Advanced Computational Simulation and Applications of Fibrous Composite Materials

Karel Frydrýšek, Vladimír Kompiš and Zuzana Murčinková

***Abstract*—**This article is focused on: 1. *Advanced computational simulation* of composite materials reinforced by short fibres. It will be shown how the reinforcing elements change stiffness of material and thermal conductivity by changing mechanical and thermal properties of both, matrix and fibres, percentage of reinforcing material and dimensions of reinforcing elements. Special computational models developed in the Slovak Republic using 1D continuous source functions along fibre axis enable to simulate fibres with matrix very effectively. 2. *Application* - New design of external fixators invented in the Czech Republic. These fixators are intended for the treatment of open, unstable and complicated fractures in traumatology and orthopaedics for humans or animals limbs. The new design is based on the development of Ilizarov and other techniques (i.e. FEM, shape and weight optimalization based on composite materials, nanotechnology, low x-ray absorption, antibacterial protection, etc.).

***Keywords*—**computational models, design, external fixators, FEM, short fibres, traumatology, biomechanics

I. Introduction

THE presented paper is focused on computational simulations of short-fibre composite materials in mechanics and applications mainly in biomechanics.

Computational simulations enable to study how properties of both, matrix and reinforcement contribute to improve material properties. Short fibres afford opportunity to obtain new materials with very different behaviour in different directions. Classical numerical methods like FEM, BEM, Fast Multipole BEM, or meshless methods are inefficient in computational simulations of such problems. Some results obtained by the Method of Continuous Source Functions (MCSF) developed by the second author, see [1], for computational simulation of behaviour such composite materials are presented.

Another practical application of composites is focused on the design of external fixators applied in traumatology and orthopaedics. These fixators can be used in the treatment of open and unstable (i.e. complicated) fractures of limbs and pelvis and its acetabulum. A few versions of fixators are presented. Numerical modelling (i.e. Finite Element Method), together with CAD modelling, experiments, material engineering and nanotechnology are presented as a support for developing of a new design of external fixators.

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II. Computational simulation of composite materials reinforced by short fibres

The assumptions of computing in MCSF are following: material of both matrix and fibre is considered to be isotropic and homogeneous; without any matrix-fibre interphase and the dimensions of the matrix are infinite (acceptable simplifications).

For the simplicity of modelling all fields are split into two parts, the homogeneous part corresponding to the homogeneous problem of the matrix without fibres and local part (local fields) containing the influence of interactions of fibres with the matrix.

1D continuous force or heat sources and force or heat dipoles distributed along fibre axes (see Fig. 1) simulate the interaction among all fibres and with the matrix in some control volume (CV) for linear elasticity or thermal problems. Mathematically, dipole is a derivative of the source function in corresponding direction. The inter-domain continuity between fibre and matrix is satisfied in discrete, collocation, points on the fibre boundaries.

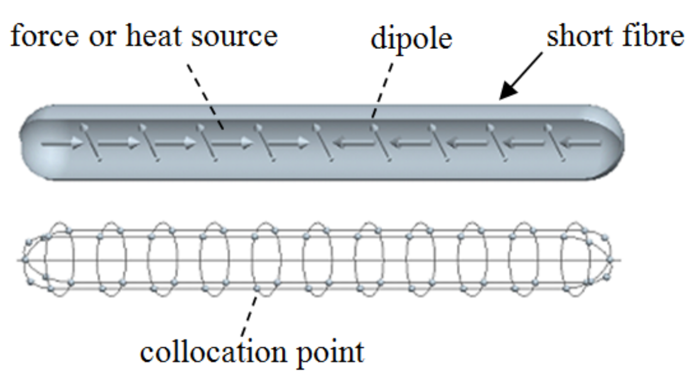

Fig. 1 Distribution of source functions and collocation points

Because of large gradients in the approximated fields, the source functions are presented by 1D quadratic NURBS (Non-Uniform Rational B-Splines) shape functions defined by discrete points along the fibre axis. Largest gradients are in vicinity of fibre ends, where also finest density of points is required in order to receive good accuracy and numerical stability of the model. Usually less than 100 equations are enough to simulate the inter-domain continuity for one fibre. If the model contains large number of fibres, the model would be large, the system of equations full and the computation time very consuming.

