A conceptual microchannel system design methodology incorporating axiomatic design theory for size-controllable monodispersed microsphere generation by a liquid chopper utilizing a PZT actuator

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A conceptual microchannel system design methodology incorporating axiomatic design theory for size-controllable monodispersed microsphere generation by a liquid chopper utilizing a PZT actuator

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Abstract: This paper proposes a design methodology for conceptual design of microchannel systems by applying axiomatic design theory (ADT). The microchannel system concerned, as an example, in this paper is for the purpose of preparing uniform microspheres based on the phase separation principle. There are two general design goals for this system: controllability of the size of microspheres and uniformity or narrow size distribution of microspheres. The conventional microchannel system designs in literature are found to be the so-called ‘coupled design’, which is regarded as a poor design, according to ADT. This paper proposes a ‘decoupled design’ process, which is considered better than a ‘coupled design’ process according to ADT. This paper demonstrates the effectiveness of such a ‘decoupled design’ process with a new microchannel system with an embedded liquid chopper utilizing a PZT actuator by simulation.

Keywords: axiomatic design theory, liquid chopper, microsphere, controllability, uniformity

1 INTRODUCTION

Emulsion in microsphere formation is an important phenomenon in the formation of foods, cosmetics, and pharmaceuticals [1]. The microsphere encapsulates beneficial agents and makes friendly environments for the agents; thus the agents stay stable over a prolonged period of time and are released as the microsphere degrades. Microspheres are prepared mainly using three approaches: solvent extraction/evaporation, phase separation, and spray-drying by mixers, colloid mills, homogenizers, and sonicators [2]. Uniformity or monodispersity of microspheres is desirable due to the constant and predictable responses of the microspheres to external fields and is required in various industrial applications such as drug delivery devices, chromatographic packing materials, and dry and liquid tones for electrophotography [3–11]. Additionally, controllability of microsphere size is eligible for different applications [12–15]. For the preparation of microspheres, a microfluidic approach based on microelectromechanical system (MEMS) technology seems to prevail for better uniformity and size controllability [16]. For the past decades, studies on chemical reactions have shown a high interest in microfluidic devices, since scaling down of a typical length to tens or hundreds of micrometres and reduction of a large amount of materials greatly increases the efficiency of development [16, 17].
For a more controllable synthesis of monodispersed microspheres in microfluidic devices, two types of conceptual designs have been developed in the literature: T-junction for crossflow and intersection for hydrodynamic flow focusing. The T-junction structure was introduced by Thorsen et al. [18] and Dendukuri et al. [3] for water-in-oil (W/O) microspheres. Tice et al. [19] investigated the three regimes of multiphase flow behaviour by capillary number (Ca) in the formation of ‘plugs’ at the T-junction. Van der Graaf et al. [20, 21] studied the influence of the properties of the aqueous phase on the process of oil-in-water (O/W) microsphere formation at the T-junction in glass microchannels and simulated the microsphere formation in a rectangular microchannel with the lattice Boltzmann method [22, 23].

The hydrodynamic flow focusing (or flow focusing) technique with immiscible fluids was applied by Ganan-Calvo and Barrero [24, 25] to form microthreads and micrometre-sized monodispersed spray in gas streams, after Knight et al. [26] reported a multistream laminar flow system in a microfluidic device to narrow or focus the middle stream (i.e. flow focusing), by increasing the two outer neighbour streams to improve mixing efficiency. The side-by-side parallel laminar streams are able to adjust the size of each stream by altering the flowrate of the multistream [27]. Later, Anna et al. [28] integrated the flow focusing geometry in a microfluidic device to produce monodispersed and polydispersed microspheres.

However, the designs of microchannels, as mentioned above, have not been studied systematically, and general design theory and methodology have not been applied to the design of microchannel systems, which may otherwise lead to some new conceptual design of microchannel systems. This observation has become an important motivation of the study presented in this paper. In this paper, a study is presented to apply a general design theory called axiomatic design theory (ADT) to the design of microchannel systems, and in particular resulted in a new conceptual design of the microchannel system introducing a liquid chopper utilizing a piezoelectric transducer (PZT), such as lead–zirconate–titanate, actuator to generate size-controllable monodispersed (uniform) microspheres. By introducing two immiscible fluids to a microfluidic device and varying the frequencies of the PZT actuator, O/W emulsion can be successfully realized forming microspheres. A stable continuous phase stream previously sheathes a dispersed phase flow in the main microchannel to control the width of it. A PZT actuator is embedded at the mouth of an external channel and the external channel is connected to the downstream of the main channel. The focused liquid flow is pinched off by the fluctuating external flows generated by the PZT actuator generating microspheres periodically. The PZT actuator operates in various frequencies. The size of the microspheres is uniform and controllable by altering frequencies of the PZT actuator. Further, a simulation was performed to verify the proposed microchannel design to generate uniform O/W microspheres using the properties of 5 per cent of poly(lactic-co-glycolic acid) (PLGA) in dichloromethane and 1 per cent of polyvinyl alcohol (PVA) in distilled water for the oil phase (dispersed phase) and the aqueous phase (continuous phase) respectively.

