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CONVECTION OF INTERNAL VARIABLE METHODOLOGY IN COMPUTATIONAL FLUID DYNAMICS SOLUTIONS FOR THIXOFORMING MODELLING

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Abstract

Thixoforming is a relatively new forming method, with high deformation of semi-solid material. From numerical point of view, such materials are difficult to simulate because of gathering some features of solid materials and some of fluids. Materials properties are history dependent like in solids, while deformations could be extremely high, like in fluids. A review of existing numerical solutions is presented in this paper, especially based on Computational Fluid Dynamics (CFD) methods with Eulerian and Arbitrary Lagrangian Eulerian (ALE) motion description. Need of new methodology for time-dependent materials behaviour simulations of thixoforming processes are pointed out. Convection of internal variable in Eulerian based simulations is introduced. Implementation as a user supplied procedure into a commercial Finite Element application ADINA-F® is shown. Results of simple thixotropic flow with some shear changes are presented.

Key words: Computational Fluid Dynamic (CFD), internal variable, thixoforming, Eulerian mesh

1. INTRODUCTION

1.1. Thixoforming processes

Thixoforming is a relatively new forming method. Material in semi-solid state with proper microstructure is formed with high speed and extremely high deformation. It is often compared with classical methods, like casting and forging. The main disadvantage of thixoforming is a required very narrow temperature range (due to semi-solid state), as well as considerable tools and dies needs. Also raw material costs are high. On the other hand, parameters of thixoformed products are better than in casting. In comparison to forging, more complicated shapes could be achieved in one step, with almost unlimited deformation. Lower energy consumption, as well as higher production speed is assured.

Thixoforming becomes interesting technology, with application in electronics, automotive and aerospace industry. Nevertheless, complicated phenomena during forming, caused by microstructural behaviour of material, constraints precision in process development, making numerical modelling necessary. Many works, provided from 70th of twentieth century demonstrate that thixoformed alloys behave as complex fluids, with some elasticity, as well as strong, nonlinear shear rate and temperature dependency. Moreover, constant shear rate microstructure evolution had been proved (Joly & Mehrabian, 1974, Kumar et al., 1994).

1.2. State of the art in thixoforming modelling

Semi-solid forming processes, like thixoforming, rheocasting, some continuous casting variants and

112 – 118

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some others, merges phenomena from fluids and solids behaviour. High deformation degree and time dependency of the material is a cause that neither structural, nor fluids computational methods are suitable. Structural solutions are commonly based on Lagrangian motion description and remeshing is required when mesh becomes too distorted. Remeshing dramatically increases time consumption and decreases solution accuracy. In the other hand, Computational Fluid Dynamics (CFD) methods, based on Eulerian or ALE motion descriptions, are not well conformable to history dependent materials properties. Nevertheless, CFD solutions seem to be more flexible and more promising than based on Lagrangian description.

Semi-solid materials are usually described as viscoplastic or elastoviscoplastic (Bellet & Moto Mpong, 2001; Kopp et al., 2003), as well as shear-thinning/shear thickening fluids or Hershel-Bulkley fluid (with yield stress). Compatibility of CFD methods with viscous, non-Newtonian fluids and structural solutions with viscoplastic material was proved by Zienkiewicz & Cormeau (1974). However, in solids computations, dynamic effects are usually omitted. In forming with high speed, like in thixoforming, dynamic effects are significant, what had been shown by Sołek et al. (2005). The main limitations of CFD methods application in metal forming modelling are caused by Eulerian motion description, which is a fundamental for CFD. At first, domain geometry during simulation has to be preserved. Second, with mesh nodes not tied to material points, history dependency could not be complied. The first problem could be resolved by employing an Arbitrary Lagrangian Eulerian motion description. ALE formulation application in FEM could be found in numerous publications (Donea & Huerta, 2003 and many others). The second problem is still not well elaborated. There are two main issues. At first, material properties could be bounded with material state history, like for example strain, and second, they could change in time with other conditions constant, like in thixotropy. In this second case, which is more interesting in thixoforming modelling, internal variable application had been applied in solid mechanics. Unfortunately, it is not trivial to transfer internal variable method into CFD techniques.

