fiber at the cross-over.

2.1.3 Geometric modelling algorithm:

To generate 3-D fibrous mesh, we took geometric modelling approach. First, two co-ordinate points in three dimensions with z co-ordinate equal to diameter of a cylindrical fiber is chosen and a cylinder is drawn around a line segment joining these two 3-D points to represent a fiber. Then, the algorithm randomly generates two 3-D points on a fiber collection surface defined by a user with the help of random number generator such that their z co-ordinates are fixed and other x and y co-ordinates lie on the line representing the edges of fiber collection area along with a radius value for that fiber. In addition, the algorithm also facilitates the selection of two 3-D points such that they are always oriented in particular direction in x-y plane. This definitive orientation is achieved by angle range supplied by a user. Thereafter, the line segment formed by an earlier selected two three dimension points is projected in x-y plane where previousfiber line segments were already projected to determine the chance of intersection of new fiber line segment with previous deposited fiber line segments. The line segment is depicted by the equation of line in 3-dimensional space. Let the new line segment and the line segment on which new line segment is projected are given by equation (1) and (2) respectively

$$L_1 = N_1 + r \times (N_2 - N_1), r \in [0,1] \quad (1)$$

$$L_2 = N_3 + s \times (N_4 - N_3), s \in [0,1] \quad (2)$$

$$r = \frac{\{(\vec{v}\cdot\vec{v})(\vec{u}\cdot\vec{w}) - (\vec{u}\cdot\vec{u})(\vec{v}\cdot\vec{w})\}}{(\vec{u}\otimes\vec{v})^2} \quad (3)$$

$$s = \frac{\{(\vec{u}\cdot\vec{v})(\vec{u}\cdot\vec{w}) - (\vec{u}\cdot\vec{u})(\vec{v}\cdot\vec{w})\}}{(\vec{u}\otimes\vec{v})^2} \quad (4)$$

Where $\mathbf{N_1}$, $\mathbf{N_2}$, $\mathbf{N_3}$, $\mathbf{N_4}$ are four position vectors in 3-D space to represent two line segment and $\vec{u} = \overrightarrow{N_1N_2}, \vec{v} = \overrightarrow{N_3N_4}$, $\vec{w} = \overrightarrow{N_1N_3}$ are vectors joining above four position vectors. If the line segment represented by equation (1) and (2) intersects, then L_1 should be is equal to L_2.Solving the equation (1)and (2) simultaneously will provide us distinct values of r and s. By examining the values of r and s, condition for intersection can be determined:

If $0 \le r \le 1$ and $0 \le s \le 1$, intersection exists

$r < 0$ or $r > 1$ or $s < 0$ or $s > 1$ line segments do not intersect.

a) If new fiber line segment is intersecting with all the underneath fibers, it is placed above the fiber line segment which is having the highest z co-ordinate value such that the two fibers lie on each other satisfying the condition of degree of cross-over (defined by user).
b) If new fiber line segment is intersecting with none of the underneath fibers, it is placed at the height equal to its radius value such that the fiber just touches the x-y plane.
c) If new fiber line segment is intersecting only some of the underneath fibers, then it is placed above the intersected line segment which is having highest z co-ordinate value such that the two fiber lie on each other satisfying the condition of degree of cross-over defined by an user.

When a fiber line segment intersects the other line segment, then it bends at a cross-over according to maximum allowable angle of bending. This angle is further determined on the basis of a fiber rigidity and its length to diameter ratio, where length is the length of the overhang part of thefiber at a junction of a cross-over. Although the bending of fiber during the electrospinning process is governed by numerous factors like physical and rheological state of polymeric fiber, the impact velocity of the fiber approaching the stationary previously deposited. However, our current algorithm allows bending angle to be supplied by user defined by the rigidity of a fiber. When new fiber line segment intersects with earlier deposited fiber line segment, the new fiber line segment is divided into head and tail part as shown in figure 1. The head and tail part of the line segments are again projected onto x-y plane to determine the numbers of fibersthey are going to have a cross-over with. Thereafter, those numbers of fiber line segments are taken in a subset matrix and searched for the minimum distance from the head or tail region. Thereafter, they need to descend vertically before touching any otherfiber line segment. This distance is calculated by the formula given by the shortest distance between two 3-D line segments shown in equation (5)