2 AXIOMATIC DESIGN: REVIEW

Design of effective systems is the ultimate goal of many fields, including engineering, business, and government. However, system design has lacked a formal theoretical framework and has been done in heuristic or empirical approaches. Systems under these approaches cause both technical and business risks because today’s systems become more complicated, and many interrelated parameters and subsystems that have not been fully understood may cause very difficult design problems [29–32]. Design theory and methodology (DTM) is a branch of engineering research devoted to the formalization of engineering design and the methods used by designers [33]. Axiomatic design theory (ADT) has been broadly used for decades due to its capability to reduce complexity of a system design. Design is an interplay between ‘what we want to achieve’ and ‘how we want to achieve it’ [34].

The customers’ needs are defined as function requirements (FRs), which describes ‘what we want to achieve’. The descriptor of ‘how to achieve it’ is defined as design parameters (DPs). To be efficient and to generate the design that meets the perceived needs, the designer must specifically state the design goals in terms of ‘what we want to achieve’ and begin the design process. Iterations between ‘what’ and ‘how’ are necessary, but each iteration loop must redefine the ‘what’ clearly. In most design practices, design decisions are made based on experience rather than using a systematic methodology, which is the case in microsystems design as well. Although experience is important because it generates knowledge and information about practical design, empirical knowledge alone is not sufficient, as it is not always reliable, especially when the context of the application changes. An initial prototype machine made by a designer is improved by all the mistakes during testing until it works, which is costly and not safe [34].
Axiomatic design theory (ADT) was proposed by Suh [35] to provide a basis for correct design decisions. ADT provides the science base to augment the designer’s experience by providing the underlying principles, theories, and methodologies so that the designer can fully utilize the creativity. ADT is a rational way to develop a complicated system that satisfies FRs and constraints at low cost and on time without mistakes [34, 35]. Design issues become easier to understand when they are analysed using the framework of axiomatic design [35–37]. The world of axiomatic design has four domains: customer domain, functional domain, physical domain, and process domain [36]. The domain structure is shown in Fig. 1.

The customer domain is characterized from the customer’s attributes (or needs) (CAs) in a product, process, system, or materials. The customer’s needs are specified in terms of functional requirements (FRs) and constraints. Design parameters (DPs) satisfy the specific FRs. Process variables (PVs) characterize an optimal process in the process domain [34]. ADT is based on two design axioms: the Independence Axiom and the Information Axiom [36].

**Axiom 1: The Independence Axiom. Maintain the independence of the FRs**

The independence of FRs must always be maintained; i.e. design decisions must always be made without violating the independence of each functional requirement from other functional requirements. The FRs are defined as the minimum number of independent requirements that characterize the design goals. Once FRs are defined based on the CAs, the FRs are mapped on to the physical domain by a suitable set of DPs, as illustrated in Fig. 2.

If the design details are missing at the highest level of design, the highest level design must be decomposed to develop the design details. As the highest level design is decomposed, the decision of the lower level design must be consistent with the highest level design intent without a violation of the independence axiom. In order to decompose FRs and DPs, a zigzag method is applied, as illustrated in Fig. 3. From an FR in the functional domain, a conceptualized design in the physical domain is determined corresponding to DP. FR1 and FR2 at the next level are created, satisfying the highest level FR for the highest level DP. Then, DP1 and DP2 are found to satisfy FR1 and FR2 respectively, by conceptualizing a design at this level. This process is continued until the FR can be satisfied without further decomposition. The final states are indicated by thick-bordered boxes, which are called ‘leaves’ [34].

