Biomechanica Hungarica III. évfolyam, 1. szám

Analysis of the mechanical behavior of discrete elements in fluids (from the continuum to the discrete)

Brigitta Krisztina Tóth, Imre Bojtár
Department of Structural Mechanics
Budapest University of Technology and Economics (BME)
brigitta.toth@mail.bme.hu

Keywords: motion of red blood cells; stresses of artery-walls; continuum modelling; discrete element method; endothelium cells

1. Introduction

In the last few years there is increasing interest in numerical models of human blood vessels. The new computer-based systems can help already to come to a decision, if it is necessary to operate a diseased segment of a blood vessel, and if it is so, how urgently.

In the past years I have measured material parameters for different constitutive models of human artery vessels, and in the course of this work the medical doctors raised a very interesting issue: *is it possible to give an estimation* with engineering models, what *collision-forces* are effected in the endothelium cells – covering the vessels wall – from the red blood cells floating in blood plasma arteries? The question is important from biomedical point of view, because the endothelium cells work in some respect as a *"switchboard",* they transfer these internal forces as commands for different biochemical reactions of a segment of vessels. The solution of this problem could help to understand the physiological processes of artery wall.

To understand this problem from engineering point of view we have to know that arteries can be modelled like tubes – with elastic wall –, in which the flowing liquid is the so called blood plasma, and the different bigger-size cells – amongst all in largest number the red blood cells – move in this plasma. The volume percent of the cellular fraction is greatly significant, so we have to examine a relatively densely "filled" fluid. The solid particles can bump with each other or with the vessels wall in the course of their motion in the fluid, and the question is exactly, how can we describe this motion and how can we calculate the contact forces during these collisions?

I would like analyze what kind of numerical model is able to examine this effect of red blood cells streaming in the different type (size) of human arteries. I evaluated in a critical analysis those numerical models, which are used in fluid mechanics nowadays, mainly examined from that point of view, how fare are they able to model the mechanical effects of solid particles floating in blood plasma. I do also computational simulations on different models held suitable – and run-able by me, of course – to calculate collision forces of cells. I have a look at separately those special cases, when the diameter of the examined artery is so small, that the red blood cells pass through them only one after the other. In such cases the mechanical effect on the vessels wall is special, it doesn't refer to the direct collision, it refers to the change is pressure produced in the course of the flow.

We would like to note that this task of biomedical problem has a great number of analogous associate in many field of the life. For instance I can mention different examples: the rock masses transported by stream of lava, as well as ice-floes break off a glacier and travelling in a river, or an alternative, typically analogous task is for example the investigation of solid slime diluted with liquid and streaming in pipes, etc. It is worth mentioning, that can be found engineering-like examples to the analysis the influence of collisions also: the ice-floes bumping against a body of a ship or a river-pier of a bridge, or forces exerted by other solid bodies require similar mechanical investigations, like I need in the solution of my work.

The complex biomechanical analysis of arteries – generally speaking the solution of coupled problems in different numerical techniques – can be solved essentially in two different ways. The one is the *continuum-base modelling,* which can occur by any *FEM* (Finite Element Method) + *CFD* (Computational Fluid Dynamics) software. I note that we have the possibility to investigate also the time-dependent analysis of bigger-size arteries with these types of modelling, since we can keep the cellular elements circulating in blood only as infinitesimal particles. But in another domain of scale, what I want to model too, the effect of the particles having extension is greatly significant. Otherwise there is an interesting question: how can we take into account the presence of cellular elements with the method referred to above, in other words till when can we increase the rate of particles "theoretically" considered in current flow, how many percent of volume occupy those? It is important to note also that at present times further researches exist, which have the aim to expand the applicability of continuum-based modelling to the modelling of particles, too. These are called *"modified finite element methods"* (see the works of *Oñate* and *Liu*).