a) Numerical models of thixotropy and thixoforming

At first, it should be noticed, that “thixoforming” and “thixotropy” does not have the same meaning. Thixotropy has wider meaning, because thixotropic behaviour could be found in paints, inks, detergents, clay suspensions, oils, food, pharmaceuticals and many others. Metal alloys in semi-solid state are only a small part of thixotropic fluids. On the other hand, during thixoforming, thixotropic effects are not apparent. There are many works, which adapts numerical models neglecting time-dependent effects and still obtaining correct results (Messmer et al., 1999; Kim & Kang, 2000; Huilgol & You, 2005). However, in many cases concerning thixotropic effects could be helpful, especially in long lasting processes, when time dependent phenomena are noticeable.

b) Numerical models of thixotropy and thixoforming with internal variable

Thixotropy models could be divided into three categories – phenomenological, direct microstructural and indirect microstructural (Mujumdar et al., 2002). Historically, first works refer direct microstructural models (Goodeve, 1939), where a number of bonds or links between the particles is a measure of microstructure. In indirect microstructural models, a scalar value of structural parameter, first introduced by Moore (1959), is used as a measure. The third approach is based on phenomenological description of thixotropic behaviour with some analytical functions. It was introduced by Slibar & Paslay (1964), but nowadays it is rather rarely employed.

c) Internal variable (***IV***) in CFD

In Eulerian/ALE description material point is not tied with mesh node. ***IV*** values could not be stored in mesh nodes, like in Lagrangian meshes. Positions of material points could be tracked during following steps, but this method constraints approximation between “material nodes” and “mesh nodes”. Also changing domains borders is a big obstacle. A better solution could be a “convection” of ***IV***. In this case, internal variable is no longer linked with material point, but its values are computed in Eulerian mesh nodes. Employing convection of ***IV*** allows evolution in time introducing. While convection equations are employed, a source term seems to be a natural mechanism for internal variable time dependency. Convection solutions in CFD methods are widely used and deeply described in many publications (Zienkiewicz & Taylor, 2000; Donea & Huerta, 2003). In most cases, iterative solution is employed, with velocity/pressure field computed in one step and convection in second. This method allows to build complicated models, concerning systems of multiply fields (velocity, pressure, mass transfer and so on), being solved in one model.

d) Internal variable in CFD solutions for thixoforming

Nowadays, solutions of thixoforming processes based on CFD and IV methodologies for unrestricted geometries are not numerous. Burgos et al. (2001) presented Finite Element computations with indirect structural model for Sn-15Pb alloy, but model geometry and boundary conditions were simplified and partially analytically transformed, what made IV convection model non-applicable in unrestricted domains geometries. Roussel et al. (2004) presented solution of rotational viscometer, but governing equation were analytically transformed. Moreover, it was based on Finite Difference Method, what makes this solution hard to apply in more complicated problems.

The most advanced works are presented by Modigell & coworkers (eg. Modigell & Koke, 1999, 2001, Koke & Modigell, 2001). Rheological model of Sn-15%Pb alloy, based on indirect microstructural method where implemented into CFD software Flow3D. Some comparisons between Newtonian and thixotropic fluids where presented, as well as comparison of numerical model computations with experimental results.

Mentioned papers shows, that rheological models of thixoforming based on CFD and indirect microstructural assumptions are very useful in most of thixoforming cases.

In this paper, implementation of numerical model of thixotropy, based on convection of internal variable, with Eulerian motion description is presented. ADINA-F commercial software has been used as a computational environment. Solution in based on Finite Element Method. There are no limitations of domain geometry and time stepping in this solution.

1.3. Numerical model of thixotropy

There are many models of thixotropic behaviour in literature. Wide review could be founded in publications of Mujumdar et al. (2002) and Barnes (1997). In this work an indirect microstructural model has been chosen:

$$\frac{d\lambda}{dt} = g\left(\dot{\gamma},\lambda\right) = a\left(1-\lambda\right)^{b} - c\lambda\dot{\gamma}^{d}, \qquad (1)$$

where a, b, c and d - constants, λ - structural parameter and $\dot{\gamma}$ - shear rate. Relationship between viscosity and structural parameter is based on Baravian et al. (1996) proposal:

$$\eta\left(\sigma,t\right) = \eta\left(\lambda\right) = \frac{\eta_{\infty}}{\left(1-K\lambda^{2}\right)}, \qquad (2)$$

$$K = 1-\left(\frac{\eta_{\infty}}{\eta_{0}}\right)^{1/2}, \qquad (3)$$

where η_0 and η_∞ are the usual limiting values of viscosity at very low and very high shear rate. Parameters of above equations are to be selected for particular material. An equilibrium value of structural parameter λ is a function of shear rate $\dot{\gamma}$. For those values, time derivative in equation (1) is equal to 0, and solution is stationary. When shear rate changes, this derivative becomes nonzero, pushing structural parameter to its new equilibrium value.