During the mapping process, all the possible different ways of satisfying the FRs need to be considered by identifying reasonable DPs, called the conceptualization process, considering all available methods such as brainstorming, morphological techniques, analogy from other examples, extrapolation and interpolation, law of nature, order-of-magnitude analysis, and reverse engineering. At a given level of the design hierarchy, an FR vector is made up representing the set of FRs in the function domain, and a DP vector in the physical domain is constituted corresponding to the DPs that satisfy the FRs.

A design equation that describes the relation between the two vectors can be expressed mathematically as

\[
[FR] = [A][DP]
\]
where \([A]\) is called a design matrix that characterizes the product design. A design matrix for a design that has \(n\) FRs and \(n\) DPs is expressed as

\[
A_{ij} = \frac{\partial FR_i}{\partial DP_j} \quad (i = 1, 2, \ldots, n) \quad (4)
\]

In a differential form, equation (1) can be rewritten as

\[
(dFR) = (A)(dDP) \quad (3)
\]

and the elements of the design matrix are given by

\[
A_{ij} = \frac{\partial FR_i}{\partial DP_j} \quad (4)
\]

In general, with \(n\) FRs and DPs, equation (1) can be rewritten in terms of its elements as

\[
FR_i = \sum_{j=1}^{n} A_{ij} DP_j \quad (i = 1, 2, \ldots, n) \quad (5)
\]

or

\[
\begin{align*}
FR_1 &= A_{11} DP_{11} + A_{12} DP_{12} + \cdots + A_{1n} DP_{1n} \\
FR_2 &= A_{21} DP_{21} + A_{22} DP_{22} + \cdots + A_{2n} DP_{2n} \\
&\vdots \\
FR_n &= A_{n1} DP_{n1} + A_{n2} DP_{n2} + \cdots + A_{nn} DP_{nn}
\end{align*} \quad (6)
\]

For a linear design, \(A_{ij}\) are constants, and for a non-linear design, \(A_{ij}\) are functions of the DPs.

If a design matrix \([A]\) is a full matrix, which is neither diagonal nor triangular, a design cannot satisfy the independence axiom, which is called a coupled design. The matrix \([A]\) must be either diagonal or triangular in order to satisfy the independence axiom.

Each of the FRs can be satisfied independently with one DP if the design matrix \([A]\) is diagonal, which is called an uncoupled design. If the design matrix is triangular, the independence of FRs can be assured if and only if the DPs are determined in an appropriate sequence, which is called a decoupled design.

**Axiom 2: The Information Axiom. Minimize the information content of the design**

Among those designs that satisfy the independence axiom, the design that has the smallest information content and the highest probability of success is the best design. The probability of success is defined as

\[
Ps = \frac{\text{common range (CR)}}{\text{system range (SR)}} \quad (7)
\]

\(Ps\) is governed by the intersection of the design range (DR) defined by the given design specification of FRs and the system range (SR), which is the distribution for performance of the designed product. If an FR is a continuous random variable, \(Ps\) can be expressed as

\[
Ps = \int_{FR-\Delta}^{FR+\Delta} \Phi(FR) dFR \quad (8)
\]

where \(\Phi(FR)\) is a system probability density function (PDF), \(\Delta\) is half of DR, and \(FR^*\) is the target value as illustrated in Fig. 4 [38].

The ordinate is the probability density and the abscissa is either the FR or DR. The system PDF is plotted over the SR for a specified FR. The distance between the target value and the mean of the system PDF is called bias. The overlap between DR and SR is called the common range (CR) and the FR is satisfied only in CR.

The area under the system PDF within CR, \(A_{cr}\), is the design’s probability of achieving the specified goal, and the information content \(I\) can be calculated as [34, 35]

\[
I = \log_2 \frac{1}{A_{cr}} \quad (9)
\]
The information content $I_i$ for a given $FR_i$ is defined in terms of the probability $P_i$ satisfying $FR_i$

$$I_i = \log_2 \frac{1}{P_i} = -\log_2 P_i \quad (10)$$

Either the logarithm based on 2 or the natural logarithm may be used. In the case of multiple FRs, $mFRs$, the information content for the entire system $I_{sys}$ is

$$I_{sys} = -\log_2 P_{(m)} \quad (11)$$

where $P_{(m)}$ is the joint probability that all $m$FRs are satisfied. In case of an uncoupled design where all FRs are statistically independent

