Minimum damping profile of micro/nano-robot and as the carrier for drug delivery: theory study

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Abstract. The use of the micro/nano-robot as a carrier for drug delivery in vivo represent a novel and innovative method in cancer/tumor therapy and related biomedical applications. In this paper, the authors firstly deduce the minimum damping profile of micro/nano-robot as it locomoting in vascular and capillaries system. Where originating from the Bernoulli’s equation, and integrating the calculus of variations with the Euler-Lagrange equation, then the profile of micro/nano-robot which the generatrix of this axisymmetric body is the 4/3 order of the curve is obtained. Following, the elastic responses of the cell indented by this profile are studied detailedly. Utilizing the method of continuum mechanics, the interior stress and displacement distributions, indentation depth, surface stress distribution (corresponding the critical rupture stress of cytomembrane) and applied force (corresponding the required force output from micro/nano-robot) are derived. Furthermore, those elastic responses indented by conical and spherical profile are computed and contrasted. Conclusively, the authors provide a design reference for the profile of micro/nano-robot as a carrier for drug delivery, and deduce the elastic responses of the cell when it penetrated by the body of micro/nano-robot.

1. Introduction

The single-cell-based nanotechnologies have been very popular in the cancer/tumor therapy [1], induced pluripotent stem cells (iPs) technology [2], medical imaging technology and related cell-engineering fields, which require delivering the nanoscale objects (therapeutic drug, or the special biomolecular factors/gene, or the medical imaging material) into the cell. The easy implement, high precision and effective target transfection are key considerations for evaluating the way of this transporting. Summarily, there are two main patterns (active and passive pattern) to complete this transportation in vivo/vitro for the single cell.

Electroporation is a typical active pattern of transportation, which combines the microfluidic with microchannel technology, and actuated by microelectrode [3], making up a nanofountain-probe (NFP) that can deliver the nanoscale objects into the cell in vitro [4]. High transportation efficiency can be achieved through electroporation, yet the damage of cell by electric field also can’t be ignored. In addition, those methods are not facilitate to implement in vivo.

Endocytosis is the other main way but a passive pattern, which utilize the natural properties of cell membrane-endocytosis effect and mediated by nanoparticle [5], to complete the drug
delivery/transportation [6]. Yet the diverse and intricate biochemical environment and fluctuating force of cell membrane, will give rise to (may misleading the bonding) low efficiency binding between nanoparticle and targeted diseased cell membrane.

Based on the analysis above, all limitations of the ways of electroporation and endocytosis will be overcame if there will be a smart micro/nano-robot [7], that be capable of initiative self-locomoting in vascular and actively penetrating the cytomembrane for drug delivery in vivo [8]. For this newly arisen robotics research area there are many related works have been done [9]. Especially for the propulsion principle which is crucial component for the safe and sustainable operation in vivo, including magnetic, ultrasound, optical, thermal, electrical, acoustic, and enzyme-functionalized, have been put forward for the micro/nano-robot [10]. However, the quantitative evaluation of penetrating force output from the micro/nano-robot which also is the applied force to puncture the cytomembrane have not been investigated, yet will be investigated in current paper.

In this paper, the authors firstly deduce the minimum damping profile of micro/nano-robot as it locomoting in vascular and capillaries system. Where originating from the Bernoulli’s equation, and utilizing method of calculus of variations and Euler-Lagrange equation, then profile of micro/nano-robot which the generatrix of this axisymmetric body is the 4/3 order of the curve is obtained. Secondly, the elastic responses of the cell penetrated by this profile of micro/nano-robot are studied systematically. Based on the elementary solution of axisymmetric problem in elastic mechanics and employing the method of contact mechanics, the interior stress and displacement distributions, the indentation depth, the normal surface stress distribution (provide a quantitative indicator to understand the critical rupture stress of cell membranes), the applied load (corresponding the required force that micro/nano-robot shall output), and their interrelationships are investigated. Finally, cases of conical and spherical profile of micro/nano-robot also be calculated and contrasted.

2. Minimum damping profile of micro/nano-robot

As the micro/nano-robot locomoting in the blood capillary or extracellular matrix, its geometric shape which suffering minimal resistance is required that within a certain propulsion power. Nonetheless, the microfluidic effect have not been considered that may make important influence in the moving process as micro/nano-robot locomoting in microfluidic environment. Yet regarding the microenvironment as the incompressible flow and leaving out the friction effect between the interface, therefore the Bernoulli’s equation [11] was introduced as follow

\[
\frac{V^2}{2} + g \cdot z + \frac{P}{\rho} = C
\]  

(1)

Moreover, the gravity effect can be neglected as the negligible difference at height dimension. Taking those factors into consideration, and consider the pressure along the x-coordinate that the micro/nano-robot suffering, as shown in figure 1-(a) which the micro/nano-robot locomoting in vascular and capillary medium.

