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OPTIMIZATION STUDY ON THE CONTOURED SHOCK TUBE FOR NEEDLE-FREE DRUG DELIVERY

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ABSTRACT

An exciting alternative of the conventional drug delivery systems has been proposed in recent times named as transdermal powdered drug delivery. The idea is to deliver drug (in powdered from) into the human skin without using any external needle. Among different proposed systems the contoured shock tube (CST) system stands out. The performance of CST device is widely analyzed by different researchers. However, there is still room for improvement of it's performance. This study aims at improving the performance of CST device by adjusting it's geometry as well as operating condition. A significant improvement in the performance is reported after proper adjustment of different features of the device.

INTRODUCTION

The contoured shock tube consists of a conventional shock tube with a supersonic nozzle connected at the end. The high pressure driver and the low pressure driven zone are separated by two polycarbonate diaphragms. The drug is stored in the drug cassette which is placed between the diaphragms. When the operation is initiated by opening the micro-cylinder, a very high pressure builds up in the driver section. Once the designated pressure is reached, the diaphragm ruptures and a high pressure transient flow is generated through the shock tube. The drug particles accelerate behind the moving shock wave. A schematic diagram is given in Fig.1.

Transdermal powdered drug delivery offers a wide range of advantages compared with the conventional systems. First and most attractive advantage is the delivery of drug without any external needle. As a result all possible contamination hazards can be avoided. As the operation of the device is very simple, no skilled expert is needed to execute the delivery process. The storage system of the drug also becomes very convenient as drugs can be stored in powdered form. Transdermal powdered drug delivery also offered prospect of much improved delivery system for some complicated drug delivery like the DNA vaccination or anti-viral drug delivery.

The first person to pioneer the field of transdermal powdered drug delivery was Stanford et al. [1]. Bellhouse et al. later modified it for human treatment [2]. The proposed system was found to be quite capable of delivering particles (protein, DNA) to the human skin with precision and accuracy [3].

In recent times Kendall et al. have designed a number of systems and studied them both numerically and experimentally [4-10]. He concluded that the performance of contoured shock tube is far better than the other devices. However, there are still lots of improvements have to be done for widespread commercial use of CST. Recently an optimization study of different particle features was conducted by the authors of this article (in print). The current study aims at optimizing the performance of CST by varying the geometry and operating conditions. A computational approach is taken as conducting repeated experiment and analysing characteristics of key components is very complex.

NOMENCLATURE

P	[Pa]	Static pressure
M		Mach number
ρ	$[kg/m^3]$	Fluid density
u	[m/s]	Gas phase velocity
u_p	m/s	Particle velocity
ρ_p	$[kg/m^3]$	Density of particles
D_p	[m]	Particle diameter
t	[s]	Time
F_D	[N]	Particle drag force

Abbreviation

CST	[-]	Contoured shock tube
CDSN	[-]	Convergent-divergent supersonic nozzle
P.S	[-]	Primary shock
S.S	[-]	Secondary shock
C.S	[-]	Contact surface
QSSF	[-]	Quasi-steady supersonic flow

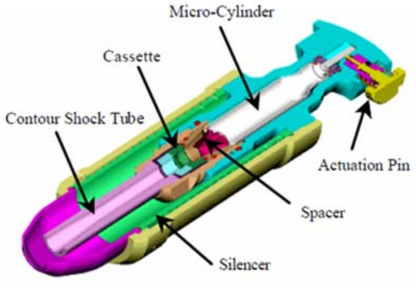


Figure 1 Schematic diagram of CST device. [6]

FLOW MODELING

The computational domain and the applied boundary conditions are shown in Fig. 2. The domain is extended to 15D×4D (D is the diameter of the nozzle exit) for better numerical accuracy. To avoid complexity the micro-cylinder is not modeled. Instead a pre-filled driver section is assumed (1550 KPa). Atmospheric pressure is specified in the driven section. An instantaneous diaphragm rupture is assumed. Only one diaphragm instead of two is considered. The particles are of 39 µm diameter with a density of 1050 kg/m^3. The wall temperature is assumed as constant with no slip condition. A general 2D axisymmetric model is used. However, 3D calculations are also conducted to investigate important features (More clearly specified in the result and discussion section). A mesh independent study is also conducted to find out the optimum mesh size. The lowest mesh size of 29,370 is chosen for the current study as no larger than 0.2% difference is observed in different mesh distributions.