$L_1 = N_1 + r \times (N_2 - N_1), r \in [0,1]$ the projected line segment

$L_2 = N_3 + s \times (N_4 - N_3), s \in [0,1]$....the new line segment

$$d_{\min} = |L_2 L_1| \quad (5)$$

Thereafter, from the minimum distance and length of head and tail part, the angle needed for bending a fibre is determined by equation (6)

$$\theta = \tan^{-1}(h/l) \quad (6)$$

Where h is minimum distance and l is the length of head or tail part of the fiber at the cross-over.Then two free ends of the head and tail part of new fiber line segment are rotated about an arbitrary line perpendicular to head or tail part of the new fiber line segments by an angle determined by above method. If the angle is less than maximum allowable angle of bending supplied by user, then the rotation of free ends of head and tail part is carried out using above angle but in all other case bending is carried out using maximum allowable angle of bending. The new points after rotation about and arbitrary axis are given by equation (7)

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \left(T^{-1} R_x^{-1} R_y^{-1} R_z R_y R_x T\right) \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} \quad (7)$$

Where x', y', z' are points after rotation, x, y, z are points before rotation, R_z,R_y,R_x,T are rotation and translation matrix respectively. Then, these new points are stored in matrix along with the point of bending as two new fibers line segments as shown in figure 1. Then using these three points, two cylinders representing the bentfibers are created.

Then two new 3-D points are determined for next placement. This entire process is repeated until the weight of fiber deposited becomes equal or more than the maximum weight of fiber supplied by user.

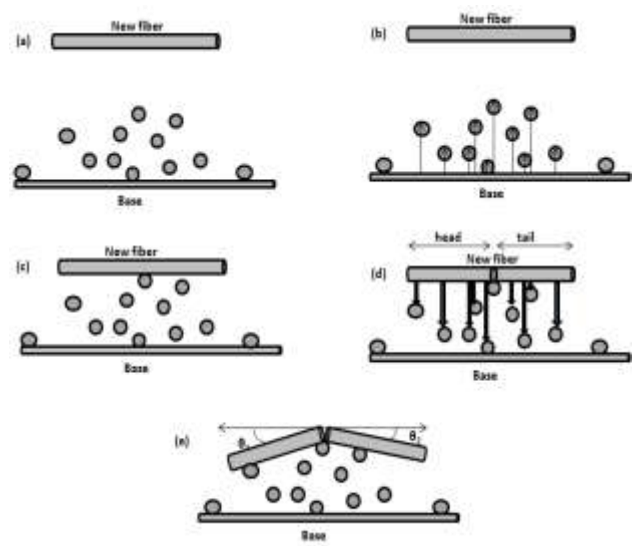

Figure 1 Diagrammatic representations of fiber mesh generation algorithm step inspired from source[8].a) A new fiber is generated above the rest of the fiberb) Height of all the fibers below the new fiber is measured such that whenever a new fiber is made to fall it just touches the fiber underneath c) The largest of all the height is taken and subtracted from height of new fiber to get distance by which it will move vertically to touch that fiber. d) The new fiber is divided into head and tail region and then steps from b to c is repeated to find the smallest distance from below fiberse) The smallest distance divided by length of head or tail region gives the tan (θ) and then end points are rotated by that angle if it is less that maximum allowable angle of rotation.

Thus, the algorithm allows the generation of 3-D fibrous mesh with number of input parameters as summarized in Table (1). The algorithm not only generates the 3-D fibrous mesh but also estimates the physical properties associated with fibrous meshes. It calculates the diameter, length, and angle distribution of fibers deposited during mesh generation. As the fibers are having extremely high aspect ratio, so we have calculated I- randomness [9] which is just the angle made by a fiber when projected onto xy-plane with that of x-axis as a parameter to represent the randomness. The quantification of the randomness is determined by skewness of the angle or orientation distribution curve. The degree of alignment is defined as the magnitude of the angular standard deviation from the mean angle in calculated I- randomness data*i.e.* lower is the angular deviation; higher is the degree of alignment and vice-versa. During bending, there is certain loss of volume (figure 1) but it is considered negligible in comparison to the total volume of fibers present in the mesh. The apparent density is calculated as ratio of mass of fiber deposited to the volume of box in which it is being collected. As the surface area to volume ratio for fibrous material is an important parameter, the surface area of fibrous mesh is calculated by summing up the surface area of all the fibers present in it. The solid volume fraction (SVF) is defined as ratio of volume of fibers present in the fiber mesh to the actual volume of box in which fibers are being collected. It is calculated as the percentage volume of box occupied by fibers. The porosity of the fiber mesh is unity minus the solid volume fraction. These parameters govern the physical and mechanical properties of fibrous mesh. The input and output parameter defined in the algorithm are summarized in the Table 1.The pore size distribution was determined indirectly by application of statistical model developed by Eischhorn and Sampson [10]. The model was implemented in an algorithm to estimate the pore size distribution in fiber mesh generated by above algorithm. Furthermore, the pore size was obtained as mean pore diameter assuming it to be circular by using an approach developed by Deng and Dodson[11]. The pore size has been expressed as a statistical relation between diameter, length and number of fibers present in a fibrous mat. Eventually, the pore size and their distribution are one of the important parameter while studying or applying them for any transport processes.

