EXPERIMENTAL AND NUMERICAL LDL TRANSPORT IN THE ARTERY

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Introduction

Atherosclerosis is a chronic systemic inflammatory disease; the end-stage of which is plaque rupture. Calculation of the interactive molecule forces open a new avenue for multiscale modeling methods which will give better insight for understanding and the prediction of LDL transport through the arterial wall.

Methods

A. Experimental setup

Ex vivo blood vessels experiments of LDL transport were performed on the isolated rabbit common carotid arteries. Blood vessel was excised and placed in the water bath. The lumen was perfused with Krebs-Ringer physiological solution (KRS), using the peristaltic pump at 1 ml/min. The perfusate was continuously bubbled with a 95% O_2, and 5% CO_2 with the pH adjusted to 7,4 at 37 C.

B. Numerical procedures

Basic principle of the DPD (Dissipative Particle Dynamics) methods is the fact that all particles have interaction with the neighbor particles which are in certain domain and force of interaction makes three inner forces: conservative, dissipative (because of stochastic behavior) and random force.

For binding LDL molecules on the arterial wall the spring force is used [Filipovic et al 2008a,b].

$$F_a = k_{sf}(1 - \frac{L_{sf}}{L_{sf}^{\max}}) \qquad (1)$$

where L_{sf} is the distance between molecule of LDL and endothelium, $L_{sf}^{\max}$ is maximum distance between molecules and k_{sf} is the stiffness coefficient.

Results

Dimension of DPD two-dimensional model are 2500x360, which is in accordance with the experimental setup. Time step is 0.0015s, and number of time steps is 10000000, so total time of calculation is 14.167h.

For bounding LDL molecules on the blood wall a spring force was used. One molecule LDL needs three receptors for bounding, so our coefficient was calculated as triple value of one chemical's incorporating.

Shear rate was calculated based on the knowing dynamic viscosity of blood and dimension of model for different applied shear stress.

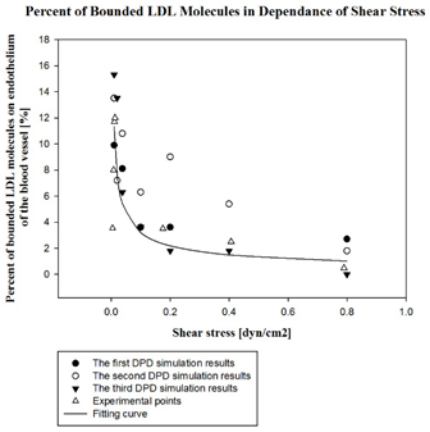

Figure 1: Results obtained from experimental measurement and DPD simulations

Discussion

In this study we compared computational results obtained from DPD simulations with experimental results for LDL transport through isolated blood vessel.

Matching of labeled LDL location between experimental and computer model shows a potential benefit for future prediction of this complex process using computer modeling. In our future investigation we will try to bring more complex model and more accurate results with discrete modeling approaches and computational chemistry.

References

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