$$P_{(m)} = \prod_{i=1}^{m} P_i \quad (12)$$

$I_{sys}$ is calculated as

$$I_{sys} = \sum_{i=1}^{m} I_i = -\sum_{i=1}^{m} \log_2 P_i \quad (13)$$

In the case of a decoupled design where all FRs are not statistically independent

$$P_{(m)} = \prod_{i=1}^{m} P_{(i|j)} \text{ for } [j] = (1, 2, \ldots, i-1) \quad (14)$$

where $P_{(i|j)}$ is the conditional probability of satisfying $FR_i$. $I_{sys}$ can be calculated as $[39]$

$$I_{sys} = -\sum_{i=1}^{m} \log_2 P_{(i|j)} \text{ for } [j] = (1, 2, \ldots, i-1) \quad (15)$$

Thus, it is found that the smallest information content $I$ represents the best design as it requires the least amount of information to achieve the design goals. Inversely, the highest probability represents the best design. If the probability is small, more information is required to satisfy $FR$.

3 PROPOSED DESIGN CONCEPT

3.1 Microfluidic device

A typical microfluidic device consists of two parts, as shown in Fig. 5: a substrate and a top plate. For easy observation during experiments, either a substrate or a top wafer should be transparent. Microchannels including inlet and outlet holes are patterned and fabricated on a top plate for better manipulation during the fabrication process.

In order to produce microspheres in microchannels, emulsion is an important phenomenon to start with. Emulsion of two immiscible fluids, oil phase and aqueous phase, in microscales has attracted high attention to generate microspheres for various applications, defining one phase as continuous phase and the other as dispersed phase. In between the two immiscible fluids, the interfacial tension and the inertial force mainly govern the dynamics of the free surface and are significantly greater than gravitational force. As the governing forces are competing, the interfacial area of the two fluids is reduced (interfacial tension dominates) or extended (inertial force dominates). By the competition of the governing forces, the dispersed phase forms to be microspheres, and the continuous phase encircles the microspheres. The Weber number $We$ represents the relative importance of the interfacial tension and inertial force, and the flow number $Ca$ signifies the relative effect of viscous forces versus interfacial tension between the immiscible fluids $[40]$. The dimensionless $We$ and $Ca$ are defined as

$$We = \frac{\rho V^2 l}{\sigma} \quad (16)$$

$$Ca = \frac{\mu V l}{\sigma} \quad (17)$$

![Fig. 4](image1)

**Fig. 4** Design range, system range, common range, and system PDF for a function requirement

![Fig. 5](image2)

**Fig. 5** A typical microfluidic device with a microchannel
where \( \rho \) is the density, \( V \) is the velocity, \( l \) is the characteristic length, \( \mu \) is dynamic viscosity, and \( \sigma \) is the interfacial tension. Thus, the smaller characteristic length (the width in this case) of the flow stream yields a higher proportion of the interfacial tension in the two-phase flow.

Functional requirements (FRs) for a microchannel design to generate uniform and size-controllable microspheres are consistancy (uniformity) and size controllability. Consistency operates uniformity of microspheres for constant and predictable responses. Various sizes of microspheres are pursued by size controllability for the controlled release of suitable active agents (i.e. antigens) from the polymeric microsphere in the field of drug delivery and the size of the microspheres is proportional to the width of the dispersed phase stream. Then, breakage can be regarded as a major functional requirement. Hence, FRs are derived as:

- \( FR_1 \): consistancy.
- \( FR_2 \): size-controllability.
- \( FR_3 \): breakage of the flow stream.

The one-to-one correspondence between DPs and FRs should be considered. To derive DP\(_1\) for FR\(_1\), continuous flow streams with consistent flowrates are necessary. A pneumatic pump can generate continuous and constant air pressures to feed fluids to microchannels. By altering the pressures, the dispersed phase stream is cut to form microspheres. The respective DPs for each FR are as follows:

- \( DP_1 \): continuous and consistent pressures for inlets.
- \( DP_2 \): to change the width of the dispersed phase.
- \( DP_3 \): to narrow the width of the dispersed phase to be cut.

### 3.2 Evaluation of typical microchannel designs for microsphere generation

Typical designs of microchannels for microsphere generation contain crossflow at the T-junction and hydrodynamic flow focusing at the intersection, as illustrated in Fig. 6. In T-junction design, the flow rate of the continuous phase (crossflow) cuts the dispersed phase into droplets to form microspheres. A higher velocity of the crossflow reduces the size of microspheres by decreasing the width of the dispersed phase. In the intersection design, sheath flows (continuous phase) break the focused flow (dispersed phase) jet into droplets to form microspheres. Similarly to T-junction design, higher flow rates of sheath flows decrease the size of microspheres by shrinking the width of the dispersed phase.