The alternative practicable analytical method is the so called *Discrete Particle Method* (DPM), which is able to treat the large-sized particles as really independent bodies. Although the behaviour of particles moving in the artery can

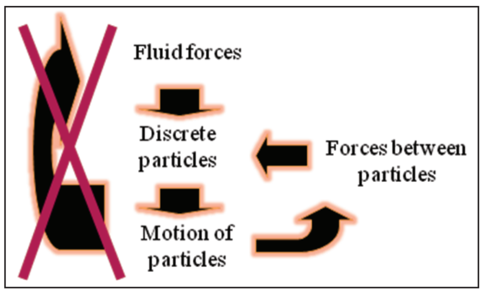

Figure 2. The flow chart of the traditional discrete element method: the motion of particles don't have a reaction on the fluid

Figure 1. Examples to "large-sized" discrete particles in streaming substance: stream of lava, glacier, red blood cells

be modelled with this method, moreover the fluid-forces can be added to the particles, a question arise: have these particles – cellular elements – a reaction on the circulating fluid surrounding them? The answer is of course, that the influence between the liquid and the body attending in continuum medium is mutual; the body has an influence on the relationship of circulation. In our opinion we ought to connect the pure discrete element modelling and the continuum-based fluid mechanics if we want to describe the required problem. Our answer is simple at first sight that we have to consider only *Newton's III. law* of motion what declare the law of action-reaction. Unfortunately this is not so easy, new developments must introduce in this field of science, like for instance the coupled new PFC3D, which connects the program based on the discrete element method with the CFD module.

2. Methods

2.1. Continuum model of particles moving in fluid

The *Computational Fluid Dynamics* (CFD) is suitable to model the behaviour of streaming fluids, heat-transfer or any other complex processes (see *Ferziger et al.*[7]). The CFD solves the equations describing the behaviour of fluid on the investigated domain, and can take into account the prescribed boundary and initial conditions on the domain (see *ANSYS CFX Theory Guide*[1]).

We can talk about multiphase flow in those cases, if more than one fluid is presented. Fluids can occupy independent regions which can partake in the same area of the fluid. The flow consisting of several components is different from these phenomena of course.

There are two available well defined fluid-models: the *Euler-Euler multiphase model* (see *Enwald et al.*[6], *Manninen et al.*[10]) and the so called *Lagrangian Particle Tracking* model. See applications and summaries in *Casey et al.*[3], in *Lun et al.*[9], in *Menter et al.*[11] and in *Clift et al.*[4].

In the next I will talk about the modelling of particle transport. The so called *Particle Tracking* model is able to describe dispersed phases, which appear discretely dispersed in the continuum substance. This model contains the independent calculation of the discrete particles with the essential conditions considering the effect to the continuum, which is made by the particles. From view point of this paper, this includes the circulation of blood and the transported cellular elements in it, too. Thus, the particle transport is attached to the multiphase models, in which case the particles are followed *Lagrangian-manner* during the flow, instead of extra *Euler-phase* modelling. We can model the entire particle-phase by a ideal sample substituting the particles. The tracking of particles is possible by the help of the common differential equations (these equations refer to place, velocity and mass). If we combine these equations with the basic mechanical equations of particles we can describe the complex behaviour of the whole system.

If the fluid contains small particles, it means the injection of millions of particles in every second. Avoid the cost of modelling the whole particles; we have the possibility to inject particles representing the real number of the particles but fewer than that. We can prescribe how many particles have to denote the followed particles. Contrary to the Euler-type multiphase computation, the calculation protection of the continuum phase doesn't contain the volume fraction occupied by the particles. This means, that the model is valid only in case of *small volume fractions.* Moreover in that case, when the model is not reliable, the volume fraction of the particles can be greater than one.

Different diverse forces can cause the motion of a particle in the fluid. We have to take into account the following forces at the equations describing the motion of particles: viscous, fluid *drag force,* buoyancy, virtual mass and pressure gradient forces, centripetal and *Coriolis-forces* in rotating frame of reference. The calculation of viscous drag forces is always important and essential. Apart from that buoyancy, what appears at one-phase flows, the difference between the densities of the particle and the continuous phase results in buoyancy too.

2.2. Discrete element modelling of particles in fluid

We can model the mechanical behaviour of complex systems composed of different particles with the help of the so called *particle-flow model.* Within the frame of this paper, if I use the word *"particle",* I don't think about the particle defined in mechanics, which has an extension negligible, and so it occupies a simple *"point"* in the place. In this paper I will always use the world "particle" as a body with *finite dimensions.* A discrete element model (see the theory from *Cundall et al.*[5]) consists of independent particles, which are able to move independently from each other, and they make interaction with each other only at contact points or by the side of their surfaces, respectively. In so far as we count particles to be rigid, as well as we consider finite normal stiffness in the course of contact problems, the mechanical behaviour of the system will be definable by the motion of particles and the interaction forces between particles (see details in *PFC3D Guide*[2]).