When the thermal conductivity of the fibre is much larger than that of the matrix, it is possible to assume in the first step of iteration procedure that the temperature in each fibre is constant. Similarly in mechanical fields, if the fibre stiffness is much larger than the stiffness of the matrix, it is supposed that the fibre is rigid in the fibre axis direction but flexible in bending. Reference temperature and displacement of each fibre is taken of the centre point of corresponding fibre in homogeneous material, i.e. in the matrix material without fibres.

Intensities of the source functions are obtained by solution of the problem. The resulting matrices are full, non-square and are solved in least square (LS) sense. As corresponding pair of fibres interact with each other, all the temperature change and rigid body displacement (RBD) of fibres by this interaction are obtained from energy and/or force equilibrium in each fibre, respectively in iteration steps taking into account finite temperature conductivity or stiffness of fibres.

Detail description of MCSF can be found in [1] and [4]. To solve the problem, the fundamental solution has to exist. Temperature field induced by a unit heat source acting in arbitrary point of infinite domain is the fundamental solution for heat problems and it is given by:

$$T = \frac{1}{4\pi\, r} \tag{1}$$

where r is the distance of the field point t and source point s, where the heat source is acting at.

The field of displacements in an elastic continuum by a unit force acting in direction of the axis x_p is given by Kelvin solution known from Boundary Element Method:

$$U_{pi}^{(F)} = \frac{1}{16\pi G(1-\nu)}\frac{1}{r}\left[(3-4\nu)\delta_{ip} + r_{,i}r_{,p}\right] \tag{2}$$

where i denotes the x_i coordinate of the displacement, G and ν are shear modulus and Poisson’s ratio of the material of the matrix (isotropic material is considered here), r is the distance between the source point s, where the force is acting with a field point t, where the displacement is introduced.

Temperature field induced by a unit heat dipole in x_i direction is:

$$T_{,i} = \frac{1}{4\pi}\left(\frac{1}{r}\right)_{,i} = -\frac{1}{4\pi}\frac{1}{r^2}r_{,i} = -\frac{1}{4\pi}\frac{x_i}{r^3} \tag{3}$$

Heat flow in x_i direction by the unit heat source (1) is given by:

$$q_i = -k\frac{\partial T}{\partial x_i} = -kT_{,i} = k\frac{1}{4\pi}\frac{x_i}{r^3} \tag{4}$$

where k is heat conductivity of the matrix. Usually the heat conductivity (Young's modulus of elasticity) of fibre is several orders higher than that of the matrix.

Similarly the heat flow by the dipole (3) is obtained from the second derivative of (1):

$$T_{,ij} = \frac{1}{4\pi r^3}\left(\frac{3x_i x_j}{r^2} - \delta_{ij}\right) \tag{5}$$

where δ_{ij} is Kronecker delta.

Heat flow through a surface with the normal n is defined as:

$$q_n = q_i n_i \tag{6}$$

Collocation points (see Fig. 1) are located on the interface between fibre and matrix. Then the intensities of the source functions can be computed by satisfying the inter-domain boundary (continuity) conditions in collocation points on the fibre-matrix interface boundaries.

In the present method, four collocation points are used on each cross-section of fibre for satisfying the boundary (continuity) conditions in perpendicular direction of fibre-matrix interface boundary. It should be stressed that the ends of a fibre should be in the form of half spheres or cylinders. It is important to satisfy the boundary conditions (b.c.) in these parts as well. Without considering of these b.c., the source functions located along the fibre axis may lead to incorrect results.

In order to find the unknown intensities of the source functions, we have to solve 1D quasi-singular equation in the form:

$$\int_{\Gamma} K(s,t)\, f(t)\, d\Gamma = g(s) \tag{7}$$

where $K(s,t)$ is kernel function, which is corresponding source function in our case, $f(t)$ is the unknown intensity of the source function, $g(s)$ is the function prescribing the b.c. and Γ is the 1D integration curve along fibres’ axes.