Modelling physical properties of fiber mesh

Electrospinning produces fibrous mesh with fibers with dimension in micron to nanometer range, which arecontinuous in nature with very high length to diameter ratio. By modulating the different input parameters of electrospinning, it is possible to make random, fused, aligned fiber meshes. Moreover, these fibrous meshes are also highly porous in nature with a very high surface area. Due to the above properties, they have been extensively explored in various applications. Porosity and pore size being the inherent property of such fibrous mesh, they need to be studied extensively and characterized thoroughly before such meshes could be used in any application. To determine the effect of various input parameters of mesh such as the radius of fiber present in the mesh, alignment of fibers, degree of cross-over among the fibers, collection area, weight of fiber deposited and stiffness of fiber indicated by the angle of bending of fibers at cross-over of another fiber on porosity or solid volume fraction, simulation of the fiber mesh generation were performed by changing the above mentioned parameters. The graphs were plotted between the solid volume fraction and various parameters to study and establish the relation between them. Further, as a statistical method was being used to predict the pore size distribution, the effect of diameter of fibers in a fibrous mat on pore size distribution was studied by keeping the number of fibers to be constant. Similar studies were performed to quantify the effect of the number of fiber on pore size distribution function keeping the diameter constant. Thus, with the help of the geometric model of fibrous mesh, simulation of physical properties can provide us useful insight into changes in physical properties due to various structural parameters of fibrous mesh

3. Results and Discussion

Electrospinning is a facsimile technique exploited primarily for fabrication of nanofibrous matrices. So, we have developed a mathematical approach to generate *insilico* geometrical model of random and aligned fiber meshes. In this model, fiber were assumed to be cylindrical in nature with very high aspect ratio lying over each other with a bend at the cross-over as observed in electrospun micro-

/nanofiberous systems. We have also developed an algorithm to generate mimickingelectrospun micro-/nanofiberous systems which can be further used for physical-mechanical simulation studies. The algorithm providesus the facilities for input of various structural parameters to obtain various physical characteristics as output from the model as listed in the Table 1. Furthermore, the algorithm enables conversion of geometric model to a surface mesh model. This feature of model enables fibrous mesh model to be converted to a solid model for any mechanical/transport analysis by finite element method. The qualitative assessment through figure 2 shows the comparison between the images of fiber meshes obtained by electrospinning and images generated from our algorithm. The gross morphology of the fibrous structure resembles quite well with the SEM images of actual electrospun fiber meshes.

Table 1: Input and output parameter in an algorithm.

S. No	Input	Output
1	Total weight of fibrous mat	Randomness
2	Fiber collection area	Solid volume fraction
3	Diameter range	Apparent density
4	Orientation angle range	Pore size and its distribution
5	Degree of cross-over	Surface area
6	Max. Angle of bending	Diameter Length and alignment

The algorithm has been developed to get a desired fibrous mesh for physical and mechanical analysis depending on its input structural properties. We have simulated the fibrous structure and studied the role of different structural factors governing the solid volume fraction of the mesh. The physical properties of any fibrous mesh were dependent on the structural features of fibers in a mesh.

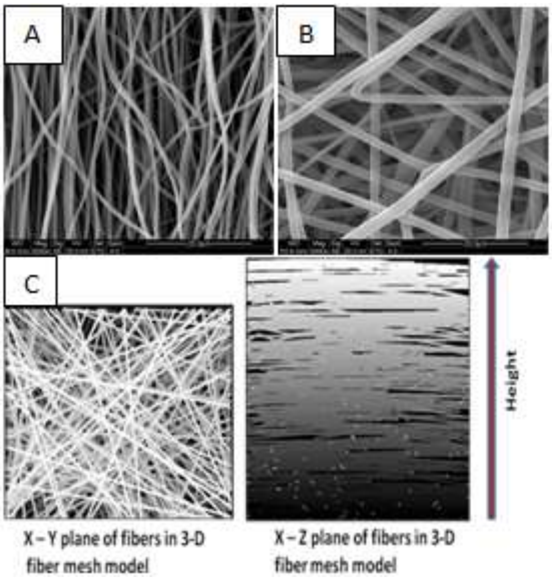

Figure 2: A) Random electrospunfiber mesh B) aligned electrospunfiber mesh C) 10X10 mm fiber mesh generated by algorithm having weight of 0.5mg and diameter of 50µm. Left is the top view and Right is the side view.