![Figure 1. Schematic illustration of the micro/nanorobot-mediated drug delivery process. (a). Schematic of the micro/nano-robot locomoting in vascular and capillaries system, where the](image)
minimum damping profile of micro/nano-robot is required. (b). When the macro/nano-robot arriving at the area of diseased cells, it will going on to actively puncture the cell membrane to inject nanoscale objections into the cell. (c). In the indentation process there are four significant variables needed to be considered: the surface stress distribution on the cytomembrane, the applied load $P$, and the contact radius $a$ and the penetrating depth $D$, which can also be used in related field like measurement of modulus of softmatter. (d). The accompanying stimulation of interior stress and displacement on the certain(targeted) protein inside the cell also are important factors for evaluating this whole processes.

Then Bernouli’s as above can be reduced and transformed to,

$$p_x = c_1 \cdot \rho \cdot v^2 \cdot \sin^2 \theta$$

where $p_x$ is the components of pressure along the $x$-axis at chosen point. $c_1$ is the arbitrary constant $\rho$ is the density of the fluid at all points in the fluid, $v$ is the speed of fluid flow at a point on a streamline.

Following, the per unit force of micro/nano-robot received can be obtained by multiply the pressure at a point with the unit area of thrust surface. Combining with the simple mathematical derivation the per unit force can be got

$$dF_x = 2\pi \cdot c_1 \cdot \rho \cdot v^2 \cdot y \cdot (y')^3 \cdot dx$$

Further, the functional expression of the total force that the micro/nano-robot received under it’s a certain profile of head shape $y(x)$, noted with $J[y]$, that can be formulated as

$$J[y] = \int dF_x = 2\pi \cdot c_1 \cdot \rho \cdot v^2 \cdot \int_0^L y \cdot (y')^3 \cdot dx$$

Among above expression, introducing the notation $W = y \cdot (y')^3$ and considering the one-dimensional Euler-Lagrange equation [12], which given by

$$\frac{\partial W}{\partial y} - \frac{d}{dx} \left( \frac{\partial W}{\partial y'} \right) = 0$$

and incorporating with the boundary conditions

$$y(0) = 0, y(L) = R$$

where $L$ is the length and $R$ is the radius at length of $L$ of the revolved axisymmetric profile of body of micro/nano-robot. Then the profile of minimum damping force that the micro/nano-robot suffering when it locomoting in vascular systems, can be deduced as

$$y = L^{3/4} \cdot R \cdot x^{3/4}$$

For keeping accordance with following processing in cylindrical coordinates, the function of the micro/nano-robot profile can be written as follow,

$$z = L \cdot R^{-4/3} \cdot r^{4/3}$$

3. Elastic responses of cell indented by the micro/nano-robot

With the above derived profile of micro/nano-robot from fluid mechanics, then it will going on to actively puncture the cytomembrane to inject the nanoscale objections into the cell, as shown in figure 1(b). The quantitative understanding of the normal surface stress distribution on cytomembrane indented by this profile, the corresponding required output force from micro/nano-robot and the interior displacement/stress distribution will be studied, as shown in figure 1(c-d). Different from adopting means of the molecular dynamics which considering the interaction potential between two atoms (or particles), but the elastic mechanics especially contact mechanics was employed to study this penetrating process.

3.1 Interior stress and displacement components
Regarding the whole problem is axisymmetric and the cylindrical coordinates system is adopted where the displacement components are \((u_r, u_z)\) and the stress components are \((\tau_{zr}, \sigma_z, \sigma_r, \sigma_\theta)\) while other components are vanish. The Young modulus of the micro/nano-robot was assumed to be stiffer far more than the cell’s modulus and the target cell can be approximately treated as an isotropic semi-space. There are two boundary conditions in this problem, as follow

\[
\begin{align*}
 u_z (0 < r < a, z = 0) &= D - g(r), & \sigma_z (r \geq a, z = 0) &= 0
\end{align*}
\]

where a is the radius of the contact area, D is arbitrarily parameter which regarded as the depth of the penetrating, \(g(r)\) is formulated to characterize the profile features of the micro/nano-robot.