Newton's law of motion gives the basic relations between the motion of particles and the forces causing them. The system of forces can be in quasi-static equilibrium – in which case the motions are remarkably small – or can be so, what causes the flowing of the particles. A much complex behaviour can be modelled, if we allow the adherence of particles by the side of their contact points, up till the time as the forces between particles are in the neighbourhood of the so called contact stiffness necessary for opening the connection. In this manner tension forces can arise between particles, so contact problems among adhered blocks can be modelled too, and in this way there is the possibility of breaking blocks into smaller-sized elements.

In addition to the traditional domain of the particle-flow analysis, by this type of modelling there is a possibility to analyze the solid bodies by specified initial- and boundary conditions. In these models we can consider the solid body as a compact set composed of numerous particles. The stresses and strains can be considered as an averaged value inside a characteristic measurement domain.

All equations of motion have to satisfy for each particle. New connections can create and they can divide in the course of the calculation. The interaction between particles can be considered as dynamic process, in which course, an ambition of continuous equilibrium is noticeable by the help of the balancing of the internal forces. We can handle the dynamic behaviour with a numerical time-stepped algorithm, where the velocity and acceleration can be treated as constant in the individual time-steps.

The course of the solution is just the same, what the explicit method of finite differences applies in case of continuum investigations. The chosen time-step has to be so small, that the error in one time-step happens only by the direct neighbours of particles, so at all times we can determine the forces acting on a particle from the adjacent particles being interaction with it. Since the velocity of the expansion of disturbance is the function of physical properties of the system, we have to choose the time-step in that manner, that it fulfils the above mentioned condition. The application of explicit numerical method opens the door to simulate nonlinear contact problems of numerous particles, without extreme memory requirement or application of iterative solutions.

The *DEM* (Discrete Element Method) calculations apply in rotation *Newton's II. law of motion* to the particles and the force-displacement law to the contacts. Newton's II. law of motion serves for determination of motion derived from contact forces acting on particles and from body forces, while the force-displacement law makes the update of contact forces caused by relative displacements by contact points possible.

3. Results

The relation of artery's diameter to the size of red blood cells determines fundamentally the modelling of discrete elements (red blood cells) streaming in the continuum medium (blood). Since our main purpose is determinate the mechanical effect acting on the so called endothelium cells, we suggest the usage of different methods in the different domains of artery size.

3.1. Middle-large arteries

We begin with the investigation of the blood streaming in an artery having radius: $r = 1.5$ mm, because in this domain of size the red blood cells start to exert significant influence on the wall. We regard as suitable for investigation the *continuum-base modelling* of this domain of size of arteries. We have the foreknowledge, that only these arteries having "larger" diameter can be examined on the basis of pure continuum modelling, when the order

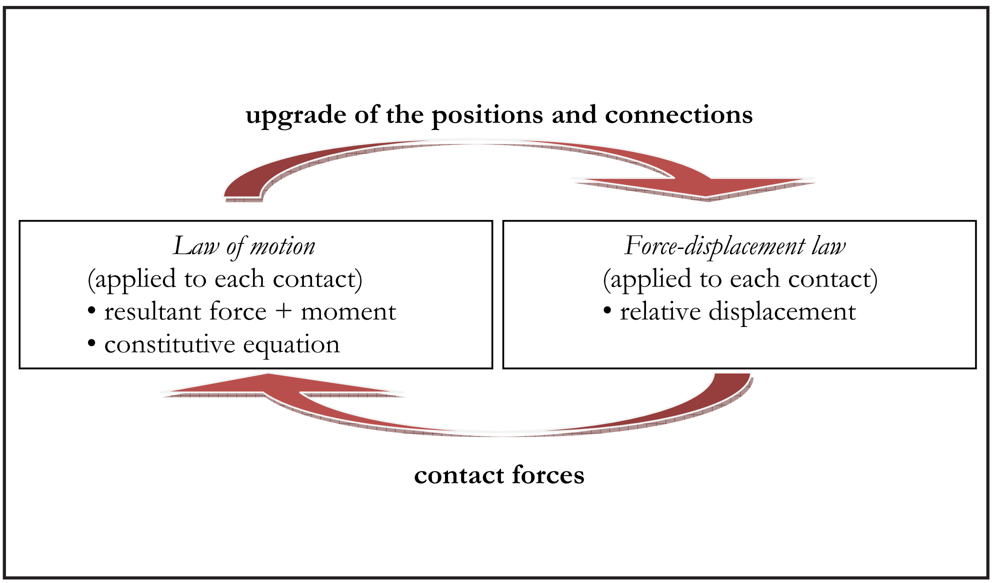

Figure 3. The course of the calculation

of magnitude of red blood cells diameter is not so significant considering the diameter of the blood vessel. We can model the sinker-like shape red blood cells as an particle having approximate diameter $d_{sphere} = 5.56 \cdot 10^{-6}\ m$.