![Fig. 6 Schematic top views of typical methods to generate microspheres in microchannels. In the microchannels, different colours of fluids signify two immiscible flows, which are continuous phase and dispersed phase, and the arrows represent directions of flows](image)

The design equation for the selected DPs and FRs in the T-junction and intersection designs is

\[
\begin{bmatrix}
FR_1 \\
FR_2 \\
FR_3
\end{bmatrix} = \begin{bmatrix}
\times & 0 & 0 \\
\times & \times & \times \\
\times & \times & \times
\end{bmatrix} \begin{bmatrix}
DP_1 \\
DP_2 \\
DP_3
\end{bmatrix}
\]

The equation clearly explains that they are coupled designs since \( FR_2 \) is achieved by \( DP_1 \), \( DP_2 \), and \( DP_3 \). Hence, from a design point of view, it is clear that the conventional microchannel system designs are poor, which may cause uncertainty and difficulty in operating systems. In order to decouple the coupled design based on ADT, \( FR_2 \) should be achieved by \( DP_1 \) and \( DP_2 \), and \( DP_3 \) must be engaged for only \( FR_3 \) for decoupled design.

### 3.3 Proposed conceptual design of the microchannel for microsphere generation

As discussed in the previous section, a better design is decoupled or uncoupled design. Since a simpler mechanism of microfluidic device for microsphere generation is preferable, a decoupled design is more suitable. In order to decouple equation (18), which makes \( FR_2 \) independent of \( DP_3 \) (decoupling), inlet
pressures to change the width of the dispersed phase stream and to break it must be separated.

Hydrodynamic flow focusing is widely used in order to squeeze and keep the width of the focused flow for cytometry applications. However, higher velocity of the focused flow is not avoidable, which yields a higher value of the Weber number. Hence, an extra force is needed to increase the interfacial tension for droplet formation. In this paper, a liquid chopper is introduced to create an extra force on the two-phase flow stream to cut off the focused flow. An embedded piezoelectric actuator drives external flows to structure a liquid chopper. With an oscillating flow, the pressure from the external channel is boosted to pinch the main stream, and finally the focused flow is cut off. A lead–zirconate–titanate (PZT) actuator is suitable to generate oscillation to the microchannel. The schematic diagram of the proposed microchannel design is illustrated in Fig. 7.

As the interests in manufacturing and assembly for small parts with a size ranging from very few millimetres down to nanometres increases, one of the commonly used materials is the piezoelectric. PZT is one of the piezoelectric materials and is widely applied for actuators to convert a strain into a force [41, 42]. A PZT actuator is a well-known device for managing very small displacements in the range of 10 pm (1 pm = 10^{-12} m) to 100 µm [43]. The displacement is proportional to the applied external voltage. The dimension changes can be adjusted with extremely high resolution for millions of cycles without wear or deterioration. The advantages of the PZT actuator are [42]:

(a) Subnanometre resolution
(b) Large force generation
(c) Submillisecond response
(d) No magnetic fields
(e) Extremely low steady state power consumption
(f) No wear and tear
(g) Vacuum and clean room compatibility

Commonly used PZT actuators have two piezoelectric modes (d_{31} and d_{33}), as shown in Fig. 8. The induced strain direction of the PZT plate is either perpendicular (d_{31}) or parallel (d_{33}) to the electric field direction [44]. The characteristic of the PZT actuator allows the proposed method for microsphere generation.

The proposed microchannel system consists of two intersections for hydrodynamic flow focusing and the liquid chopper. The middle stream is focused by the sheath flows hydrodynamically from the first intersection to downstream. The width of the focused stream does not depend on the magnitude of applied pressures but rather on the ratio of the side pressure from the sheath flow to the inlet pressure of the middle flow, which is proportional to the flow velocities. After being focused, a higher velocity of the focused flow is not avoidable, which makes the focused flow stable. A fluctuating external flow is

![Fig. 7 Schematic diagram of proposed microchannel design and microsphere generation](image)

![Fig. 8 Schematic cross-sectional view of two piezoelectric modes by the electric field. When the electric field is applied through the PZT plates, the PZT plates deform perpendicular (d_{31}) and parallel (d_{33}) to the electric field. Once the electric field is off, the PZT plates return to the original shape](image)
introduced to the focused stream at the second intersection by a PZT actuator. By structuring a liquid chopper, the fluctuating external flow pinches the stable focused flow, and the flow is disconnected to form droplets, which are emulsified to microspheres.

