Hydrodynamic Simulation of an Orbital Shaking Test for the Degradation Assessment of Blood-Contact Biomedical Coatings

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Abstract. Biomedical coatings are used to promote the wear resistance and the biocompatibility of a mechanical heart valve (MHV). An orbital shaking test was proposed to assess the durability of the coatings by the amount of eroded material due to the surrounding fluid. However, the shaker's rotating conditions and the corresponding physiological condition were still lack of understanding. This study implemented numerical simulations by establishing a fluid dynamic model to evaluate the intensity of the shear stress under various rotating speed and diameter of the shaker. The results are valuable to conduct *in vitro* tests for estimating the performance of biomedical coatings under real hemodynamic conditions and can be applied to other fluid contact implants.

Introduction

Mechanical heart valve (MHV) is widely used in the replacement of human heart valve and ventricular assist devices. In order to reduce the failure after valve transplantation, there is a biocompatible coating to modify prostheses' surface [1]. During the serving time of an MHV *in vivo*, its coating is constantly subjected to the shear stress caused by the blood flow. In general, when the valves are moving from opening to closing, the average flow rate is greater than 0.8 m/s due to the venturi effect [2,3,4]. The biocompatible coatings may lose their function and even be removed from the surface, of which the intensity of the shear stress and the duration are two major factors that cause the long-term degradation of the coatings.

To examine the adhesion strength between biocompatible coatings and MHV, the samples with collagen-heparin composite coating were immersed in containing tubes filled with physiological saline, incubated at 37°C, and then shaken on an orbital shaker for different durations [5]. The remained material on the substrate was measured and compared. It is a simple and easy way to evaluate the long-term performance of any biomedical coating, organic or inorganic, on the blood contact device. However, the shaker's rotating conditions, including the rotating speed and diameter, and the corresponding physiological condition was still lack of understanding.

In this work, an orbital shaker is chosen for simulating the fluid condition in heart and blood vessels, the remained amount of coated heparin after the experiment is regarded as indicators of the binding at different rotating speeds and diameters. A preliminary analysis of the biocompatible coatings degradation in dynamics condition is presented, and a previous experimental work was also investigated [6].

Materials and Method

Problem Description. Fig. 1(a) shows a commercially available orbital shaker. The container on the orbital shaker being translated along the path is illustrated in Fig. 1(b), where (x, y) , (x', y') , R , and ω

represent the fixed global coordinate, the orbitally-moving coordinate on the container, the radius of rotating path, and the rotating speed. As the sample and the fluid inside the container were both moving with the path in the same rotating speed, a simulation model was established by exploiting moving boundary technique of the computational domain.

Fig. 1 (a) The orbital shaker in this study, (b) the rotating path of the container, with a coated sample and PBS solution, and the relation equation of the fixed global coordinate (x, y, z) and the orbitally-moving coordinate (x', y, z'). ω is the rotating speed in rad/s, R is the radius of the rotating path in mm, and t is the time in second. The A-A view is the cross section of the container to illustrate the detail status of the fluid.

Simulation setup. In this model, the computational area was composed by two domains, the surrounding air domain and the container domain. The dimensions and material properties of the domains are summarized in Table 1 and Table 2.

The simulation was carried out with the commercial computational fluid dynamic (CFD) software. The fluid had a multiphase property and a k - ϵ turbulence model was applied. The solution was modelled as a mixture of water and air, which was incompressible, viscous, and isothermal. By means of this model, the shear flow was accessed in the flow.

Rotating speed and diameter of the shaker were two independent variables in the simulation. The rotating speed of the shaker was varied from 60 rpm to 300 rpm and the rotating diameter of the shaker was 1 cm, 3 cm and 5 cm respectively.

Table 1 Properties of the surrounding air domain.

Diameter [mm]	100
Height [mm]	20
Density [kg/m^3]	1.225
Viscosity [$\text{kg/(s}\cdot\text{m)}$]	0.00001789

Table 2 Properties of the container domain.

Diameter [mm]	30
Height [mm]	20
Liquid level [mm]	10
Air Density [kg/m^3]	1.225
Solution Density [kg/m^3]	998.2
Solution Viscosity [$\text{kg/(s}\cdot\text{m)}$]	0.001003

Result and Experimental application

In this section we present the results of our numerical simulations for five rotating speeds and three rotating diameters of the shaker. Fig. 2 demonstrates a typical trajectory and liquid distribution at four positions where the rotating speed and diameter are 120 rpm and 1 cm.

