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Numerical Simulation of Production of Microspheres from Polymer Emulsion in Microfluidic Device towards using in Drug Delivery Systems

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Abstract

The production of microspheres from polymer emulsions using microfluidic devices has shown great potential for drug delivery applications due to their ability to encapsulate and release drugs in a controlled manner. In this study, the effects of velocity, density, viscosity, and surface tension, as well as channel diameter, on microsphere generation were investigated using Fluent Ansys software. The software was programmed with the physical properties of the polymer emulsion such as density, viscosity and surface tension. Simulation will then be performed to predict fluid flow and microsphere production and improve the design of drug delivery applications based on changes in these parameters. The effects of capillary and Weber numbers are also studied.

The results of the study showed that the size of the microspheres can be controlled by adjusting the speed and diameter of the channel. Narrower microspheres resulted from narrower channel widths and higher flow rates, which could improve drug delivery efficiency, while smaller microspheres resulted from lower interfacial surface tension. The viscosity and density of the polymer emulsion significantly affected the size of the microspheres, it`s higher viscosities and densities producing smaller microspheres.

The loading and drug release properties of the microspheres created with the microfluidic technique were also predicted. The results showed that the microspheres can efficiently encapsulate drugs and release them in a controlled manner over a period of time. This is due to the high surface area to volume ratio of the microspheres, which allows for efficient drug diffusion. The ability to tune the manufacturing process using factors such as speed, density, viscosity, channel diameter, and surface tension offers a potential opportunity to design drug delivery systems with greater efficiency and fewer side effects.

Keywords: Polymer emulsion, Microfluidic, Numerical simulation, Microspheres, Drug delivery and release mechanism.

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Introduction

Because of their biocompatibility and biodegradability, natural polymer emulsions have received interest in the manufacturing of microspheres [1]. Droplet creation, droplet break-up, coalescence, and solidification are all steps involved in the synthesis of microspheres from natural polymer emulsions [2]. However, emulsion parameters such as viscosity, density, and surface tension can have a substantial impact on these processes and the resultant microspheres.

The viscosity of the emulsion affects the size and shape of the droplets. Higher viscosity can lead to smaller droplet size and higher dispersion, while lower viscosity can lead to larger droplet size and higher monochromatic dispersion. Likewise, the density and surface tension of an emulsion can affect the production and breakdown of droplets, and thus the size and uniformity of the microspheres [2].

Fluid flow and microfluidic geometry could potentially play a role in microbead production. To create beads with precise properties, numerical models are used to determine the appropriate flow rate and channel shape. For example, simulations show that narrower channels produce smaller droplet sizes and higher mono-dispersity, while larger channels produce larger droplet sizes and higher polydispersity [3].

The finite volume methodology, which is frequently used in microfluidic devices, is a computer method for modeling liquid flow and emulsion droplets. ANSYS16.1 Fluent is a commercial software tool that models fluid flow and heat transfer in complicated geometries using the finite volume approach. ANSYS16.1 Fluent was used to investigate the creation of microspheres in microfluidic devices, including those created from natural polymer emulsions [4]. Simulations can assist enhance the process of microsphere creation by anticipating the behavior of emulsion droplets and liquid flow.

Numerical simulations with ANSYS16.1 Fluent software based on finite volume engineering can be a useful tool for optimizing the generation of microspheres from natural polymer emulsions in microfluidic devices, influence of viscosity, density, surface tension, velocity and microfluidic geometry.

Numerical Simulation:

Methods for modeling two-dimensional multiphase non-Newtonian flows in microfluidic for the production of microspheres are as follows:

1. Define the geometry of the microfluidic device, including channel size and input and output locations.
2. Determine fluid parameters for each phase, including viscosity, density, and surface tension, as well as the rheological properties of non-Newtonian fluids.
3. Create the governing equations for emulsion droplet flow and mass transfer in the microfluidic device. The Navier-Stokes equation for fluid flow, the continuity equation for mass transfer, and the relevant boundary conditions for the intake and outflow are often included in the equations.
4. Using the finite volume approach or another suitable numerical method, discretize the governing equations and solve for the velocity and pressure fields in the microfluidic device.
5. Take into consideration the surface tension and interfacial forces between the fluid and emulsion droplets to account for droplet deformation and break-up.
6. Predict the creation and behavior of emulsion droplets in the microfluidic device using numerical modeling, and adjust operational parameters such as flow rate and shape to obtain the required microsphere qualities.

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a. Governing Equations:

The governing equations for two-dimensional multiphase non-Newtonian flow in microfluidics can be derived from the Navier-Stokes equation for fluid flow coupled with the continuity equation for mass transfer of the emulsion droplets. The equations can be further modified to account for the non-Newtonian behavior of the fluid.

The Navier-Stokes equation for non-Newtonian fluid flow in two dimensions can be written as:

$$\rho(\partial u/\partial t + u\partial u/\partial x + v\partial u/\partial y) = -\partial p/\partial x + \nabla\bullet\tau + Fx \quad \text{.....1}$$

$$\rho(\partial v/\partial t + u\partial v/\partial x + v\partial v/\partial y) = -\partial p/\partial y + \nabla\bullet\tau + Fy \quad \text{.....2}$$

where ρ is the density of the fluid, u and v are the velocities in the x and y directions, respectively, p is the pressure, τ is the stress tensor, and Fx and Fy are the external forces acting on the fluid in the x and y directions, respectively.