Hence, by decoupling equation (18), the design equation of the proposed design becomes

\[
\begin{bmatrix}
FR_1 \\
FR_2 \\
FR_3
\end{bmatrix} = \begin{bmatrix}
x & 0 & 0 \\
x & x & 0 \\
x & x & x
\end{bmatrix} \begin{bmatrix}
DP_1 \\
DP_2 \\
DP_3
\end{bmatrix} = \begin{bmatrix}
FR_1 \\
FR_2 \\
FR_3
\end{bmatrix}
\]

The lower levels selected for \( FR_1 \) are as follows:

- \( FR_{11} \): consistancy.
- \( FR_{12} \): constant flowrate of the sheath flows.

In order to satisfy the consistency of the microfluidic system, the most important design parameter is constant pressure. Thus, the \( DP_1 \) required for \( FR_1 \) are as follows:

- \( DP_1 \): continuous and consistent pressures for inlets.
- \( DP_{11} \): constant pressure for sheath flows.
- \( DP_{12} \): constant pressure for middle flow.

The design equation for \( FR_{1s} \) and \( DP_{1s} \) for the selected lower level yields an uncoupled design as

\[
\begin{bmatrix}
FR_{11} \\
FR_{12}
\end{bmatrix} = \begin{bmatrix}
x & 0 \\
0 & x
\end{bmatrix} \begin{bmatrix}
DP_{11} \\
DP_{12}
\end{bmatrix} = \begin{bmatrix}
FR_{11} \\
FR_{12}
\end{bmatrix}
\]

The lower levels selected for \( FR_2 \) and \( FR_3 \) and \( DP_2 \) and \( DP_3 \) required for \( FR_2 \) and \( FR_3 \) respectively are as follows:

- \( FR_2 \): size-controllability.
- \( FR_{21} \): to change the flowrate of sheath flows.
- \( FR_{22} \): constant flowrate of the middle flow.
- \( DP_2 \): to change the width of the dispersed phase.
- \( DP_{21} \): to alter the flowrates of sheath flows activating the PZT actuator in external channels.
- \( DP_{22} \): constant pressures for the middle flow.
- \( FR_3 \): breakage of the flow stream.
- \( FR_{31} \): to increase the flowrates of sheath flows.
- \( DP_3 \): to narrow the width of the dispersed phase to be cut.
- \( DP_{31} \): to increase the air pressure for sheath flows.

The design equations for \( FR_{2s} \) and \( DP_{2s} \) and for \( FR_{3s} \) and \( DP_{3s} \) are

\[
\begin{bmatrix}
FR_{21} \\
FR_{22}
\end{bmatrix} = \begin{bmatrix}
x & 0 \\
0 & x
\end{bmatrix} \begin{bmatrix}
DP_{21} \\
DP_{22}
\end{bmatrix}
\]

\[
\{ FR_{31} \} = [\times ]\{ DP_{31} \}
\]

4 SIMULATION STUDY

4.1 Governing equations

Two immiscible fluids, oil phase and aqueous phase, are introduced to the microfluidic device by inlet pressures for the middle flow and sheath flows. At the first intersection, the immiscible fluids come into contact downstream, and the middle flow is squeezed by the sheath flows, constructing hydrodynamic flow focusing, as shown in Fig. 9.

The width of the focused flow is calculated by the conservation law as

\[
\frac{m_{in}}{\rho_a v_a h D_a} = \frac{m_{out}}{\rho_1 v_1 h D_1 + \rho_2 v_2 h D_2 + \rho_3 v_3 h D_3} + \rho_1 v_1 D_1 + \rho_2 v_2 D_2 + \rho_3 v_3 D_3
\]

\[
v_a = \frac{\rho_1 v_1 D_1 + \rho_2 v_2 D_2 + \rho_3 v_3 D_3}{\rho_a D_a}
\]
where \( \dot{m}_{in} \) and \( \dot{m}_{out} \) are mass flowrates of the inlet and outlet flows, \( \rho \) is the density of the flow, \( v \) is the velocity of the flow, \( D \) is the width of the microchannel, \( h \) is the height of the microchannel, and the subscripts 1, 2, 3, and \( a \) represent the inlet 1, inlet 2, inlet 3, and average property of the outlet respectively. Likewise, the conservation of mass requires that the amount of fluid crossing the centre channel must equal the amount of fluid crossing the focused stream as

\[
\rho_1 v_1 h D_1 = \rho_v v_f \frac{\pi}{4} d^2
\]