GOVERNING EQUATIONS

Gas flow modeling

The flow physics was modeled solving the unsteady Reynold's Average Navier-Stokes equation,

$$\frac{\partial W}{\partial t}+\frac{\partial F_i}{\partial x_i}=\frac{\partial^2 G}{\partial {x_i}^2}+H \qquad (1)$$

In our present study the k- ω standard model was used as it was found to predict the experimental results with higher accuracy. The turbulence kinetic energy, k and the specific dissipation rate ω for standard k- ω are obtained from the following transport equations,

$$\frac{\partial(\rho k)}{\partial t}+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\delta}{\partial xj}\left(\Gamma_k\frac{\partial k}{\partial x_j}\right)+G_k-Y_k+S_k \qquad (2)$$

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial}{\partial x_i}(\rho\omega u_i)=\frac{\delta}{\partial xj}\left(\Gamma_\omega\frac{\partial \omega}{\partial x_j}\right)+G_\omega-Y_\omega+S_\omega \qquad (3)$$

Particle transportation modeling

Discrete Phase Model (DPM) in Ansys Fluent is used to model the particle transportation through the shock tube. The fluid phase is treated as a continuum by solving the N-S equations, while the dispersed phase is solved by tracking a large number of particles through the calculated flow field. The equation of motion for the particle is,

$$\frac{du_{\mathrm{p}}}{dt}=F_D(\vec{u}-\vec{u}_p)+\frac{\vec{g}(\rho_p-\rho)}{\rho_p}+\vec{F} \qquad (4)$$

F_D is gas drag force which is calculated by,

$$F_D=\frac{3\mu C_D Re}{4\rho_p d_p^2} \qquad (5)$$

Re is particle Reynolds number which is calculated by,

$$Re=\frac{\rho d_p\left|\vec{u}_p-\vec{u}\right|}{\mu} \qquad (6)$$

The drag correlation used in the current study was proposed by Igra et al and incorporated in Ansys fluent by user defined function (UDF) [12]. The correlation is,

$$\log_{10} C_D = 7.8231-5.8137\log_{10}\mathrm{Re}+1.4129(\log_{10}\mathrm{Re})^2$$
$$-0.1146(\log_{10}\mathrm{Re})^3 \qquad (7)$$

NUMERICAL SCHEME USED

Fluent 14, a commercial CFD application software is chosen to numerically simulate the flow field. The working gas behavior is considered as ideal gas and the viscosity variation with respect to temperature is modeled using sutherland law. The flux component of the governing equation is discretized using upwinding Roe vector different splitter scheme. The time integration for the governing equations are carried out using second order explicit schemes in order to capture the main feature of the unsteady flow. The governing equations are solved in a coupled manner. An overall second order accuracy is maintained.