The stress tensor can be expressed in terms of the strain rate tensor D and the constitutive equation for the non-Newtonian fluid as:

$$\tau = 2\mu D + \sigma(I - \exp(-\lambda|D|\hat{}2)), \quad \text{.....3}$$

where μ is the dynamic viscosity of the fluid, σ, λ are constants related to the non-Newtonian behavior of the fluid, and I is the identity matrix.

The continuity equation for mass transfer can be written as:

$$\partial\rho/\partial t + \partial(\rho u)/\partial x + \partial(\rho v)/\partial y = 0 \quad \text{.....4}$$

where ρ is the density of the emulsion droplets, u and v are the velocities in the x and y directions, respectively.

b. Computer Program:

For numerical simulations of multiphase non-Newtonian flow in microfluidic devices, ANSYS16.1 Fluent can be employed. The finite volume approach is used by ANSYS16.1 Fluent to discretize the governing equations and solve for the velocity and pressure fields in the microfluidic device. To mimic the behavior of emulsion droplets in the device, the program can additionally integrate interfacial pressures and surface tension effects.

The following stages are involved in the numerical solution of the governing equations using ANSYS16.1 Fluent:

1. Using ANSYS Design Modeler, define the geometry of the microfluidic device.

2. Configure the simulation settings, including fluid characteristics, non-Newtonian fluid rheological properties, starting and boundary conditions, and operational parameters.

3. Using the appropriate meshing technique.

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4. Define the multiphase model and non-Newtonian fluid model to simulate the behavior of the emulsion droplets and the non-Newtonian fluid in the microfluidic device.

5. Set up the boundary conditions for the inlet and outlet, including the flow rate and pressure.

6. Solve the governing equations using the finite volume method and obtain the velocity and pressure fields in the microfluidic device.

7. Post-process the simulation results to analyze the behavior of the emulsion droplets and optimize the operating parameters.

Materials and practical test:

The continuous phase (water phase) was 2 % poly (lactic acid) PVA in water and the dispersed phase (oil phase) was 10 % poly (l-lactic acid) (PLLA) in chloroform. This data was taken from [5].

The formation of microspheres was simulated from a microfluidic system by the ANSYS(Workbench16.1), where a two-dimensional geometry was used to obtain microspheres. The length of plate is (1260 nm) and the width is (480 nm). The effect of density, velocity, viscosity, surface tension, and the channel geometry on the microsphere were studied. Table 1 and Fig.1, show the experimental properties of continuous and disperse phases and 2D scheme of microfluidic respectively. Figures 2 and 3 indicate the schematic of microfluidic device and the boundary conditions respectively. Table 2, show the model and geometry specifications.

Table 1: Experimental Properties of Continuous and Dispersed Phases [5].

	Density kg/m3	Viscosity kg/m-s	Velocity m/s	Contact angle	Interfacial tension N/m
Water phase	998	0.00103	0.015	175	0.006
Oil phase	1470	0.00303	0.015		

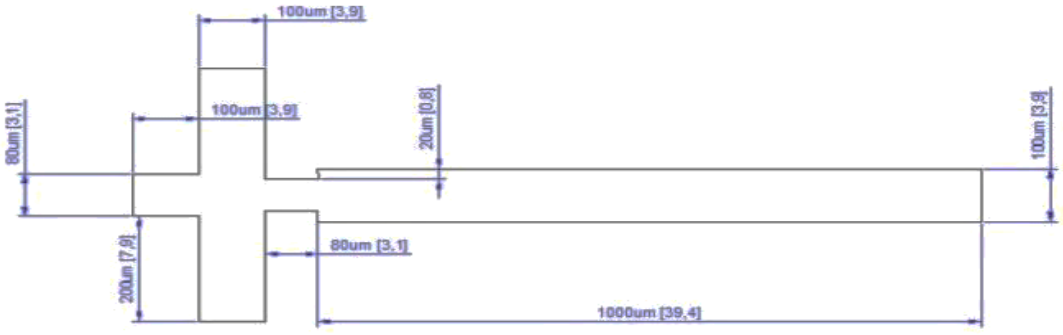

Figure 1. 2D Schematic of Microfluidic Device.

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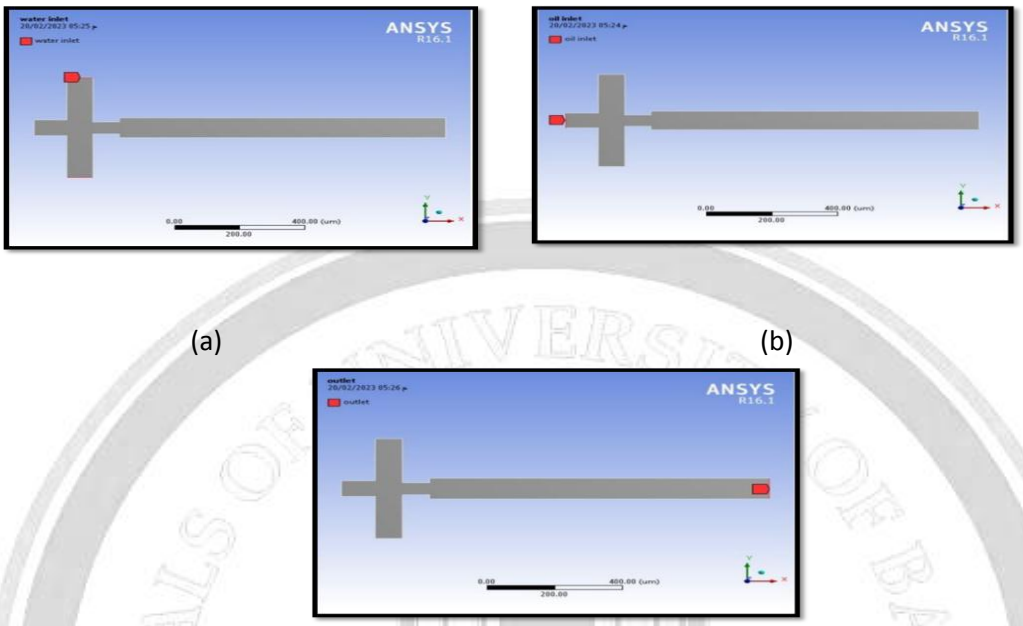

Figure 2: Boundary Conditions Used (a) Inlet Water Phase. (b) Inlet Oil Phase,(c) Outlet Microspheres.