From the simulation of random fiber mesh generation, we found that solid volume fraction (SVF) remain constant with increasing weight of fiber deposited (figure 3A) provided other parameters like collection area, radius of fiber, degree of cross-over and degree of bending were kept constant. This lead to an increase in thickness of fiber mat deposited although SVF remained same. Thus the packing of fibers remained same in fibrous mesh although the mass of fiber deposited increases. The packing fraction depends on the way of deposition of fibers. When collection area was increased, the solid volume fraction increased linearly (figure 3B) with it for same mass of fiber deposition while other parameters like degree of bend, degree of cross-over, radius of fibers were kept constant. The thickness of the fiber mat decreased with the increase in fiber collection area and there was exponential relationship between thickness and collection area. Due to increase in collection area with constant mass of fiber deposited, the packing fraction might have changed but when the mass of fiber deposited is very high, the SVF becomes constant with slight increase in collection area. When radius of fiber deposited decreases, there is exponential increase in surface area of fibrous mat. These are the essential features of fibrous material, so these properties need to be studied extensively before any application.

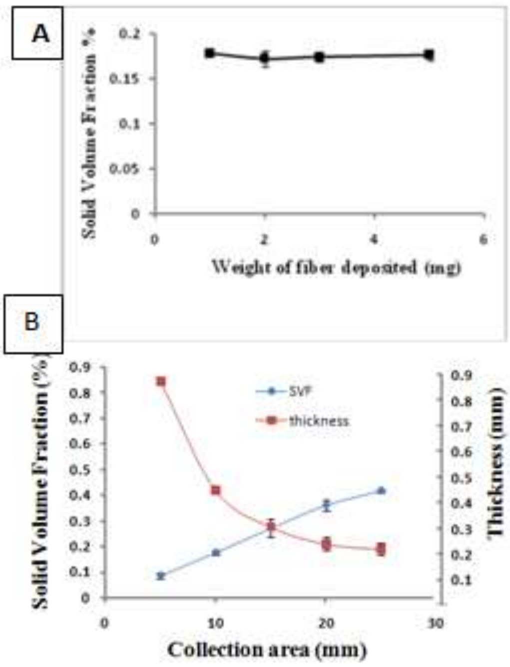

Figure 3 : A) Variation of solid volume fraction with weight of fiber deposited keeping radius of fiber-5micron, degree of cross-over-1, degree of bend -10 degree and fiber collection area- 10X10mm^{2}B) Variation of solid volume fraction and thickness of sample with collection area keeping radius of fiber -5micron, wt -0.1mg, degree of cross-over -1 and degree of bend - 10 degree

A graph was plotted between the solid volume fraction and degree of bend while keeping all other parameters such as mass of fiber deposited, radius of fibers, collecting area, degree of cross-over and density of material to be constant. This degree of bend is overall representation of nature of polymeric material; rheological state of the fiber deposited etc. From the, figure 4A it was clear that solid volume fraction increased with increase in bending angle, but then it became nearly constant indicating that SVF percentage increases with decrease in fiber stiffness but to a certain extent only. Thereafter material stiffness had limited role in the porosity or solid volume fraction. The SVF increased with decrease in the degree of cross-over, at higher value, as seen in the figure 4B, the SVF was nearly constant but at very low value like 0.01, the solid volume fraction increased to a significant amount. The fiber meshes with high degree of cross-over may be having properties comparable to solvent cast rather than electrospun fiber mesh.

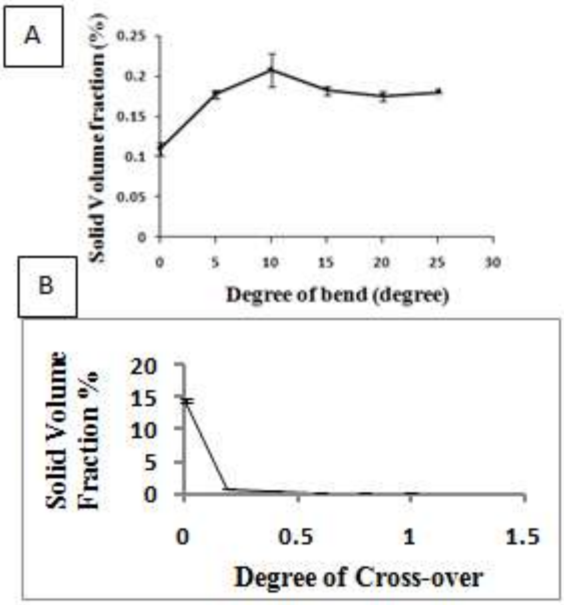

Figure 4: A) SVF vs. Degree of bending of fibers with radius of fiber - 5micron, wt- 0.5mg, degree of cross-over -1 and fiber collection area -10X10mm^2 SVF vs. Degree of cross-over among fibers with radius of fiber -5 micron, wt-0.5mg, degree of bending-10 and fiber collecting area-10X10mm^2