(26)

\[
d = \sqrt[4]{\frac{4\rho_1 v_1 h D_1}{\pi v_f}}
\]

(27)

where the cross-section of the microchannel is circular and \( v_f \) is the velocity of the focused stream. Assuming that the fluid stream is a fully developed laminar flow inside the microchannel, the velocity profile inside the section \( D_a \) is parabolic-distributed when

\[ v_f = v_{max} = 1.5 v_a \]

(28)

Thus, the width of focused stream is represented as [45]

\[
d = \sqrt[4]{\frac{4\rho_1 v_1 h D_1}{\pi v_f}} = \frac{4\rho_1 v_1 h D_1 \rho_a D_a}{1.5\pi(\rho_1 v_1 D_1 + \rho_2 v_2 D_2 + \rho_3 v_3 D_3)}
\]

(29)

The focused flow keeps the width without any disturbance and flows to the second intersection where an external flow is driven by a PZT actuator with a frequency \( f \) (Hz).

In this simulation study, only the second intersection in the microchannel was simulated by varying the frequency of the PZT actuator. A commercial computational fluid dynamics package, COMSOL MULTIPHYSICS, was used to perform the numerical simulation of the proposed novel microsphere formation method applying the properties of poly(lactic-co-glycolic acid) (PLGA) in dichloromethane and 1 per cent of polyvinyl alcohol (PVA) in distilled water for the continuous oil phase and the dispersed aqueous phase respectively. The simulation could be simplified by designing the model geometry in three dimensions, as illustrated in Fig. 10.

The flows in the system during the simulation are laminar and immiscible. The oily focused flow is the dispersed phase (PLGA solution) and the aqueous sheath flows and the external flow are the continuous phase (PVA solution) in this study. The intersection for the simulation is initially filled with the immiscible fluids, and the properties of the fluids are given in Table 1.

The governing equations for this method are as follows:

Continuity equation:

\[ \nabla \cdot \mathbf{u} = 0 \]

(30)

Momentum equation:

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + \mathbf{F}_{ext} \]

(31)

Table 1: Properties of the fluids

<table>
<thead>
<tr>
<th></th>
<th>Continuous phase flow</th>
<th>Dispersed phase flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1000</td>
<td>1450</td>
</tr>
<tr>
<td>Kinematic viscosity (m²/s)</td>
<td>1.7016 x 10⁻⁶</td>
<td>2.99 x 10⁻⁶</td>
</tr>
<tr>
<td>Dynamic viscosity (kg/m s)</td>
<td>1.7016 x 10⁻³</td>
<td>4.34 x 10⁻³</td>
</tr>
</tbody>
</table>
where \( \rho \) is density (kg/m\(^3\)), \( u \) is velocity (m/s), \( t \) is time (s), \( \eta \) is dynamic viscosity (Pa s), \( p \) is pressure (Pa), and \( F_{tr} \) is the interfacial tension force (N/m).

Additionally, a level set equation for tracking the interfaces and shapes is defined as

\[
\frac{\partial \Phi}{\partial t} + u \cdot \nabla \Phi = \gamma \nabla \cdot \left( -\Phi(1 - \Phi) \frac{\nabla \Phi}{|\nabla \Phi|} + \varepsilon \nabla \Phi \right)
\]

where \( \Phi \) is the level set function, and \( \gamma \) and \( \varepsilon \) are numerical stabilization parameters. The density and viscosity are calculated from

\[
\rho = \rho_1 + (\rho_2 - \rho_1)\Phi
\]

\[
\eta = \eta_1 + (\eta_2 - \eta_1)\Phi
\]

where \( \rho_1, \rho_2, \eta_1, \) and \( \eta_2 \) are the densities and viscosities of the continuous phase and the dispersed phase [46]. Parabolic velocity profiles were specified at inlets with zero pressure at the outlet of the intersection. The wetted boundary condition applied to all solid boundaries. The contact angle between the fluid interface and the solid wetted wall is specified as 135\(^\circ\). In reality, it is considered that multiphase flow is one of the most difficult topics in CFD simulation, causing the results of theory and experiment not always to be exact [47].