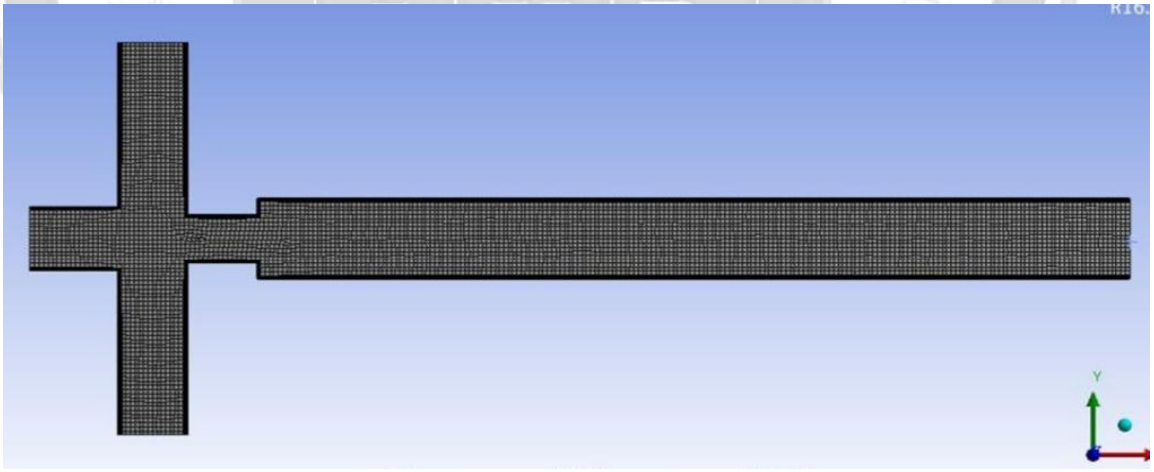

Figure3. Meshing (2D Quad Elements) of 2D Microfluidic.

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Table 2: Model and Geometry Specifications

Object Name	Geometry
State	Fully Defined
Definition	
Source	D:\9Z\9z_files\dp0\FFF\DM\FFF.agdb
Type	DesignModeler
Length Unit	Micrometers
2D Behavior	Plane Stress
Bounding Box	
Length X	1260. µm
Length Y	480. µm
Properties	
Volume	1.512e+005 µm³
Surface Area(approx.)	1.512e+005 µm²
Scale Factor Value	1.
Statistics	
Bodies	1
Active Bodies	1
Nodes	8955
Elements	8583
Mesh Metric	None

Results and Discussion:

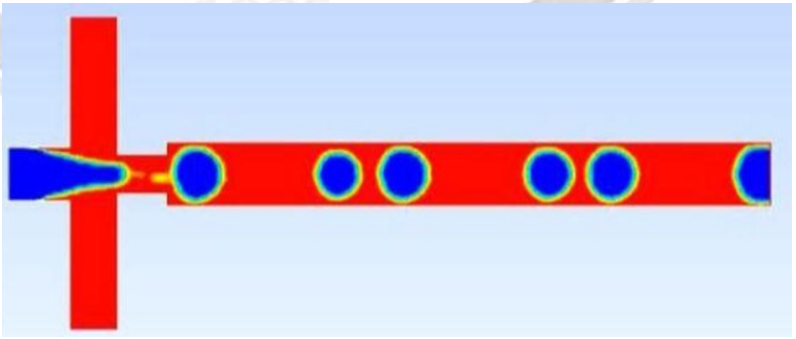

Figure 4. 2D Contours of Microspheres Production from Polymer Emulsion flowing in Microfluidic Devices Numerically According to Data in Table 1.

Figure 4 shows the microspheres formation according to the data in table 1, after many modifications. This figure is used as reference to further investigation in this study.