Further simulations were carried out to study the role of radius of fiber and the relative alignment of fiber on the solid volume fraction. From the figure, it was clear that solid volume fraction holds linear relationship with diameter of fibers (figure 5A). The solid volume fraction increased with increase in radius of fibers in the mesh. Similar trends were observed in the fiber mesh where fibers were either bend or straight. The SVF of fiber mesh decreased in aligned fiber mesh system as compared to random fiber mesh system. This may be due to the increased packing arrangement of fibers in aligned state which leaves very less void space. In the random fiber mesh, there no such packing arrangement thus resulting in increased porosity.

Thepore size distribution is inherent property of fibrous mesh and it needs to be characterized as it is of importance in tissue engineering, filtration etc. The pore size distribution function variation with radius of fibers in a fibrous mat is shown in the figure 5B. As the diameter or the number of fibers in the mesh was increased, there was decrease in pore size and increase in number of pores with small size variation. Thus, pore size and its distribution are governed by radius of fibers which can controlled during a fabrication process.

Thus, these properties being essential for any applications need to be characterized *insilico* to arrive at the structural parameters of the fiber meshes which is required to be manipulated during the fabrication process without much trial and error.

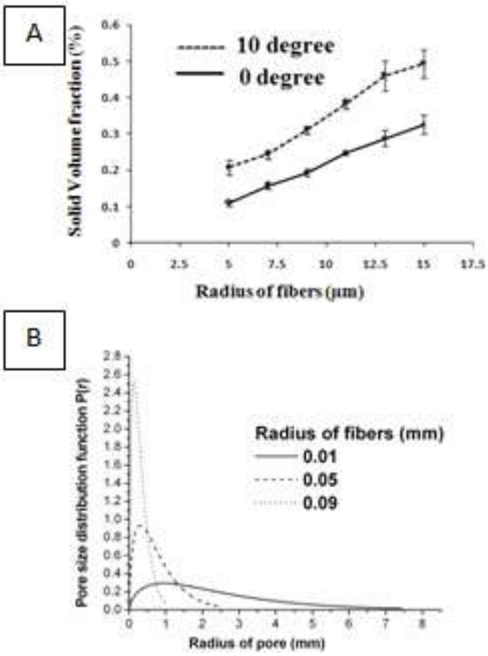

Figure A) 5 SVF % vs. Radiuskeepingwt-0.5mg, degree of cross-over-1 and fiber collecting area-10X10mm^{2}B) Graph of pore size distribution function variation with radius of fibre

4. Conclusion

Polymeric micro-/nano-fibers have potential for a variety of applications e.g. tissue engineering, filter media, biosensors, textiles etc. Many of these applications depend on the porosity and pore size distribution of these micro-nanofiber meshes that need to be characterized before any application. We have successfully designed and developed an algorithm for generation of an insilico geometric model of the micro-/nano-fiber meshes. The algorithm of geometric model enables the variation of different structural parameters of fiber meshes. Thus, this tool enables us to generate fiber meshes computationally with varied structural properties for physical, mechanical and transport phenomenon analysis. Our physical analysis suggested the dependence of diameter, degree of cross-over, degree of bending, mass of fiber mesh etc. on the porosity, surface area and pore size distribution. Thus above method will not only save numerous attempts of trial and error method of parameter optimization during fabrication of micro-/nanofibrous materials but also save time, energy and resources.

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Author Profile

Prasoon Kumar received the BE in Biotechnology from Birla Institute of Technology, Mesra, Ranchi and MTech in Biosciences and Bioengineering from Indian Institute of Technology, Kanpur in 2008 and 2010, respectively. During 2010-2011, he stayed at Central Scientific Instruments Organization (CSIO-CSIR), as a Project Assistant (level-III). He is now pursuing PhD in Mechanical Engineering from IITB-Monash Research Academy (2011-Present), Mumbai. His research interests are micro-/nanofabrication, micro-/nanofluidics, biomaterials, Image processing and Tissue engineering.

Rishav Kumar is currently pursuing B.Tech. in Electronics and Communication Engineering from International Institute of Information Technology, Hyderabad. His research interests are robotics, signal and image processing, programming languages.