Based on the elementary solutions deduced by Sneddon [13], the components of displacements and stress variables can be expressed in form of function \(\psi(\zeta)\) and considering \(r = \rho \cdot a\), thus

\[
\begin{align*}
 u_z (\rho, z) &= H_0 \left[ \psi(\zeta) \cdot \left( \frac{\lambda + \mu}{\lambda + 2\mu} \cdot \frac{z}{a} + \frac{a}{\zeta} \right) \cdot \zeta^{-1} \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right] \\
 \sigma_z (\rho, z) &= -\frac{2\mu \cdot (\lambda + \mu)}{\lambda + 2\mu} \cdot H_0 \left[ \psi(\zeta) \cdot \left( 1 + \frac{\zeta}{a} \cdot \frac{z}{a} \right) \cdot \frac{1}{\zeta \cdot a} \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right]
\end{align*}
\]

where \(H_0\) denotes the Hankel transform, \(\lambda, \mu\) are known as Lame constants, and the \(\psi(\zeta)\) denotes the function that related the profile of micro/nano-robot. Combining with the boundary conditions, the above two solutions can be reduced to a pair of dual integral equations which had been solved by Sneddon [13]. Substituting the minimum damping profile of micro/nano-robot (as shown in Equation (8) into the solution of dual integral, thus

\[
\begin{align*}
 \psi(\zeta) &= \frac{2}{\pi} \cdot D \cdot \sin \zeta - \frac{L}{2} \cdot \frac{a^{4/3}}{R} \cdot \beta \left( \frac{5}{3} \cdot \frac{1}{2} \right) \cdot \zeta \cdot \left[ \cos \zeta + \zeta \cdot \int_0^1 t^{7/3} \cdot \sin(\zeta \cdot t) \, dt \right] \\
 \text{and substituting the } \psi(\zeta) \text{ into the normal stress components Equation (12) and considering the stress on the contact periphery } \sigma_z (r = a, z = 0) = 0, \text{ then having}
\end{align*}
\]

\[
\begin{align*}
 2D \cdot \frac{7}{3} \cdot \frac{L}{9} \cdot \frac{a^{4/3}}{R} \cdot \beta \left( \frac{5}{3} \cdot \frac{1}{2} \right) &= 0, \quad \psi(\zeta) = \frac{28}{9 \pi} \cdot \frac{L}{a} \cdot \frac{a^{4/3}}{R} \cdot \beta \left( \frac{5}{3} \cdot \frac{1}{2} \right) \cdot \int_0^1 t^{7/3} \cdot \sin(\zeta \cdot t) \, dt
\end{align*}
\]

Furthermore, other four components which firstly derived by Sneddon also can be rewrote in form of function \(\psi(\zeta)\):

\[
\begin{align*}
 u_\rho (\rho, z) &= H_1 \left[ \psi(\zeta) \cdot \left( \frac{\lambda + \mu}{\lambda + 2\mu} \cdot \frac{\zeta}{a} \cdot z - \frac{\mu}{\lambda + 2\mu} \cdot \frac{a}{\zeta} \cdot \zeta \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right) \\
 \tau_{z\rho} (\rho, z) &= -\frac{2\mu \cdot (\lambda + \mu)}{\lambda + 2\mu} \cdot H_1 \left[ \psi(\zeta) \cdot \frac{\zeta}{a^2} \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right] \\
 \sigma_{\rho\rho} (\rho, z) &= -\frac{2\mu \cdot (\lambda + \mu)}{\lambda + 2\mu} \cdot H_1 \left[ \psi(\zeta) \cdot \left( 1 - \frac{\zeta}{a} \cdot \frac{z}{a} \right) \cdot \frac{1}{\zeta \cdot a} \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right] + \frac{2\mu \cdot (\lambda + \mu)}{\rho \cdot a \cdot (\lambda + 2\mu)} \cdot H_1 \left[ \psi(\zeta) \cdot \left( \frac{\mu}{\lambda + \mu} - \frac{\zeta}{a} \cdot \frac{z}{a} \right) \cdot \zeta \cdot e^{\frac{-\zeta z}{a}}; \zeta \to \rho \right]
\end{align*}
\]
\[ \sigma_{\theta \theta}(\rho, z) = \frac{2\mu \cdot \lambda}{\lambda + 2\mu} \cdot H_0 \left[ \psi(\zeta) \cdot e^{\zeta z} \cdot \frac{1}{\zeta} \cdot J_0(\zeta \rho) \right] \]

\[ - \frac{2(\lambda + \mu) \cdot \mu}{\rho \cdot a \cdot (\lambda + 2\mu)} \cdot H_1 \left[ \psi(\zeta) \cdot \left( \frac{\mu}{\lambda + \mu} \cdot \frac{-\zeta}{a} \cdot z \right) \cdot \zeta^2 \cdot e^{\zeta z} \right] \cdot \zeta \to \rho \]  

By substituting the expression of \( \psi(\zeta) \) as shown in Equation (15) into the Equations (11,12,16-19), all elastic responses of the displacement and stress components in the cell which indented by the minimum damping profile of micro/nano-robot \( z = L \cdot R^{4/3} \cdot r^{4/3} \) can be obtained respectively.