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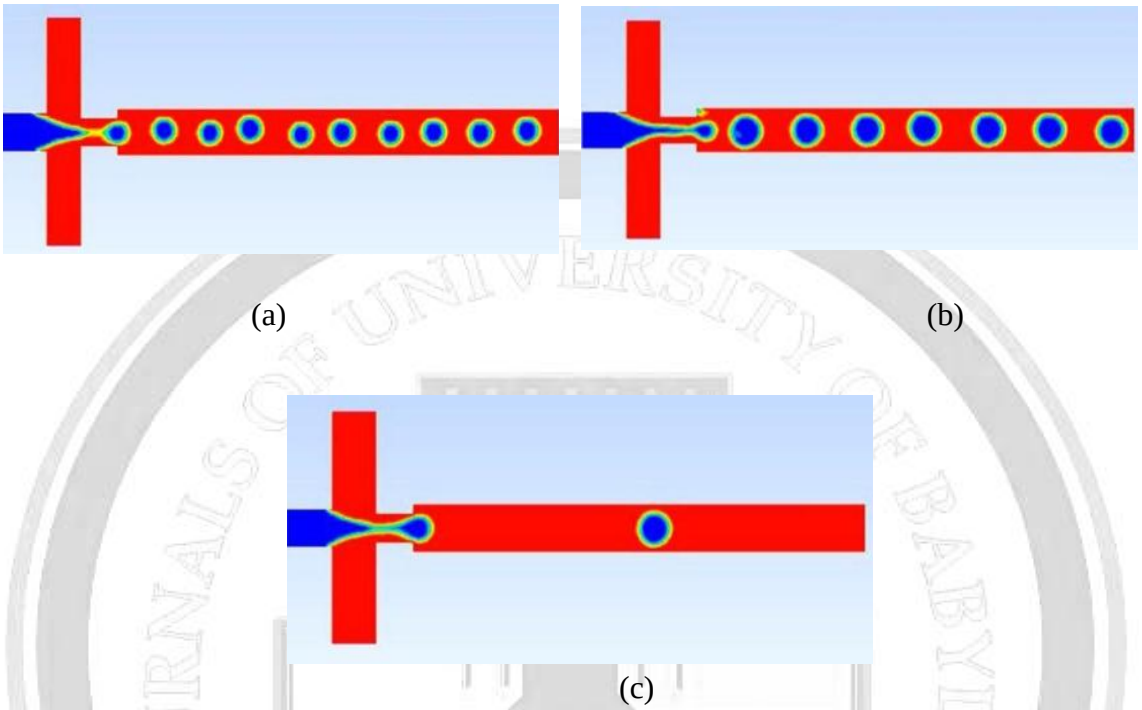
Velocity Effect:



(a) (b)

(c)

Figure 5: 2D Contours of Microspheres in a Microfluidic at Velocity of Water Phase is 0.07 m/s and Oil Phase Velocity, (a) (0.07 m/), (b) (0.05 m/s), (c) (0.015 m/s).

In a microfluidic device, the velocity of the oil phase can significantly affect the formation of microspheres in an emulsion. Figure 5, shows that the decreasing in the velocity of the oil phase from 0.07 to 0.015 m/s effects on the number, size, shape, and distribution of microspheres. Decreasing the velocity of the oil phase can lead to a decrease in the number of microspheres and increase in the size of microspheres formed from 40 to 65 um. This is because a lower velocity of the oil phase results in a lower frequency of droplet formation and larger microspheres [1]. Decreasing the velocity of the oil phase can lead to a change in the shape of the microspheres formed. Lower velocities produce more spherical droplets, while higher velocities produce more elongated droplets. Slowing the oil phase can also lead to a smaller spread of the microsphere sizes. This is because the lower velocities produce more consistent droplet sizes, resulting in less fluctuations in the diameters of the microspheres. . It's vital to remember that slowing down the oil phase might lengthen the time it takes to make a certain number of microbeads. This can have an effect on the performance of the microfluidic device and should be taken into account while optimizing microsphere production. Lowering the velocity of the oil phase can result in more stable microspheres with a more uniform size distribution. Lowering the speed causes more consistent droplet generation, which can lead to more uniform microspheres. Furthermore, reduced velocity can reduce shear-induced stresses, which can enhance droplet coalescence or emulsion break-up, leading in more stable microspheres.

The drug loading capacity of the microspheres can also be affected by the oil phase velocity. Lower speeds can lead to larger microspheres with higher surface-to-volume ratios,

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i.e., greater drug loading capacity. In addition, the reduction in induced shear stress can limit the degradation or loss of bioactive molecules during emulsification, resulting in higher drug availability. The velocity of the oil phase can potentially influence the process of drug release from microspheres. Lower velocity, in particular, can result in microspheres with a more porous structure, which can contribute to quicker drug release. Furthermore, lower shear-induced stresses can limit the production of microspheres with non-uniform drug distribution, resulting in more predictable drug release kinetics.

Density Effect:

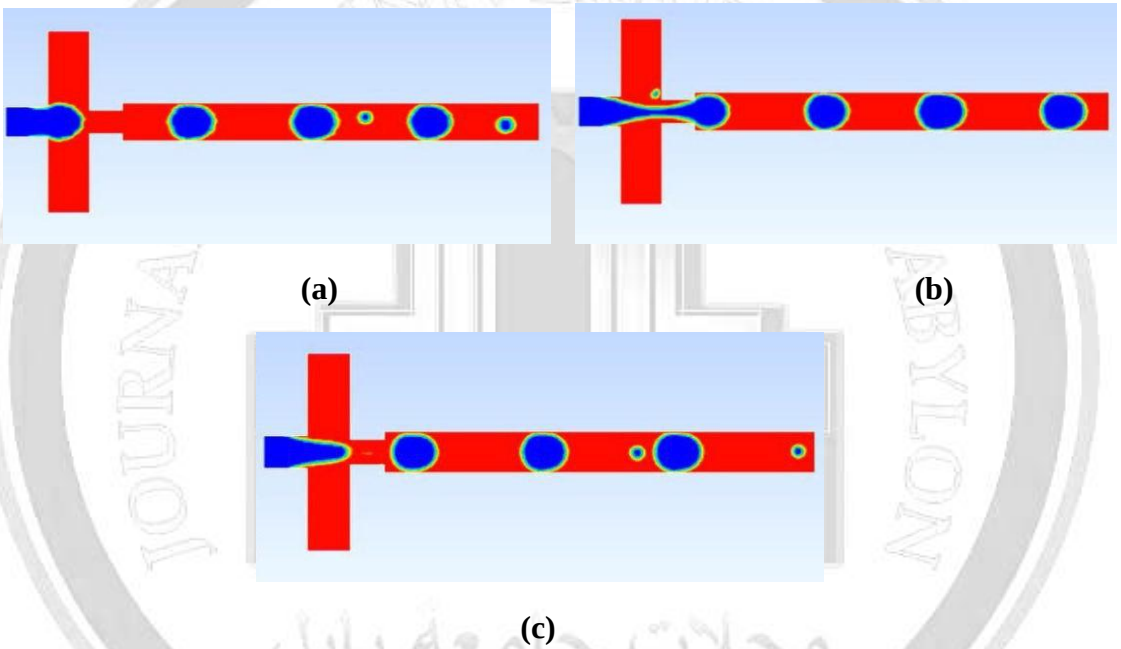

Figure 6: 2D Contours of Microspheres in a Microfluidic at the Density of Oil Phase (a) (1470 kg/m3), (b) (735 kg/m3), and, (c) (367 kg/m3

According to Figure 6, reducing the density of the oil phase leads to bigger microspheres because the lowered density can result in a slower flow rate and lower shear forces. This can result in softer mixing and emulsification, resulting in bigger, more uniform droplets. The influence on the form of the microspheres, on the other hand, may be less evident. Larger droplets may have a more spherical form. Changes in the density of the oil phase can also alter the dispersion of microspheres. A reduction in density might result in a greater variation of droplet sizes due to the softer mixing and emulsification process forming a wider range of droplet sizes.

The capacity of microspheres to keep their size, shape, and characteristics over time is referred to as their stability. In general, lower density oil phase microspheres may be less stable than higher density oil phase microspheres because they are more prone to coalescence or aggregation. With a lower density oil phase, bigger microspheres with a higher surface area-to-volume ratio can develop. This larger surface area may allow the microspheres to load and transport more medicines or other payloads. Drug release from microspheres can occur via a number of methods, including diffusion, degradation, and erosion. The density of the oil

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phase may influence these processes by affecting the size, shape, and stability of the microspheres, as well as the characteristics of the materials employed to create them. For example, if the oil phase density is too low and the microspheres are less stable, the payload may be released more quickly owing to increased exposure to external influences.

Viscosity Effect:

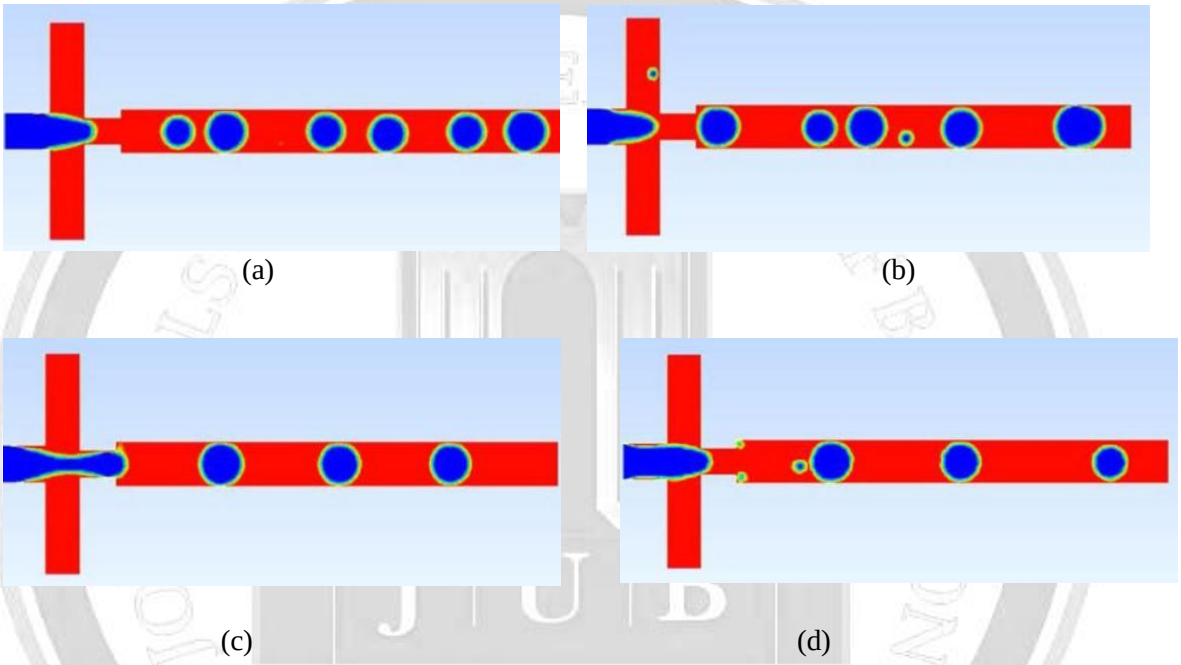

Figure 7: 2D Contours of Microspheres in a Microfluidic at Oil Phase Viscosity (a) (0.01kg/m-s), (b) (0.00606 kg/m-s), (c) (0.001515 kg/m-s), and (d) (0.0001 kg/m-s).

The shear viscosity of the oil phase can influence the size of microspheres. In general, a lower shear viscosity might result in bigger microspheres because it allows for quicker mixing and emulsification of the oil and water phases (see Figure.7). The influence of shear viscosity in the oil phase on microsphere form is less evident. Some studies have discovered that decreased shear viscosity can result in larger spherical microspheres, whereas others have found no impact because it allows for more exact control over droplet size during emulsification, a lower shear viscosity oil phase might result in a narrower dispersion of microsphere sizes. The shear viscosity of the oil phase can impact the stability of microspheres. High shear viscosity can result in less stable microspheres because the droplets are more prone to coalescence or aggregation. This effect, like the influence on microsphere shape, is less apparent and may be dependent on other factors such as the surfactant employed and the manner of microsphere creation.