a) Implementation in ADINA-F software

Equations (1)-(3) has been implemented as a user supplied procedures of ADINA-F commercial application. ADINA-F software supports iterative solution of coupled model with Navier-Stokes equation system for velocity/pressure fields and convection/diffusion equation for mass transfer. Internal variable has been introduced as a "virtual species" into convection/diffusion equation. Due to numerical stability, diffusion term of equation is not equal to zero, but diffusion coefficient is very small (artificial diffusion). Structural parameter time derivative is transformed into source term:

$$\Phi = \frac{d\lambda}{dt} Sf, \qquad (4)$$

where S is finite element surface/volume in 2D/3D space, respectively and f is a constant. In ADINA-F user supplied procedures, some limitation occurs. In this case, the most significant is a necessity of viscosity computing in mesh nodes, while source terms are computed for elements. Moreover, in user supplied procedures, shear rate values are available only in mesh nodes. That concerns using averaged shear rate values over each element for source computation. Viscosities are computed for each mesh node with structural parameter value computed by ADINA-F solver with convection/diffusion equation system.

b) The model

The case of 2D, axi-symmetric flow in narrowing pipe was chosen (Fig. 1). No-slip boundary condition on outer surface of flow was assumed. Temperature effects were neglected. Flow velocity in axis of symmetry was chosen as a load. Geometry of the model has been simplified due to simplify validation of rheology model and its implementation.

Numerical simulation covers a part of real process, starting from stationary situation with non-zero shear stress, so starting IV value is not equal to zero. Because its distribution could not be found analytically, a few initial steps of simulations does not describe real phenomena, but are used for determination of stationary IV distribution. In initial step, structural parameter value in whole domain was equal to zero. Accordingly to equation (1), it was non-equilibrium state and first steps of simulation had no physical meaning. After those "initial" steps, equilibrium values of structural parameters and shear rates were achieved. After that, some shear jumps and shear drops had been introduced with time intervals necessary for equilibrium state attainment.

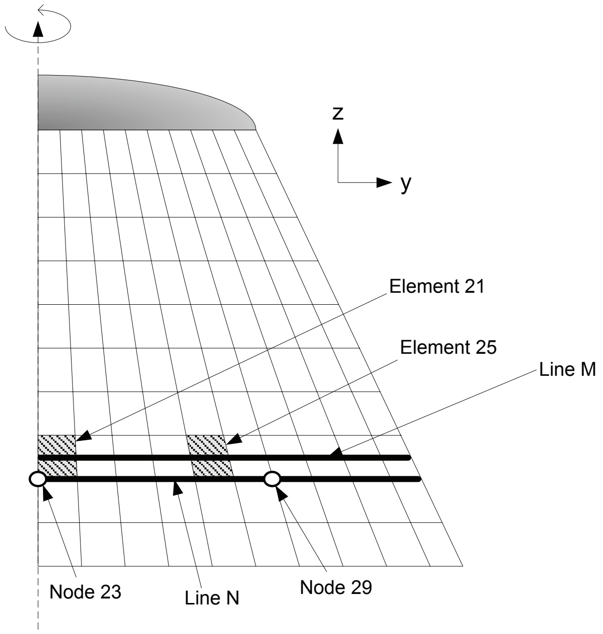


Fig. 1. *Model geometry.*

2. RESULTS

The most significant variables for recording thixotropic behaviour are effective viscosity and shear stress. Also velocities and internal variable values are interesting. Variation of these parameters in time is presented in figure 2. Due to postprocessor