5 RESULTS AND DISCUSSION

The channel was initially filled with immiscible flows, which are the continuous phase and the dispersed phase. Parabolic velocity profiles were specified at inlets with zero pressure at the outlet of the intersection. The interfacial tension \( \sigma \) for this simulation was 4.6 mN/m, which is the interfacial tension between 5 per cent of polylactic-co-glycolic acid (PLGA) in dichloromethane and 1 per cent of polyvinyl alcohol (PVA) in distilled water. For the simulation, the width of the focused flow, \( a \), was set to 2 \( \mu \)m, and the velocity of the sheath flow \( v_3 \) is considered as the same value as that of \( v_f \). These parameters were satisfying \( FR_3 \) to pinch the focused flow when an external flow was fed in. The external flow driven by the PZT actuator has the same property of the sheath flow, aqueous phase (PVA solution). By controlling the PZT actuator, the velocity of the external flow is defined during the simulation as

\[
v_e = v_f (1 + |A \sin(2\pi ft)|)
\]

Fig. 11 Snapshots of droplet formation at \( f = 1 \) MHz
where $A$ is the amplitude, $f$ is the frequency (Hz), and $t$ is time (s). The external flow is continuous and propagates the fluctuation generating instability to the main stream.

In Fig. 11, the formation of the microsphere in the microchannel is illustrated at different simulation times. The simulation shows that the external flow is introduced with high pressure to the main stream, and the focused stream is interrupted (see Fig. 11(a)). Shortly after, the focused flow is squeezed, and an oval-shaped bulb is produced (see Fig. 11(b)). The neck of the bulb is pinched off and the bulb is disconnected from the main focused stream, forming a droplet, and travels downstream (see Fig. 11(c) and (d)). This process occurs periodically with a very uniform size of the droplets.

During the periodic droplet formation process, the oscillation from the external channel transmits high pressures to the main stream, facilitating the neck being pinched off. The formation of the microsphere occurs after the neck of a liquid bulb is pinched off. The microsphere formation does not depend on only the applied external force to the flow but also the width of the focused flow as well as the geometry change of the microchannel [48]. However, only the applied external fluctuating force generated by the PZT actuator will be considered here because the simulation was set up with the uniform channel geometry and a fixed size of the width of the focused flow. The size of the microspheres by the different frequencies of the PZT actuator is shown in Fig. 12. By varying frequency $f$ from 1 to 2.1 MHz, the generated microsphere sizes were between 1.74 and 3.65 μm in diameter with about 2.4 per cent of coefficient of variation ($CV = \frac{(standard\ deviation/average\ diameter)}{100%}$ [49]), which signifies that the proposed method can be manipulated to achieve the controllability and the uniformity in the formation of microsphere generation.

6 CONCLUSION

In this paper, a microchannel design methodology has been proposed for uniform and size-controllable microsphere generation applying axiomatic design theory (ADT). The general design goals of the microchannel systems are uniformity and controllability of microsphere sizes. Employing ADT, the conventional two microchannel system designs were evaluated as coupled designs, but they may cause failure during operation. A decoupling process was proposed to develop a decent microchannel system design, a liquid chopper utilizing a PZT actuator. The decoupled microchannel system design was simulated to generate uniform O/W microspheres by using the phase separation principle.

A stable hydrodynamically focused flow is interrupted by the fluctuating flux generated by a PZT actuator in the microchannel. The initiated high pressure of the oscillating external flux overcomes the interfacing forces of the two-phase flows, and the focused flow is pinched off, which is characterized as a liquid chopper. The liquid chopper is activated in various frequencies, altering the frequency of the PZT actuator, and different sizes of uniform microspheres with 2.4 per cent of coefficient of variation can be generated. The size and size distribution of the microspheres determines the characteristics and performance of the microspheres.

This simulation study proves that this novel microchannel design can achieve tunable microspheres with uniform size and reveals a high potential for an emulsification process, which can be widely applied in numerous fields, thus demonstrating the effectiveness of incorporation of such a decoupled design process for this particular type of microchannel system.

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REFERENCES


29 Engelhardt, F. Improving systems by combining axiomatic design, quality control tools and designed experiments. Res. in Engng Des. – Theory and Concurrent Engng, 2000, 12, 204–219.
35 Suh, N. P. The principles of design, 1990 (Oxford University Press, USA).