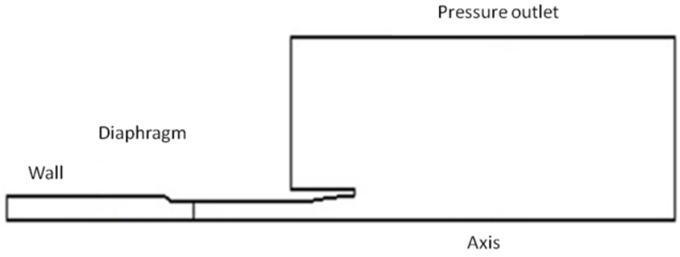


Figure 2 Computational domain and the boundary conditions

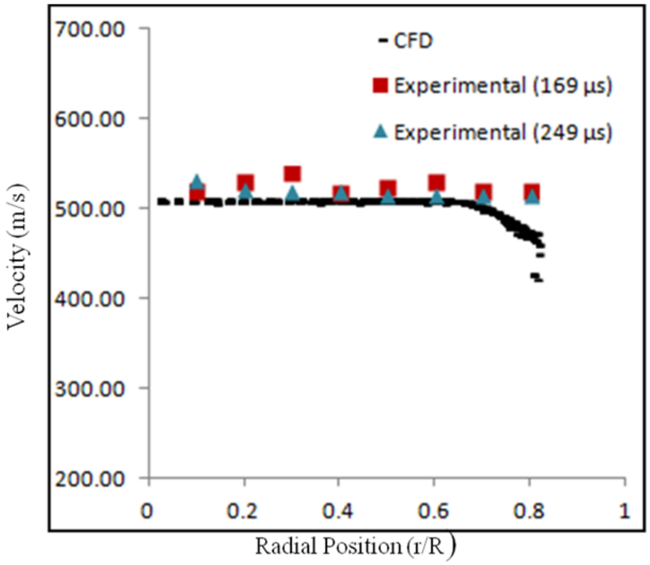


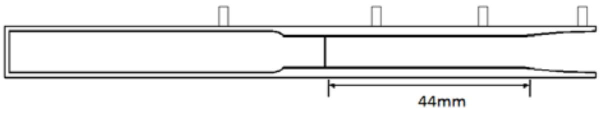
Figure 3 Numerical and experimental particle exit velocity

VALIDATION

The adopted numerical model is validated by comparing the experimental particle exit velocity with the numerically calculated particle exit velocity. The experimental results are obtained from a study conducted by Liu et al where they studied the performance of CST device [6]. The geometry and the operating conditions are kept exactly same in the numerical study. The numerical results demonstrate a good match with the experimental results (Fig 3). Thus it can be concluded that the simulation scheme used for the current study can predict the CST operation with sufficient accuracy.

RESULTS AND DISCUSSION

One of the most important parts of the CST device is the shock tube. The shock tube is responsible for accelerating the gas flow thus accelerating the particles behind it. So fixing the proper shock tube length to make maximum utilization of the shock tube is vital. In an attempt to do so, the length of the shock tube is varied from 44mm to 74mm arbitrarily just to find the optimum point, where particles are no longer accelerating by the gas flow. For our further study 44mm is regarded as cases-I and 74mm shock tube is regarded as cases-II. A schematic diagram is also shown for both cases in Fig. 6 to make it clearer. The basic idea is to allow maximum acceleration of particles inside the shock tube by selecting the appropriate length.



Case-I

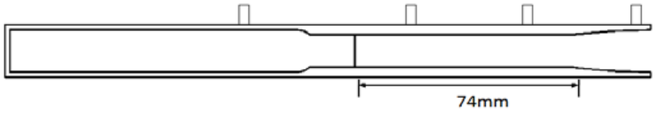


Figure 4 Considered cases for optimization of shock tube length

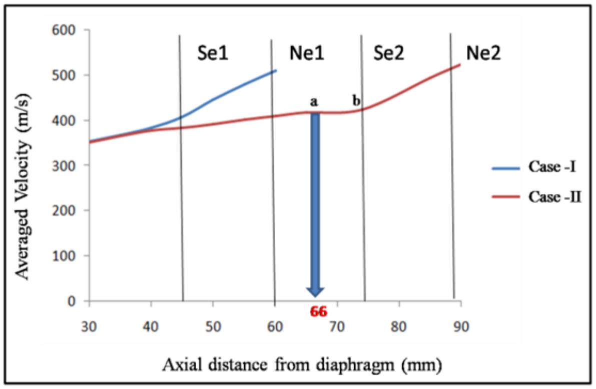


Figure 5 Axial velocity profile of particle for case I & II

The velocity profile of particle for both cases is plotted in Fig. 5. The position of the shock tube as well as the nozzle exit is marked as Se and Ne. For both cases it can be observed that the particles are accelerating up to the shock tube exit then continuing to accelerate at a higher rate inside the supersonic nozzle. However, for case-II particles continues to accelerate up to 66mm instead of restricting within 44mm. Once the particles are accelerated up to 66mm, particles exit velocity demonstrate a constant value (a to b) before passing out of the nozzle. So by increasing the shock tube length up to 66mm maximum utilization of the shock tube system can be ensured. Therefore for the new optimized device the shock tube length is fixed as 66mm.