Fig. 2 The shapes and surfaces (in blue) of the liquid (in red) in the container during a period, where the container is rotated at 120 rpm, i.e. the period is 2 s, along an orbital path with 1 cm diameter. For each position, from left to right, the simulating time is 0.625 s and the time increment is 0.5 s. The coordinate is xyz system.

Dynamic performance in the rotational speed and diameter variation. To evaluate the variable hydrodynamic condition in terms of the erosion from the flow acting on the surface of an MHV, the instantaneous viscous shear stresses can be obtained by the CFD model established in this work.

After a very short transient procedure, the flow inside the container was proven, from period to period, to be steady and well-posed at any specific position of the orbital path as indicated in Fig. 2. The distributions of the shear stress vector for three rotating diameters on the bottom surface at the simulating time of 2.5 s are visualized in Fig. 3 in isometric and top view. The rotating speed of these cases were kept at 120 rpm. The average and maximum shear stresses along an arbitrary diameter on the bottom surface of the container are shown in Fig. 4. The distributions of the shear stress are similar, which suggests that the rotating diameter has little effect on the shear stress of the bottom surface.

Fig. 3 The isometric view (upper) and top view (lower) of the shear stress distributed on the bottom surface of the container. The shaker's rotational speed is 120 rpm and the rotational diameter is 1 cm (left), 3 cm (middle) and 5 cm (right), respectively. The coordinate is x'yz' system.

Fig. 4 The variation of (a) the average shear stress, and (b) the maximum shear stress along an arbitrary diameter on the bottom surface of the container with three rotating diameters. (Rotating speed = 120 rpm).

In Fig. 5, the distributions of the shear stress vector for three rotating speeds on the bottom surface at the simulating time of 2.5 s are also illustrated by isometric view and top view. The rotating diameter of these cases were kept at 1 cm. The average stress and maximum stress are shown in Fig. 6. It is worthy of notification that the trend of the stresses is more significant than the those in Fig. 4 with the rotating diameters, especially during the rotating speeds between 180 to 240 rpm. Therefore, the rotating speed of orbital shaker is suggested to be the major parameter to set up the shear stress level of the long-term erosion test in this study.

Experimental application. In the experimental study, we present the degradation assessment of two coatings by the application of orbital shaker. These samples were both grade 2 titanium substrates treated with dopamine, poly-L-lysine, and then coated with heparin/collagen multilayers and a heparin outmost layer. Electrostatic layer-by-layer technique was conducted to build these coatings and the amount of heparin were measured by toluidine blue O test [6]. The samples with 4 and 9 multilayers in this study were coded with Ti/Dop/(Hep_Col)₄/Hep and Ti/Dop/(Hep_Col)₉/Hep, respectively.

Fig. 5 The isometric view and top view of the shear stress distribution on the bottom surface of the container. The shaker's rotational diameter is fixed at 1 cm and the rotational speed is adjusted to 60 rpm, 120 rpm, 180 rpm, 240 rpm and 300 rpm respectively from left to right. The coordinate is $x'yz'$ system.

Fig. 6 The variation of (a) the average shear stress, and (b) the maximum shear stress along an arbitrary diameter on the bottom surface of the container with five rotating speeds (rotating diameter = 1 cm).

Fig. 7 shows the quantitative analysis of the coatings by the remaining heparin from the beginning to the fifteen days. The rotating speed of the orbital shaker was kept at 120 rpm and the rotating diameter, in 1 cm. It can be observed that the heparin/collagen coatings were significantly removed by the fluid for the first two days. The samples with 9 multilayers, even having nearly the same heparin at the beginning, could maintain higher heparin content. However, when the tests exceeded four days, the degradation of both coatings reached a low and steady condition until the fifteen days. According to the numerical results in this study, the average shear stress and maximum shear stress actuated on the coatings were 0.1 and 0.4 Pa, which can be assessed and compared with the real physiological conditions.

Fig. 7 Heparin density of two samples, Ti/Dop/(Hep_Col)₄/Hep and Ti/Dop/(Hep_Col)₉/Hep, from the beginning to the 15th days of the tests conducted by the orbital shaker (N = 3).

Summary

As the degradation of the biomedical coatings are caused by the shear stress and the actuating duration, this work provides a numerical evaluation of the shear stress in the container of an orbital shaker to investigate the mechanism of the degradation. The rotational speed of the shaker is verified

to be the major operating parameter that can change the shear stress of the flow in the container. By applying the results to the experimental investigation, the correlation of biomedical coating's degradation in the fluid-contact conditions and its shear stress levels was demonstrated.

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