Lowering the oil phase's shear viscosity has the potential to boost the drug loading capacity of microspheres by resulting in more uniform microspheres with a larger surface area-to-volume ratio. This impact, however, may be affected by other factors such as the kind of medicine and the technique of drug loading. The influence of oil phase shear viscosity on

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drug release processes can be complex since it affects the size, shape, and stability of microspheres, as well as drug characteristics and drug loading technique. This finding is consistent with the findings of researchers in [2].

Channel Diameter Effect:

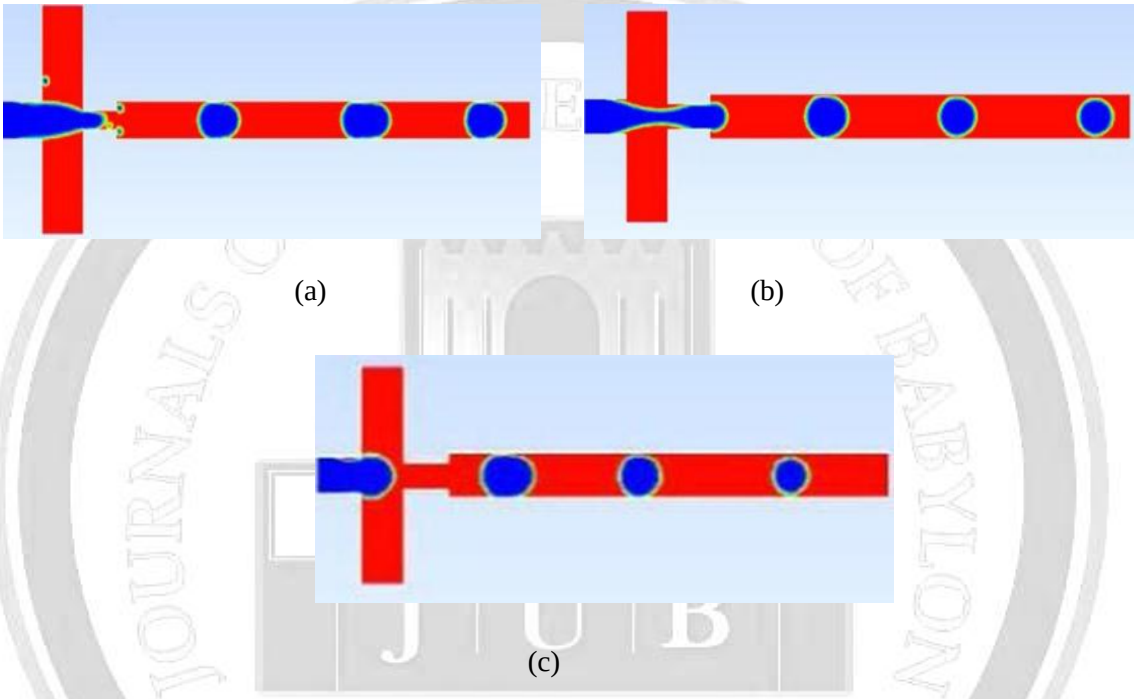

Figure 8: 2D Contours of Microspheres in a Microfluidic at Channel Diameter (a) (50um), (b)(25um), and, (c) (12um).

The diameter of microfluidic channels used to prepare microspheres can have significant effects on their properties. The size of microspheres can be affected by the diameter of the microfluidic channels. In general, Figure 8, indicates that the smaller channel diameters can lead to smaller microspheres, as they allow for more precise control over droplet size during emulsification. Some studies have suggested that smaller channel diameters can lead to more spherical microspheres, while others have found no significant effect. Smaller channel diameters can result in a narrower distribution of microsphere sizes, as they allow for more precise control over droplet size during emulsification. The stability of microspheres can be affected by the channel diameter. In general, smaller channel diameters can lead to less stable microspheres, as they may be more prone to coalescence or aggregation. However, this effect may depend on other factors such as the surfactant used and the method of microsphere formation.

The diameter of microfluidic channels can potentially affect the drug loading capacity of microspheres, as it can affect the size and surface area-to-volume ratio of the microspheres. The effect of channel diameter on drug release mechanisms can be complex, as it can affect the size and stability of microspheres, as well as the properties of the drug and the method of drug loading.

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Surface T tension Effect:

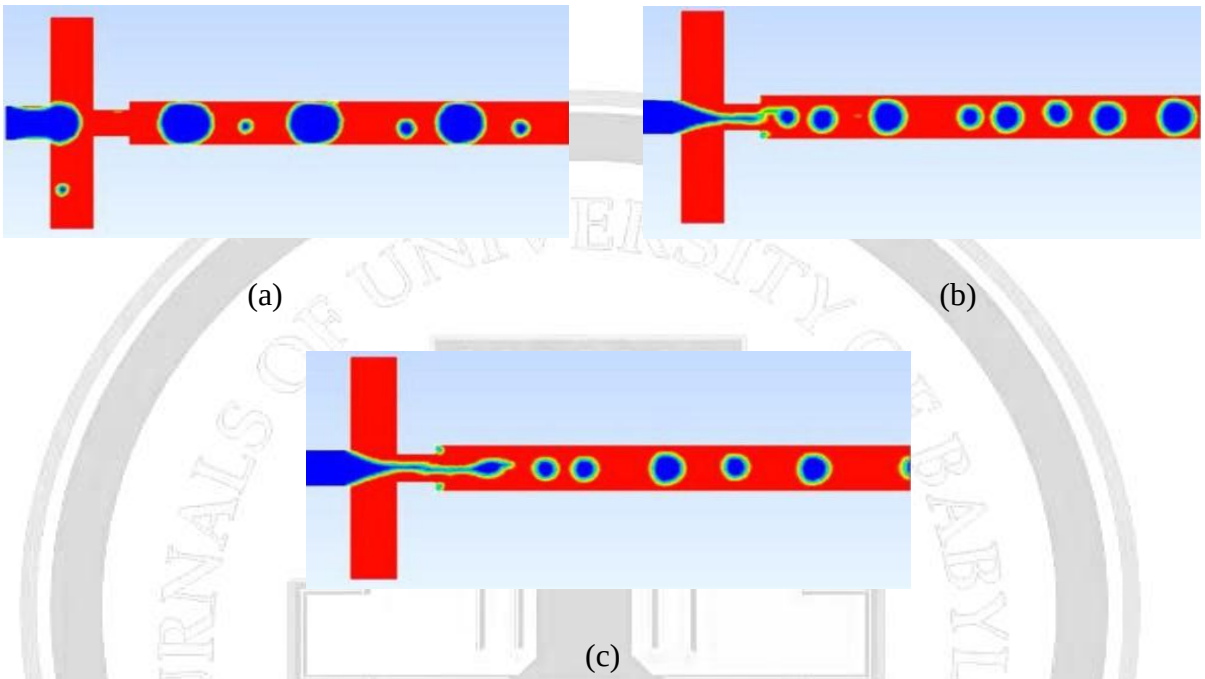

Figure 9: 2D Contours of Microspheres in a Microfluidic at Interfacial Surface Tension of the Emulsion (a) (0.01 N/m), (b) (0.001 N/m) and (c) (0.0005 N/m) .

The interfacial surface tension of an emulsion can has significant effects on the properties of microspheres formed from the emulsion. Figure9: shows that the size of microspheres affected by the interfacial surface tension of the emulsion. In general, a lower interfacial surface tension led to smaller microspheres, as it allows for faster mixing and emulsification of the oil and water phases [3]. The effect of interfacial surface tension on microsphere shape is less clear, but the lower interfacial surface tension can lead to more spherical microspheres. Lowering the interfacial surface tension of the emulsion result in a narrower distribution of microsphere sizes gradually, as it allows for more precise control over the droplet size during emulsification. The stability of microspheres can be affected by the interfacial surface tension of the emulsion. In general, lower interfacial surface tension can lead to less stable microspheres, as the droplets may be more prone to coalescence or aggregation. However, like the effect on microsphere shape, this effect is less clear and may depend on other factors such as the surfactant used and the method of microsphere formation.

Lowering the interfacial surface tension of the emulsion can potentially increase the drug loading capacity of microspheres, as it can lead to smaller and more uniform microspheres with a higher surface area-to-volume ratio. However, this effect may depend on other factors such as the type of drug and the method of drug loading. The effect of interfacial surface tension on drug release mechanisms can be complex, as it can affect the size, shape, and stability of microspheres, as well as the properties of the drug and the method of drug loading.

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Initiation of the First Microsphere:

The effect of velocity, density, viscosity, channel diameter, and surface tension on the initiation of the first microsphere can depend on the specific microfluidic device and emulsification method being used. In general, the initiation of the first microsphere can be influenced by the balance between the forces acting on the fluids in the microfluidic channels. Increasing the velocity of the fluids in microfluidic channels can increase the shear forces acting on the fluids, which can promote droplet formation and facilitate the initiation of the first microsphere. Similarly, decreasing the channel diameter can increase the pressure drop across the channel, which can also promote droplet formation and facilitate the initiation of the first microsphere. Furthermore, the surface tension of the fluids can play a role in the initiation of the first microsphere. Lower surface tension can reduce the energy required for droplet formation and promote the initiation of the first microsphere. On the other hand, higher surface tension can increase the energy required for droplet formation and make it more difficult to initiate the first microsphere. In addition, the density and viscosity of the fluids can also affect the initiation of the first microsphere. Higher density and viscosity can increase the resistance to droplet formation and make it more difficult to initiate the first microsphere.

The initiation of the first microsphere in microfluidic devices can be influenced by a range of physical parameters, and optimizing these parameters can be important for achieving successful microsphere production.

Capillary Number and Weber Number:

The capillary number and Weber number are two important dimensionless numbers in microfluidics that can have significant effects on the properties of microspheres. Increasing the velocity of the fluids in microfluidic channels can increase the capillary number and Weber number. The capillary number is a measure of the balance between viscous and capillary forces, while the Weber number is a measure of the balance between viscous and inertial forces. A higher capillary number can lead to smaller and more uniform droplets during emulsification, while a higher Weber number can lead to more turbulent flow and droplet breakup. Increasing the density of the fluids in microfluidic channels can decrease the capillary number and increase the Weber number. This is because the capillary number is inversely proportional to the density of the fluids, while the Weber number is directly proportional. A lower capillary number can lead to larger and less uniform droplets during emulsification, while a higher Weber number can lead to more turbulent flow and droplet breakup. Increasing the viscosity of the fluids in microfluidic channels can increase the capillary number and decrease the Weber number. Decreasing the channel diameter in microfluidic devices can increase the capillary number and Weber number. This is because the capillary number is inversely proportional to the channel diameter, while the Weber number is directly proportional. Decreasing the surface tension of the fluids in microfluidic channels can increase the capillary number and decrease the Weber number. This is because the capillary and Weber number is inversely proportional to the surface tension of the fluids. The capillary number and Weber number can then affect the properties of microspheres formed from the emulsions. For example, smaller and more uniform droplets can lead to smaller and more uniform microspheres, while more turbulent flow and droplet breakup can

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lead to less stable microspheres. Additionally, the drug loading capacity and drug release mechanisms of microspheres can be affected by their size and stability.