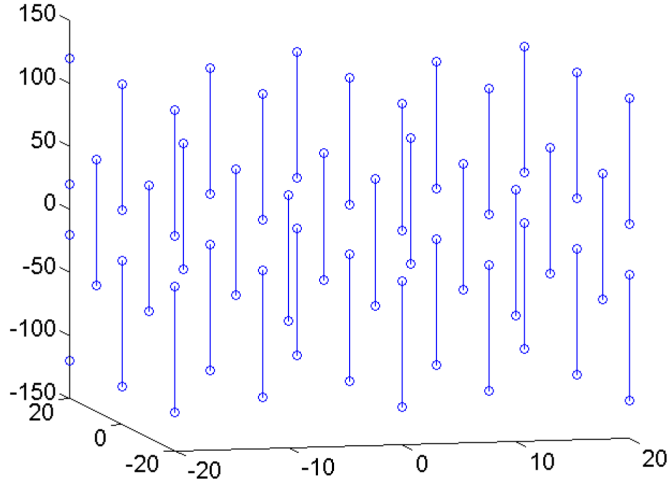

Fig. 2 Patch of fibres

Computational models involve either regularly or random distributed straight fibres in patches. Figure 2 presents in axonometric view of 38 regularly distributed straight fibres. The fibres overlap in the fibre direction. Such model can be used also for homogenization but only for regularly distributed fibres, because the heat and temperature is not homogeneous in the patch. For general case, it is necessary to define the b.c. along the control volume and the collocation points must be so, that they will satisfy the b.c. in good accuracy because of large gradients in corresponding fields there.

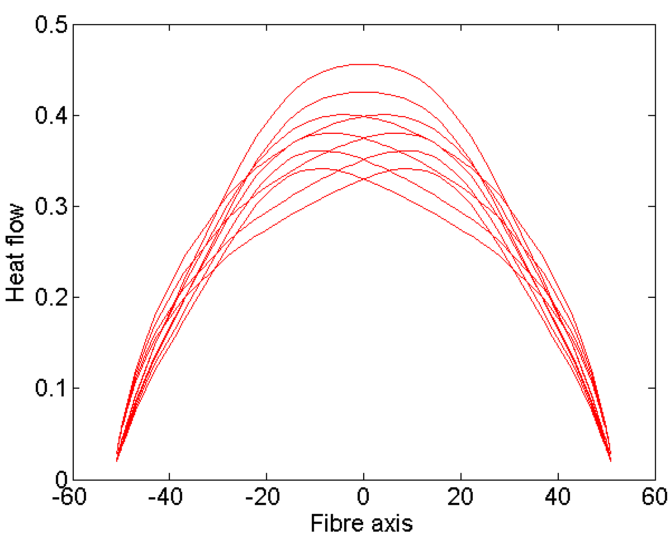

Fig. 3 Heat flow

Heat flow and temperature gradient to that in the middle of corresponding fibre are presented for regularly distributed patch fibres in 5 × 5 × 3 layers of fibres as shown in the Fig. 2. Heat conductivity of fibres was 1000 times larger than that of the matrix. The aspect ratio of fibres was 1:50. Figure 3 presents the heat flow and Fig. 4 the temperature gradient in the 6th, convergent iteration step.

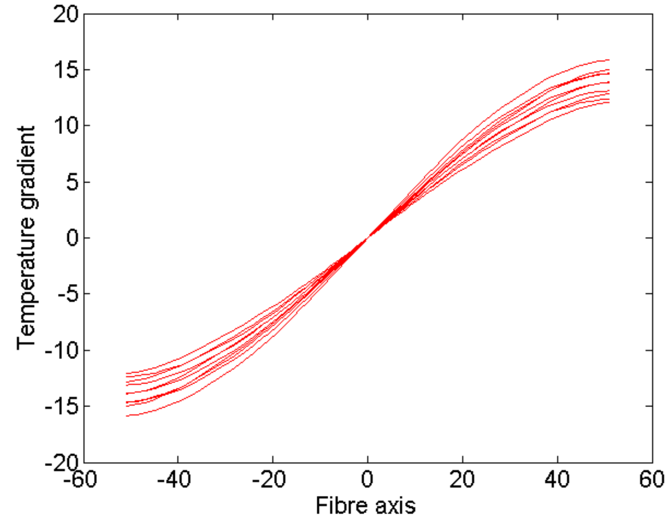

Fig. 4 Temperature gradient

The temperature in the upper layer of fibres, which is +70 in the middle point of fibres decreases in the composite from -22.7 in the corner of the patch up to -30.7 in the middle fibre. All quantities are chosen dimensionless because of linear problem.

In case of linear elasticity problems, the distribution of heat flow and temperature is analogical to stress in fibre axis and displacements.