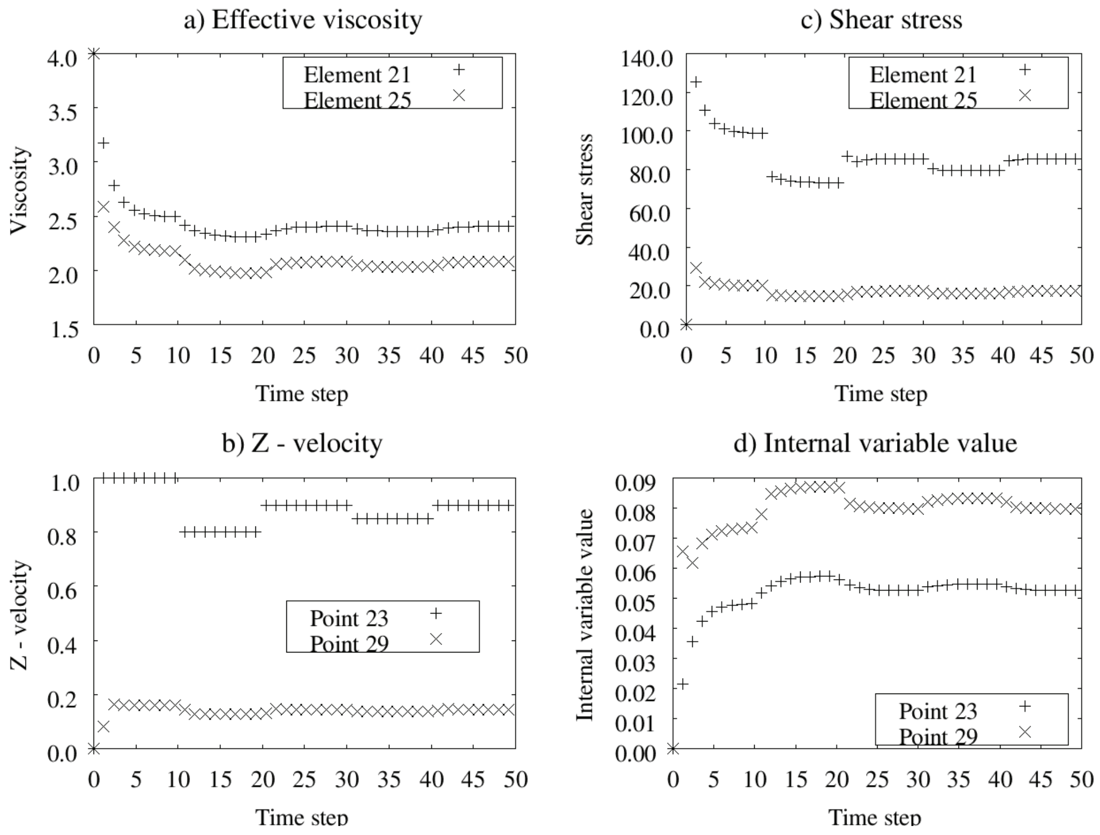
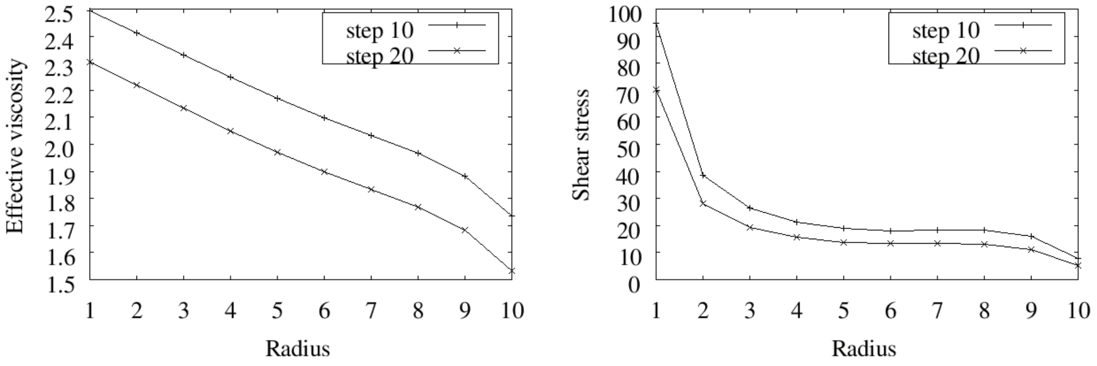