We want to find out the possibilities and limitations of the modelling by the so called *particle transport* method. The modelling of the whole particle phase in the continuum fluid occurs by the assistance of only a few tracking particles. The red blood cells constitute the predominant majority of the cellular elements flowing in the blood plasma, for this reason we have the primary goal modelling only these elements.

On the *Figure 4* – above on the left side – it can be seen the function of the inflow. We approach the physiological pulsating pressure with this function, which is perceptible by this size of artery. Next to it – to the right – the modelled schematic "artery-elbow" is visible. At the third position of the *Figure 4* it can be seen the path of the tracked particles, which zigzagged motion shows fairly the ability of bumping against each other. The colours of particles tracks signify their velocity. Finally on the fourth place of the *Figure 4* we can see the von Mises-stresses acting on the wall by the red blood cells. (Since this was a short time running of the program, the majority of the particles are still before the bend, for this reason the coloured plots are observable mainly at the entrance part of the artery.)

The so called hematocrit (Ht or HCT) or packed cell volume (PCV) or erythrocyte vol-

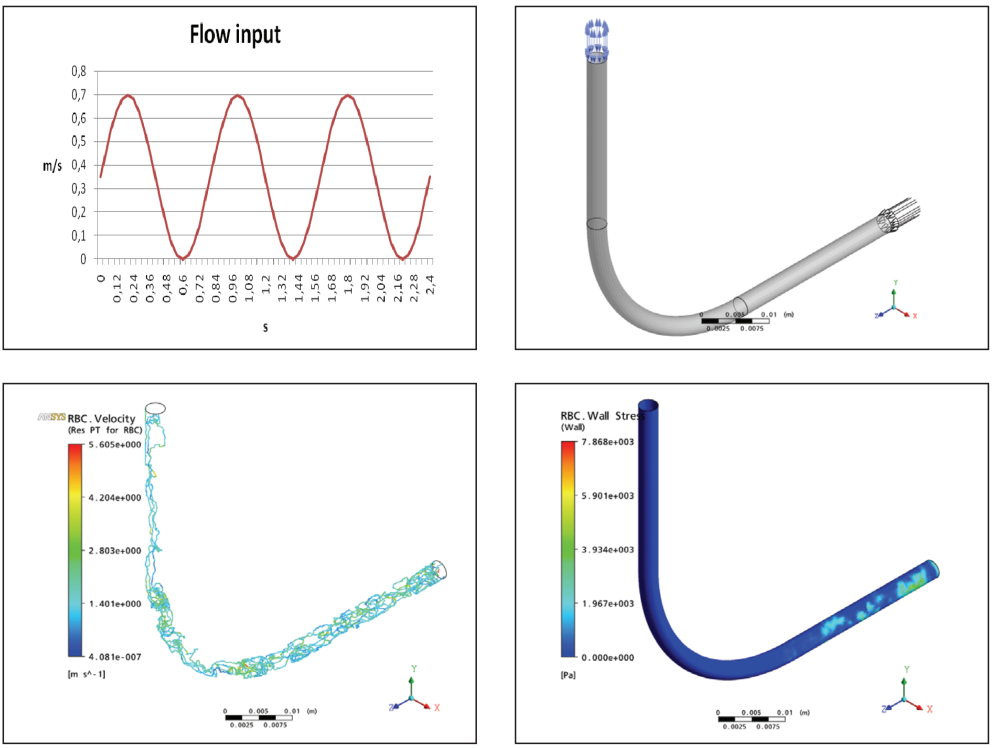

Figure 4. Flow input, schematic model of an artery-elbow, velocity of the tracked particles, wall stresses caused by red blood cells

ume fraction (EVF) is the proportion of blood volume that is occupied by red blood cells. It is normally about 48% for men and 38% for women in the physiological normal range. We had regard to this at the parameter calibration of the following pictures model. I note, that it is necessary to treat cautiously the obtained results, since the pure continuum-base modelling leaves out of consideration the dispersed particle-phase by equation of the continuum phase. Exactly therefore we recommend the application for liquids slightly saturated by particles.