Mechanical properties of composite material reinforced by short fibres are even more complicated to simulate and generally require three times more equations to solve the problem [1] and [4] as the basic source functions are forces vectors (in the heat flow the heat source is scalar) and its derivatives are tensor functions. However, the behaviour of computational model is very similar to the presented problems.

Application of fibrous composites are presented in the following text.

III. External fixators for treatment of complicated fractures (medical point of view)

Changes in lifestyle, emergency situations and accidents in the world, increased age and development of endoprosthetics are connected with increased occurrence of any kind of limb's fractures in recent years, see [9] and Fig. 5. Hence, good treatment of fractures is a challenge for the surgeons in the branch of traumatology and orthopaedics, see Fig. 6.

Fig. 5: Example of complicated fracture

Fig. 6 X-ray of periprostheticRorabeck type II fracture – lateral view (source internet [12]) before application of external fixator

There is still continuing debate which treatment option is optimal for these patients. There is no consensus on the technique to be used but logically it must be minimally invasive to decrease mortality and morbidity, see [5] and [14] – [16]. Stable osteosynthesis obtained by minimal invasive techniques assures more rapid fracture union.

External fixators can be applied in traumatology, surgery and orthopaedics for treatments such as open and unstable (complicated) fractures, limb lengthening, deformity correction, consequences of poliomyelitis, foot deformities, hip reconstructions, etc. Hence, external fixators can be used for treatment of humans and animals, for example see Fig. 5, 6, 7 and 8.

Fig. 7: Examples of complicated fracture and application of external fixators (after operation)

Fig. 8 Examples of complicated fracture and application of external fixators (three months after the operation - see [5])

IV. External fixators for treatment of complicated fractures (engineering point of view)

Scientific and technical developments, together with medical care and medical practice, bring new demands for designs of external fixators. These demands should be solved by:

- Applications of new smart materials (outer parts of fixators must be x-ray invisible, antibacterial protection based on metal-based nanoparticles on the surface, material tests; proper mechanical properties), for example see Fig. 9. This part is performed according to the theory presented in the chapter II.
- New design (weight optimalization, patient's comfort, easy to assembly).
- Measuring of the real loadings (experiments).
- Numerical modelling and experiments (FEM, SBRA Method, strain gauges, see [10], [11] and [13]).

These points which are mutually connected are discussed in references [2] and [3].

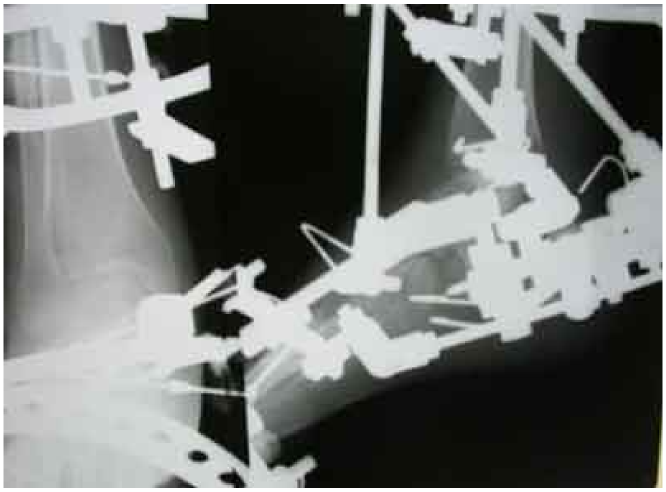

Fig. 9 Problems with high X-ray absorption (It is difficult to see broken limbs because there is so much metal parts. Hence applications of non-metalic composites are suitable)

Some solved examples (based on the theory of composites presented in the chapter II of this article) are presented in Fig. 10, 11, 12 and 13 (fixator for treatment of pelvis and acetabular fractures, see references [2], [3], [5] and [8]) and in Fig. 7, 14 and 15 (fixator for treatment of limb fractures, see reference [2], [7] and [8]).