Fig. 2. *Variables variation in time.*

capabilities, velocities and internal variable values have been recorded in nodes (no. 23 and 29) while viscosities and shear stresses has been recorded in elements (no. 21 and 25). Variables variations as a function of radius are shown in figure 3. Time steps 10 (with higher shear rate) and 20 (with lower shear rate, both after IV distribution stabilization) have been chosen for presentation. Velocities and internal variable values had been recorded on nodes' line N, when viscosities and shear stresses on elements' line E. Distribution of the most important variables are also presented in figure 4.

a) Effective viscosity

c) Shear stress



b) Z - velocity

d) Internal variable value

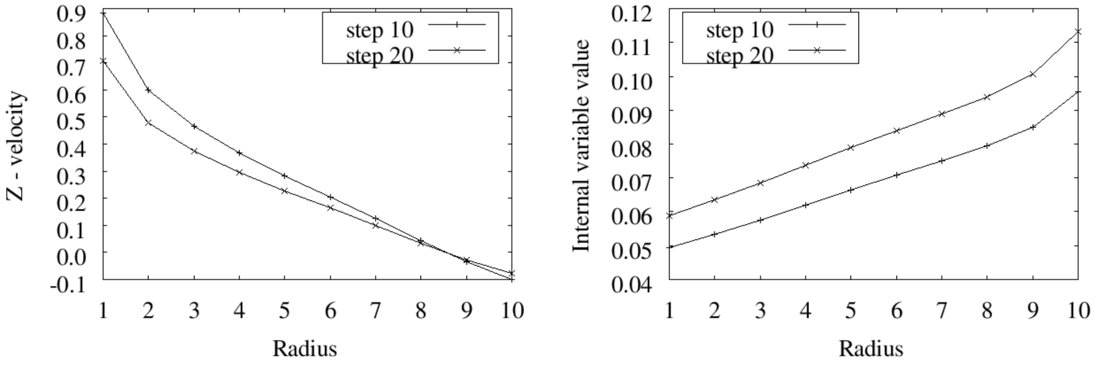


Fig. 3. *Variables variations in radius*

3. DISCUSSION

Thixotropic effects could be observed as a reaction for shear rate jumps and drops, which could be noticed in Fig. 2. Direct consequence of shear rate changes is an evolution of internal variable value (Fig. 2d). This value describes internal structure of material, which influences viscosities and shear stresses in fluid (Fig. 2a,b). Equilibrium distributions of velocity, shear rate and internal variable (structural parameter) are also shown in figure 4. Internal variable, viscosities and shear stresses values behaviour are qualitatively agreeable with results presented by Koke & Modigell (2003), Burgos et al. (2001) and Martin et al. (1994)

4. CONCLUSIONS

Achieved results agree with results of theoretical and practical works presented in literature. Indirect microstructural model of thixotropy has been successfully implemented into the commercial ADINA-F software. It is possible now to perform more complicated simulations, including thermal effects and dies interactions, based on ADINA Fluid Structures Interactions and Thermal Mechanical Coupling modules.

In the future works, more realistic processes will be introduced, including rheometrical tests, as well as semi-industry tests. Rheological model parameters for particular thixoformed alloys will be also identified.