3.2. Arterioles

At the domain of the *arterioles* (small arteries) – which can be considered as the "entrance-door" of the capillary vessels – the shape of the endothelium cells begins to play significant role. The endothelium cells covering the artery-wall are seen in the *Figure 5* below in blue colour, and their nuclei are distinctly visible as bulging in the lumen of the artery. It is observable on the *Figure 5* too, that these cells are in possession of internal stiffening. In the course of the collision of red blood cells to the wall, the endothelium cells give signals by the help of the cellular connecting-structures (modelled by five leglets, piece by piece of the endothelium cells, see also the *Figure 5*) as the results of the forces acting on their faces. These signals determine essentially the answers and reactions of the artery wall. On account of all these we propose the *discrete element method* to model this domain of artery-size. (See other application in *Li et al.*[8] and in *Tipthavonnukul et al.*[12])

On the above mentioned *Figure 5* you can see some results of simulation made by this method. The connected to one another yellow particles represent the "doughnut-shape" of the red blood cells. In the course of the discrete element modelling the red blood cells and the blood plasma are modelled by the help of particles. In so far if as we want to model the continuum phase with fine particles filling closely the entire range of the fluid phase, it will not give correct results, since we will observe the so called "tightness-symptom" of particles. No matter how we reduce the size of the particles modelling the continuum, the countable discrete particles will never substitute the continuum. This is why we advice the modelling the continuum phase only by a few distributed particles (see the small green particles on the *Figure 5*). This gives the possibility can take into account not only the effect of the continuum phase (green particles on the figure below) on the red blood cells (yellow particles on the figure below), but we have the chance to consider the back action, namely the effect of red blood cells on the continuum phase, too.

On the *Figure 6* we can see the forces arising from collision of the red blood cell to the under and to the upper wall. Red colour represents tensile forces and black colour shows the compressive forces. (A small tension is always present in the endothelium cell from the motion of the fluid.)

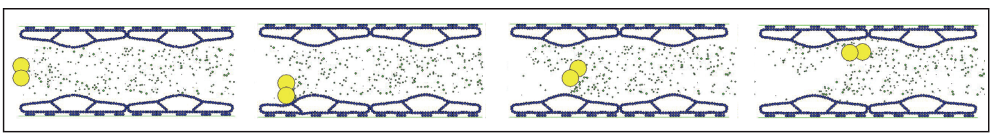

Figure 5. Motion of a red blood cell (yellow particle) in the blood plasma (representing green particles). The walls of the 2 dimensional artery consist of endothelium cells (blue cells with inner stiffening and with 5 leglets)

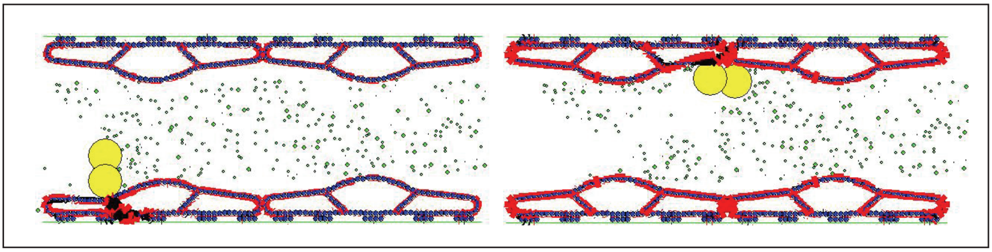

Figure 6. Collision of the red blood cell (yellow particle) to the under and the upper wall. Tensile forces are in red colour and compression in black

3.3. Capillary vessels

In the capillary vessels – smallest blood vessels – the size of the red blood cells can reach (in extreme case it can exceed, too) the diameter of the artery. In the present case it is no longer the collision of the red blood cells to the wall what mainly produce the reaction of the endothelium cells. The red blood cells march through the capillary *one by one,* and the shear forces arising by this motion acting the main role. On account of these we propose to return to the *continuum-based* modelling. We made a simplified mixed model to the investigation the effect of the red blood cells moving in the capillaries. In this model not only the continuum phase takes effect the particle inside it, but the back-action could be model also.