Optimization:

Optimizing the effect of the different parameters on microspheres specifications can involve adjusting the values of these parameters to achieve desired microsphere properties. It may be beneficial to adjust the fluid flow rates and the composition of the fluids, the surfactant in microfluidic channels to achieve a specific velocity range, a specific density range, a specific viscosity range, and a specific surface tension range that results in the desired droplet size and distribution. Increasing the velocity, viscosity, density and decreasing the surface tension can result in smaller droplets, but it is important to ensure that the droplets remain stable and do not experience coalescence or breakup.

In addition to these optimizations, it is important to consider other factors that can affect microsphere properties, such as the choice of polymer used for microsphere formation, the method of drug loading, and the method of drug release. By carefully controlling these parameters, it may be possible to optimize microsphere properties such as size, shape, distribution, drug loading, and drug release mechanisms for specific applications.

Conclusions:

1.The production of microspheres from polymer emulsion in microfluidic devices has shown great potential for drug delivery applications.

2. In this study, the effects of velocity, density, viscosity, channel diameter, and surface tension on the production of microspheres using Fluent Ansys16.1 program were investigated.

3.The numerical results showed that the velocity of the fluid flow has a significant impact on the production of microspheres. Higher velocities lead to smaller droplet sizes, which can potentially improve drug delivery efficiency.

4.The density and viscosity of the polymer emulsion also affected the droplet size, with higher densities and viscosities leading to smaller droplets.

5. both the channel diameter and surface tension played important roles in the production process. Smaller channel diameters and higher surface tensions led to smaller droplets, resulted in more stable droplets.

6.The interaction between the fluid and the channel walls was also found to affect the production of microspheres. The simulations also showed that the microspheres produced in the microfluidic device had good drug loading and releasing capabilities. The microspheres could effectively encapsulate drugs and release them in a controlled manner over a prolonged period of time.

7.the study demonstrated that the production of microspheres from polymer emulsion in microfluidic devices can be optimized by adjusting the velocity, density, viscosity, channel diameter, and surface tension. The ability to control these parameters provides a promising approach for developing drug delivery systems with improved efficacy and reduced side

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effects. Overall, the numerical results of this study provide valuable insights into the production of microspheres for drug delivery applications using microfluidic devices.

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ARTICLE
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محاكاة عددية لإنتاج الكريات المجهرية من مستحلب البوليمر في جهاز الجريان المايكروي لاستخدامها في أنظمة توصيل الأدوية

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الخلاصة

أظهر إنتاج الكرات المجهرية من مستحلبات البوليمر باستخدام أجهزة الجريان المايكروية إمكانات كبيرة لتطبيقات توصيل الأدوية نظرًا لقدرتها على تغليف الأدوية وإطلاقها بطريقة خاضعة للرقابة. في هذه الدراسة، تم فحص تأثيرات السرعة والكثافة واللزوجة والتوتر السطحي، وكذلك قطر القناة، على توليد الكراة المجهرية باستخدام برنامج ANSYS. تمت برمجة البرنامج بالخصائص الفيزيائية لمستحلب البوليمر مثل الكثافة واللزوجة والتوتر السطحي. لإجراء المحاكاة والتنبؤ بتدفق السوائل وإنتاج الغلاف المجهري وتحسين تصميم تطبيقات توصيل الأدوية بناءً على التغييرات المذكورة كما تمت دراسة تأثيرات أرقام capillary وWeber.

أظهرت نتائج الدراسة أنه يمكن التحكم في حجم الكرات المجهرية عن طريق ضبط سرعة وقطر القناة. فقد ا نتجت الكرات المجهرية الضيقة عن عرض قناة أضيق ومعدلات تدفق أعلى ، مما قد يحسن كفاءة توصيل الدواء ، بينما انتجت الكرات المجهرية الأصغر عند انخفاض التوتر السطحي البيني. أثرت لزوجة وكثافة مستحلب البوليمر بشكل كبير على حجم الكرات المجهرية، حيث ان زيادة اللزوجة والكثافة تنتج كرات مجهرية أصغر.

كما تم التنبؤ بخصائص التحميل وإطلاق الدواء للكرات المجهرية التي تم إنشاؤها باستخدام تقنية ميكروفلويديك. أظهرت النتائج أن الكرات المجهرية يمكنها تغليف الأدوية بكفاءة وإطلاقها بطريقة خاضعة للرقابة على مدى فترة من الزمن. ويرجع ذلك إلى ارتفاع مساحة السطح إلى نسبة الحجم للكرات المجهرية، مما يسمح بنشر الدواء بكفاءة. وقد توفر القدرة على ضبط عملية التصنيع باستخدام عوامل مثل السرعة والكثافة واللزوجة وقطر القناة والتوتر السطحي فرصة محتملة لتصميم أنظمة توصيل الأدوية بكفاءة أكبر وتأثيرات جانبية أقل.

الكلمات الدالة: المستحلب البوليمري، الموائع الدقيقة، المحاكاة العددية، الكريات الدقيقة، آلية توصيل الدواء وإطلاقه.