In the standard contoured shock tube the diaphragm rupture pressure is specified as 1550kPa. With this rupture pressure, the gained particle exit velocity is 510 m/s [11]. Moreover particle distribution is fairly limited in the nozzle exit plain. In an attempt to generate a higher particle exit velocity as well as distribute particle into a wider area, diaphragm rupture pressure of 3000 kPa is proposed. As the intention of conducting this study is to investigate the exit condition of particles in details, 3D CST model is used for more accurate results.

Particle velocity distribution in the nozzle exit for rupture pressure 3000kPa is plotted in Fig 6. Particles seem to gain a higher exit velocity of 605 m/s compared to the previous 510 m/s. Also particles are distributed up to radial position 0.85 whereas it was restricted up to 0.75 in the previous cases.

To get a more clear view of the particle distribution in the nozzle exit plain, simulated particle distribution is shown in Fig. 7. It seems that the particles are spatially distributed throughout the whole nozzle surface. No stream of particle is observed to be concentrated in any particular section. This is a big improvement in the performance of CST device.

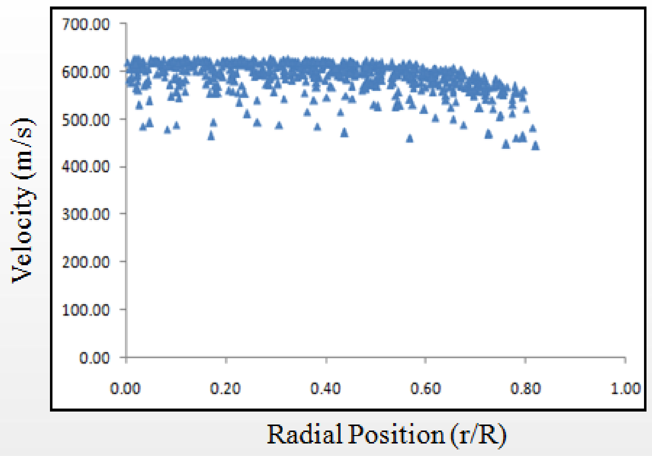


Figure 6 Particle velocity distribution is the nozzle exit for rupture pressure 3000 kPa

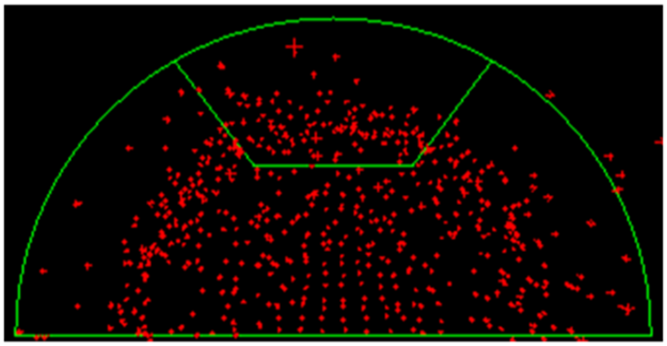


Figure 7 simulated particles distribution in the nozzle exit

CONCLUSION

A numerical approach has been adopted in order to optimize the performance of contoured shock tube by varying it's geometry and operating conditions. The length of the shock tube was varied from 44mm to 75mm and the diaphragm rupture pressure is varied from 1550kPa to 3000kPa.

Initial results suggest that, increasing the shock tube length allows particles to further accelerate before entering into the nozzle. Thus the shock tube length is fixed as 66mm.

It has also been observed that the higher rupture pressure produces higher particle exit velocity with wider distribution. Thus the rupture pressure is fixed as 3000kPa.

Although, these results help to design an improved contoured shock tube device, a more in depth study is necessary to analyse gas and particle interaction in the adjusted conditions. This could be the focus of future work on CST.

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