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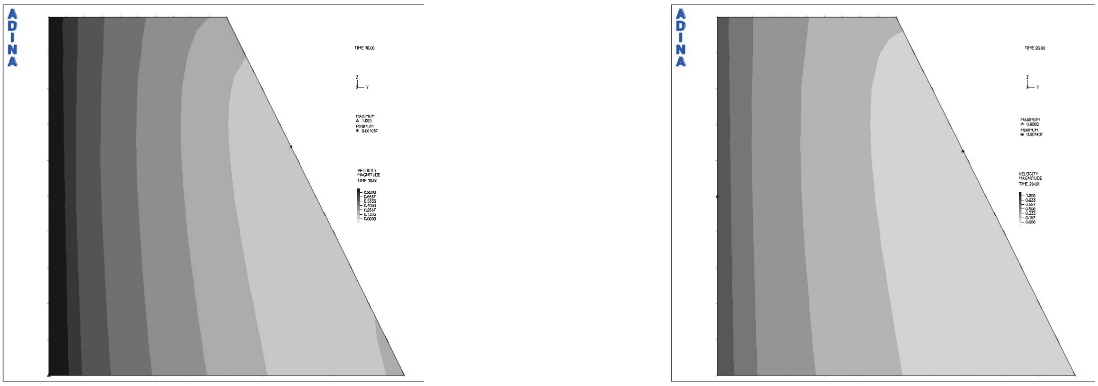
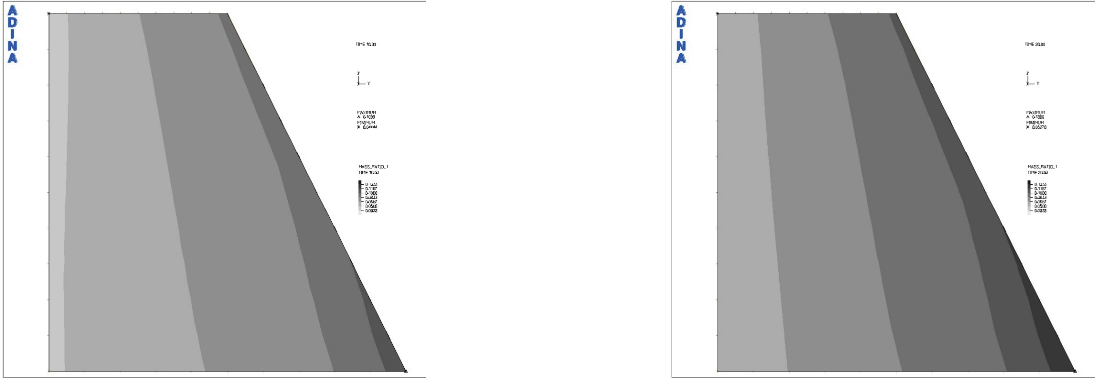
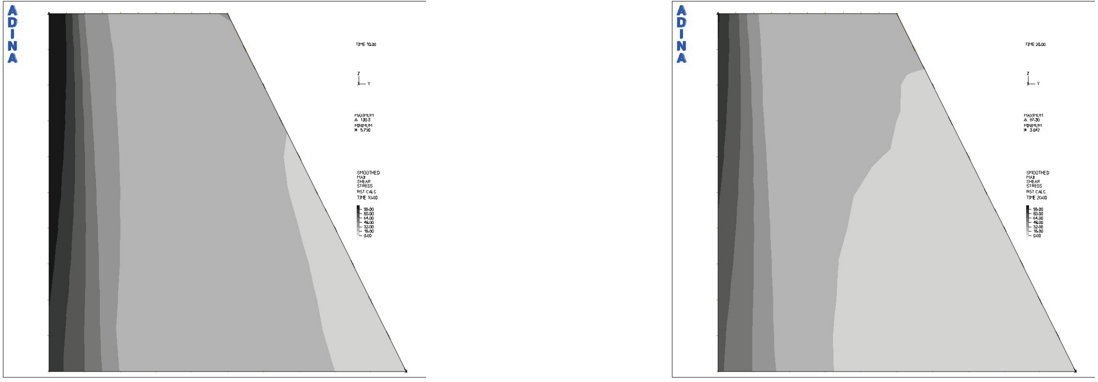


Velocity magnitude (step 10) Velocity magnitude (step 20)



Structural parameter (step 10) Structural parameter (step 20)



Maximal shear stress (step 10) Maximal shear stress (step 20)

Fig. 4. *Main variables distribution in 10th and 20th time step.*

REFERENCES

Baravian, C., Quemada, D., Parker A., 1996, Modelling thixotropy using a novel structural kinetics approach: basis and application to a solution of iota carrageenan, *J. Texture Stud*. 27, 371–390.

Barnes, H., 1997, Thixotropy – a review, *J. non-Newton. Fluid Mech*., 70, 1–33.

Bellet, M., Moto Mpong, S., 2001, Determination of the constitutive equation parameters of a thixotropic Al alloy and FEM modelling of the thixoforming process, in: *Proc. NUMIFORM 2001*, ed. Mori, Lisse, 1087-1092.