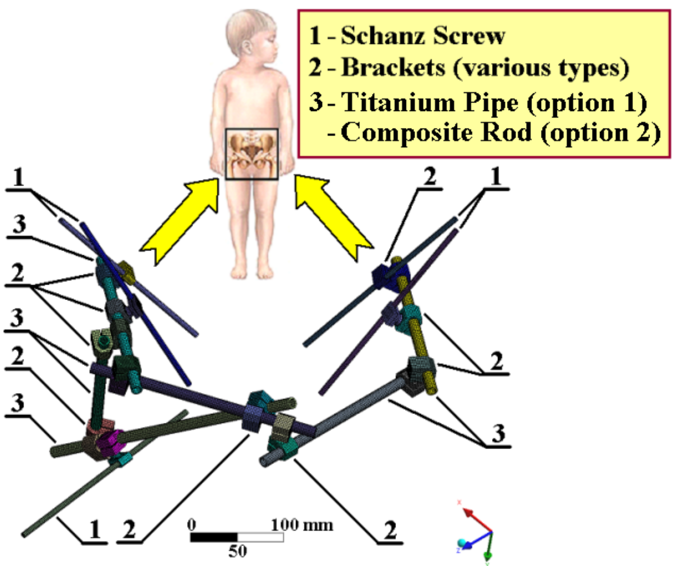

Fig. 10 Application of external fixator for treatment of pelvis and its acetabulum

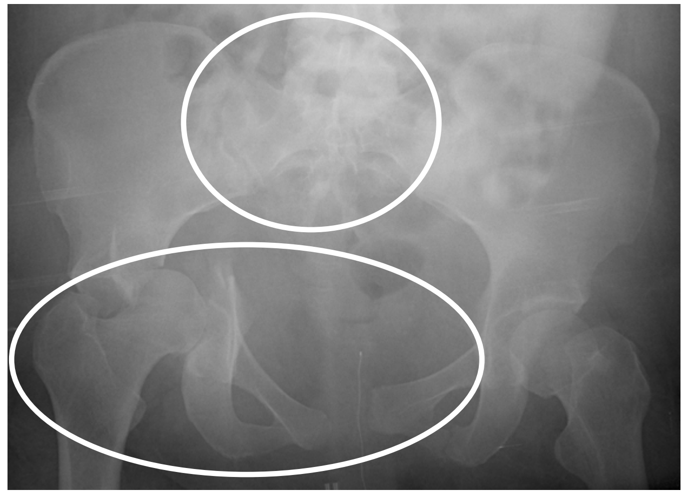

Fig. 11 Anteroposterior radiograph - fracture of pelvis and its acetabulum

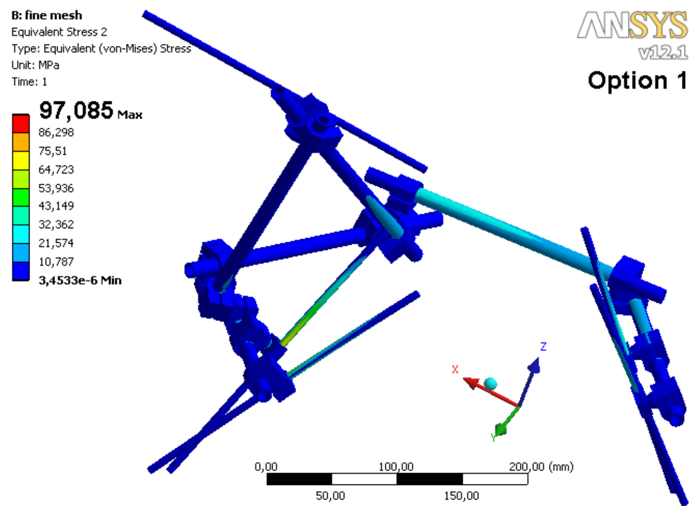

Fig. 12 "Option 1" - FE modelling of external fixator for pelvis and acetabulum (equivalent von Mises stresses /MPa/ for tensile loading 100 N)

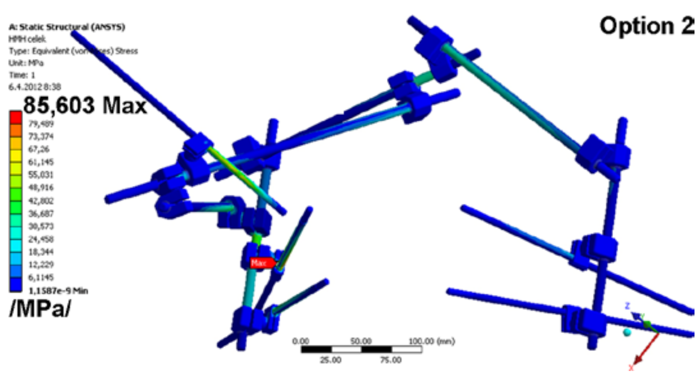

Fig. 13 "Option 2" - FE modelling of external fixator for pelvis and acetabulum (equivalent von Mises stresses /MPa/ for tensile loading 100 N)