### 3.2 Penetration depth, normal surface stress and applied force

Noting the result about penetrating depth in Equation (14), it can be easily calculated as

\[ D = \frac{7}{6} \cdot L \cdot \left( \frac{a}{R} \right)^{4/3} \cdot \beta \left( \frac{5}{3}, \frac{1}{2} \right) \]  

Furthermore, by substituting Equation (15) into Equation (12) and setting \( z = 0 \), the surface normal stress can be computed as

\[ \sigma_n(r, 0) = -\frac{E}{(1-v^2)} \cdot \frac{14}{3\pi} \cdot \beta \left( \frac{5}{3}, \frac{1}{2} \right) \cdot L \cdot \left( \frac{a}{R} \right)^{4/3} \cdot \left\{ \cdot F, \left[ -\frac{1}{6} \cdot \frac{1}{2} \cdot \frac{5}{6} \left( \frac{r}{a} \right)^2 \right] - \left( \frac{r}{a} \right)^{4/3} \cdot \sqrt{\pi} \cdot \Gamma \left( \frac{5}{6} \right) \cdot \Gamma^{-1} \left( \frac{1}{3} \right) \right\} \]  

Finally, the applied force \( P \) is defined as

\[ P = -2\pi \cdot \int_0^a \sigma_n(r, 0) \cdot r \cdot dr \quad 0 < r < a \]  

by substituting Equation (21) into above expression and integrating with Equation (20), the applied force \( P \) depends on penetrating depth \( D \) can be evaluated as

\[ P = \frac{E}{(1-v^2)} \cdot \frac{8}{7} \cdot \frac{7}{6} \cdot \beta \left( \frac{5}{3}, \frac{1}{2} \right)^{-3/4} \cdot L^{-3/4} \cdot R \cdot D^{7/4} \]  

Actually, the same results of penetration depth \( D \), normal surface stress distribution and applied force \( P \) also can be calculated from known formulas [14], and the difference from here is the mathematical derivations where the obtain of the formula of normal surface stress distribution is based on the full known of \( \sigma_n(r, z) \) and then setting \( z = 0 \), whereas the interior stress distributions are failed to be presented in existing classical formulas.

### 4. Comparison of elastic responses indented by three different profiles

In this section, the values of interior stress and displacement distributions, penetrating depth, normal surface stress, and applied force indented by three different profiles of micro/nanorobot will be computed and contrasted successively. Where the generatrix of the axisymmetric indenter of the micro/nanorobot: 1 order curve of the generatrix (conical profile), 4/3 order curve of the generatrix (minimum damping force), 2 order curve of the generatrix (spherical profile), will be studied respectively.

#### 4.1 Comparison of interior stress and displacement components

Like the treatment methods in Section 3 where the obtainment of function of \( \psi(\zeta) \) for the minimum damping profile (4/3 order curve of the generatrix of indenter), the functions of \( \psi_{\text{Conical}}(\zeta) \) and \( \psi_{\text{Spherical}}(\zeta) \) for conical and spherical profile can be derived analogously as below,

\[ \psi_{\text{Conical}}(\zeta) = k \cdot a \cdot \frac{1 - \cos \zeta}{\zeta}, \quad \psi_{\text{Spherical}}(\zeta) = \frac{4}{\pi} \cdot \frac{a^2}{R} \cdot \left( \frac{\sin \zeta}{\zeta^2} - \frac{\cos \zeta}{\zeta} \right) \]  

(24,25)

where \( k \) is the slope of conical indenter, \( R \) is the radius of spherical indenter.
By substituting the functions of $\psi(\zeta), \psi_{\text{Conical}}(\zeta)$ and $\psi_{\text{Spherical}}(\zeta)$ into the Equations (11-12, 16-19) respectively, the corresponding stresses and displacements distributions indented by those three different profiles of micro/nano-robot can be obtained. For the less computation and the convenience of comparison, the values of stress and displacement only on the line 1 ($z=r$) in the interior of cell (half space), as depicted in figure 1-(d), are numerically calculated as shown in figure 2.