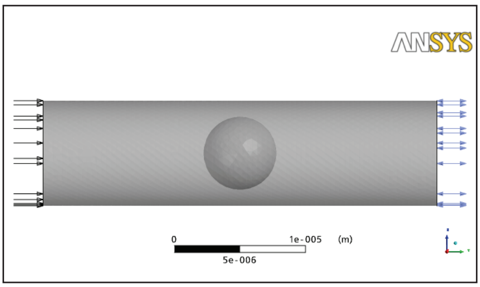

Figure 7. Geometry of a capillary vessel within a schematic red blood cell

4. Discussion

We have the aim to scientific investigate those domains of size of arteries, where the effect of the red blood cells on the wall is significant, and it is impossible to model the whole blood circulating in the blood vessels as continuum medium, thus we have to separate the blood to the plasma and to the cellular elements (mainly the red blood cells) streaming in it. We think different methods are suitable for modelling of different size of arteries. By the middle-large

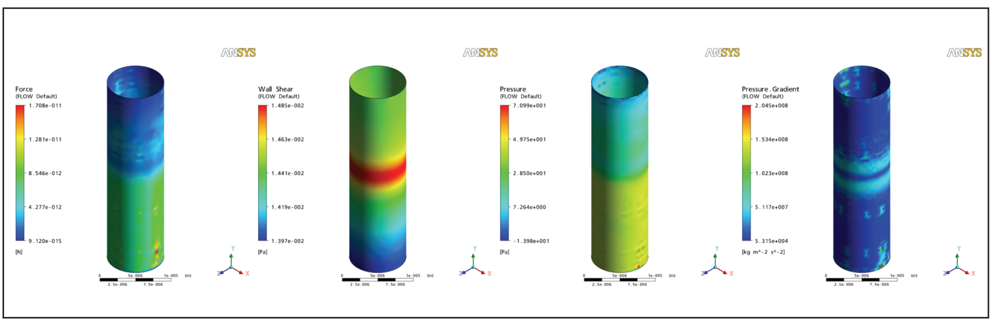

Figure 8. Results on the wall: Force, Wall shear, Pressure, Pressure Gradient

arteries repute convenient the continuum-based modelling, and inside this the so called particle tracking method. As soon as the tube-diameter size decrease and we reach the arterioles, the discrete element method gives the possibility to the modelling, and finally by the capillary vessels according to our suggestion is necessary to return to the continuum-based models.

References

1. ANSYS CFX-Solver Theory Guide. ANSYS CFX Release 11.0., ANSYS Europe, 1996–2006.
2. PFC3D, Particle Flow Codein 3 Dimensions, THEORY AND BACKGROUND, Itasca Inc.
3. *Casey M, Wintergerste W.* Best Practice Guidelines, ERCOFTAC Special Interest Group on Quality and Trust in Industrial CFD, Report, 2000.
4. *Clift R., Grace JR, Weber ME.* Bubbles, Drops and Particles, Academic Press, New York, USA, 1978.
5. *Cundall PA, Strack ODL.* A Discrete Numerical Model for Granular Assemblies, Géotechnique 1979;29:47–65.
6. *Enwald H, Peirano E, Almstedt AE.* Eulerian Two-Phase Flow Theory Applied to Fluidisation, Int. J. Multiphase Flow, Suppl., 1996;22: 21–66.
7. *Ferziger JH, Peric M.* Computational methods for fluid dynamics, Springer, Berlin.
8. *Li L, Holt RM.* Simulation of Flow in Sandstone with Fluid Coupled Particle Model. In: Rock Mechanics in the National Interest (Proceedings of the 38th U.S. Rock Mechanics Symposium, 2001 July; Washington, D.C.), Rotterdam: Balkema, 2001;1:165–172.
9. *Lun CKK, Savage SB, Jeffery DJ, Chepurniy N.* Kinetic Theories for Granular Flow: Inelastic Particles in Couette Flow and Slightly Inelastic Particles in a General Flow Field, J. Fluid Mech., 1984;140:223–256.
10. *Manninen M, Tavassalo V.* On the Mixture Models for Multiphase Flow, VTT Publications, 1996.
11. *Menter F.* CFD Best Practice Guidelines for CFD Code Validation for Reactor Safety Applications, Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis (ECORA), European Commission, 5th EURATOM FRAMEWORK PROGRAMME, 1998–2002.
12. *Tipthavonnukul S, Chan D.* Numerical Simulation of Granular Particles Moving in Fluid Flow. In: Discrete Element Methods: Numerical Modeling of Discontinua (Proceedings of the Third International Conference, 2002 September; Santa Fe), Reston, Virginia; ASCE. 2002;104–106.

Brigitta Krisztina Tóth
Department of Structural Mechanics
Budapest University of Technology and Economics (BME)
H–1111 Budapest, Műegyetem rkp. 3.