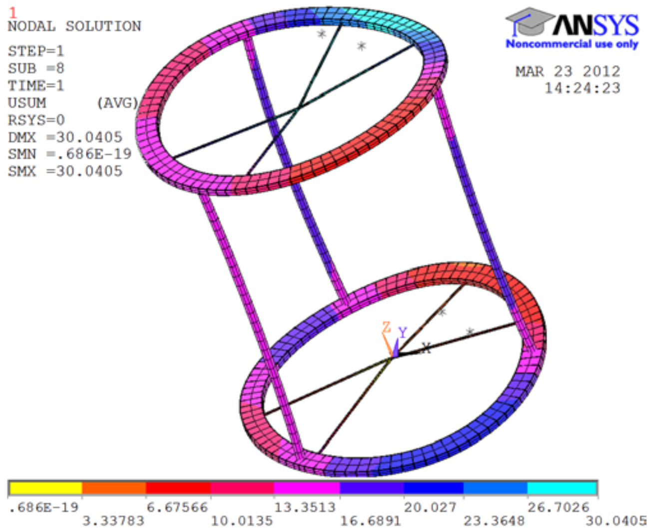

Fig. 14 FE modelling of external fixator - Ilizarov apparatus (overloading, total displacements in the structure)

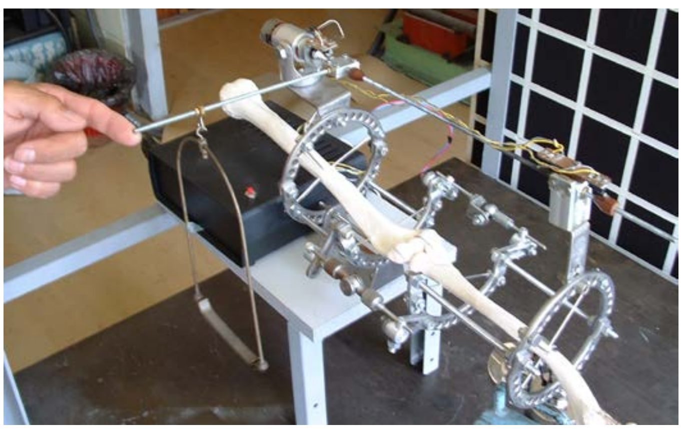
Fig. 15 Experimental measurements - external fixator (Ilizarov apparatus)

V. Conclusions

This article presents international cooperation between Czech and Slovak scientists.

Applied Mechanics - point of view: Only a brief description with references for the computational models and numerical results are presented in this paper. They document that present models are able to evaluate contribution of reinforcing fibres and to obtain all parameters necessary for homogenized material properties. Theory and applications in biomechanics are presented.

Medical point of view: Any kind of fractures make an important therapeutical problem for their individual and specific character. Their diversity from other types of fractures consists in the fact that they are fractures of bone with the implants of total arthroplasty and therefore the method of treatment must often be different from therapeutical as in case of other types of fractures. Among the general risk factors we can include osteoporosis, rheumatoid arthritis, treatment with corticosteroids and naturally other diseases which may affect healing processes of patients. Emergence of these fractures can be additionally caused by technical problems e.g. anterior notching of the femoral cortex of total knee arthroplasty, damage of proximal femur at application of the total hip arthroplasty and other. Among other possible complications there can be postoperative treatment and patient's personality – early weight bearing. The complications may occur at conservative treatment as well as after the surgical treatment and they are affected by right evaluation of fracture and right choice of the treatment method and also by the patient preparation and leading of the treatment including rehabilitation and weight bearing.

Engineering point of view: Report about the new ways to design of external fixator, based on the results of previous research, was presented. Hence, the new designs and materials of fixators will satisfy the ambitious demands of modern traumatology, surgery and economics. The results of experiments fit quite well with numerical modelling. According to the results, the improvements in the designing of external fixators for treatment of limb fractures are evident. VŠB - Technical University of Ostrava together with University Hospital of Ostrava and Trauma Hospital of Brno are now in the middle of a process creating new designs for external fixators. Hence, they are in cooperation with the Czech producers MEDIN a.s. (Nové Město na Moravě, Czech Republic). Therefore, all results could not be published in this paper due to confidentiality reasons.

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