![Figure 2](image-url)

**Figure 2.** Displacement and stress distributions along the line 1: $z=r$ (as shown in figure 1-(d)) of half space (cell) indented by three different profiles of micro/nano-robot, where the generatrix of axisymmetric indenter is $z=r; z=r^{4/3}; z=0.5r^2$ respectively. And the range of line 1 ($z=r$: 0~1.5 (um) with interval distance 0.05 (um)), the Poisson ratio of half space (cell) $\nu=0.49$ and the unified penetration depth $D=1$ (um) are set. (a) and (b) indicate the values of two displacement component $U_z$ and $U_r$. (c)-(f) show the values of four stress components $\sigma_{rr}, \sigma_{zr}, \sigma_{\theta\theta}$ and $\sigma_{zz}$ respectively, where the common part of $-E/1-\nu^2$ are departed and the value at original point (0,0) of stress components $\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{zz}$ are infinite which are not be marked in plots.

### 4.2 Comparison of penetration depth, normal surface stress and applied force

For the penetration depth indented by conical and spherical profile of micro/nano-robot, by substituting the profile of $z=r; z=0.5r^2$ into the solution of dual integral and considering the boundary condition $\sigma_z(r=a, z=0)=0$ for this type of incomplete contact, as the obtain of Equation (14) then the following relationships can be obtained,

$$D_{\text{Conical}} = \frac{\pi \cdot a \cdot k}{2}, \quad D_{\text{Spherical}} = \frac{a^2}{R}$$ \hspace{1cm} (26,27)

Furthermore, by substituting the Equations (24,25) into the normal stress components and setting $z=0$ in Equation (12), the normal surface stress distribution indented by conical and spherical profile can be computed respectively as below,

$$\sigma_{zz,\text{Conical}}(r,0) = \frac{-E}{2(1-\nu^2)} \cdot k \cdot \cosh^{-1}(\frac{2D}{\pi \cdot k \cdot r}), \quad \sigma_{zz,\text{Spherical}}(r,0) = \frac{-E}{(1-\nu^2)} \cdot \frac{2}{\pi \cdot R} \cdot \left(D \cdot R - r^2\right)^{1/2}$$ \hspace{1cm} (28,29)
Having the stress distribution of normal surface as above, the applied force can be easily deduced that based on the Equation (22), thus,

\[ P_{\text{Conical}} = \frac{E}{(1-v^2)} \cdot \frac{2}{\pi} \cdot k \cdot D^2, \quad P_{\text{Spherical}} = \frac{E}{(1-v^2)} \cdot \frac{4}{3} \cdot R^{1/2} \cdot D^{3/2} \]  

(30,31)

Immediately, those results of penetration depth \( D \), normal surface stress distribution and applied force \( P \) also can be found are identical with using the known formulas[14]. Figure 3 illustrate the numerical results of above relationships where the same contact radius \( a=1 \), and penetrating depth \( D=1 \) is fixed respectively.

Figure 3. Elastic responses of cell indented by three different profile of micro/nano-robot, where the generatrix of axisymmetric indenter is \( z=r \), \( z=r^{4/3} \), \( z=0.5r^2 \) respectively. (a) show the relationship between penetration depth \( D \) and contact radius \( a \); (b) indicates the normal stress distributions on the surface of membrane which proving a quantitative indicator to understand the critical rupture stress of cell membrane, and the common part of \((E/1-v^2)\) are departed from plot (b) and (c); (c) presents the relationship between applied force \( P \) and penetration depth \( D \) which can be used in related field like measurement of modulus of softmatter, and \( P \) also corresponding the required force output from micro/nano-robot.

5. Conclusions
In this paper, the minimal resistance profile of micro/nano-robot firstly be derived when it locomoting in the fluid environment of vascular systems. Originating from the Bernouli’s equation, combining the variational method with the one-dimensional Euler-Lagrange equation, the profile of 4/3 order curve of generatrix of axisymmetric body was obtained. Secondly, the elastic responses of the cell are studied as it was penetrated by the micro/nano-robot, which based on the Hankel transform and the elementary solution of Sneddon for solving contact mechanics. The normal surface stress distribution on the cytomembrane and the applied load \( P \) are derived respectively, which the former variable \( \sigma_{zz}(r, z=0) \) indicates the critical rupture stress of cytomembrane and the latter one \( P \) corresponding the required force that the micro/nano-robot shall output to penetrate the cell membrane. Especially the interior stress and displacements distribution of the cell are explicitly derived for the first time as we known.

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