Donea, J., Huerta, A., 2003, *Finite Element Methods for Flow Problems*, John Wiley & Sons Ltd., Chichester.

Goodeve, C. F., 1939, A general theory of thixotropy and viscosity, *Trans. Faraday Soc*., 35, 342-358.

Huilgol, R.R., You, Z., 2005, Application of the augmented Lagrangian method to steady pipe flows of Bingham, Casson and Herschel–Bulkley fluids. *J. non-Newton. Fluid Mech*., 128(2-3), 126–143.

Joly, P. A., Mehrabian, R., 1976, The rheology of partially solid alloy. *J. Mater. Sci*., 11, 1393-1418.

Kapranos, P., Liu, T.Y., Atkinson, H.V., Kirkwood, D.H., 2001, Investigation into the rapid compression of semi-solid alloy slugs, *J. Mat. Proc. Technol*., 111, 31–36.

Kim, N. S., Kang, C.G., 2000. An investigation of flow characteristics considering the effect of viscosity variation in the thixoforming process. *J. Mat. Proc. Technol*., 103, 237–246.

Koke, J., Modigell, M., 2003, Flow behaviour of semi-solid metal alloys. *J. non-Newton. Fluid Mech*., 112, 141-160.

Kopp, R., Choi, J., Neudenberger, D., 2003. Simple compression test and simulation of an Sn15% Pb alloy in the semi-solid state, *J. Mat. Proc. Technol*., 135, 317–323.

Kumar, P., Martin, C. L., Brown, S., 1994, Constitutive modelling and characterization of the flow behaviour of semi-solid metal alloy slurries – I. The flow response, *Acta Metall. Mater*., 42, 3595-3602.

Martin, C. L., Kumar, P., Brown, S., 1994, Constitutive modelling and characterization of the flow behaviour of semi-solid metal alloy slurries – II. Structural evolution under shear deformation, *Acta Metall. Mater.*, 42, 3603-3614.

Messmer, G., *Simulation of a Thixoforging Process of Aluminium Alloys with Flow-3D*. Internet, http://www.thixoschmieden.de/misc/Veroeffentlichungpdf/Mrglish.pdf.

Modigell, M., Koke, J., 1999, Time-Dependent Rheological Properties of Semi-Solid Metal Alloys, *Mechanics of Time-Dependent Materials*, 3, 15-30.

Modigell, M, Koke, J., 2001, Rheological modelling on semi-solid metal alloys and simulation of thixocasting processes. *J. Mat. Proc. Technol.*, 111, 53-58.

Moore, F., 1959, The rheology of ceramic sleeps and bodies, *Trans. Br. Ceramic Soc.*, 58, 470-494.

Mujumdar, A., Beris, A. N., Metzner, A. B., 2002, Transient phenomena in thixotropic systems, *J. non-Newton. Fluid Mech.*, 102, 157-178.

Roussel, N., Le Roy, R., Coussot, P., 2004, Thixotropy modelling at local and macroscopic scales, *J. non-Newton. Fluid Mech.*, 117, 85-95.

Slibar, A., Paslay, P. R., 1964, On the technical description of the flow of thixotropic materials, Proceeding of International Symposium on Second Order Effects in Elasticity, *Plasticity and Fluid Dynamics*, 1, 314-330.

Sołek, K., Stuczyński, T., Białobrzeski, A., Kuziak, R., Mitura, Z., 2005, Modelling thixocasting with precise accounting of moving front of material, *Mater. Sci. Technol.*, 21, 551–558.

Zienkiewicz, O. C., Cormeau, I. C. 1974., Visco-plasticity - plasticity and creep in elastic solids - a unifed numerical solution approach, *Int. J. Numer. Methods Eng*, 8, 821-845.

Zienkiewicz, O. C., Taylor, R., L., 2000, *The Finite Element Method*, Butterworth-Heinemann, Oxford.

METODA KONWEKCJI ZMIENNEJ WEWNĘTRZNEJ W ROZWIĄZANIU Z ZAKRESU KOMPUTEROWEJ MECHANIKI PŁYNÓW (CFD) DLA TIKSOFORMINGU

Streszczenie

Tiksoforming jest stosunkowo nową metodą formowania. Polega ona na nadawaniu znacznego stopnia odkształcenia materiałowi w stanie stało-ciekłym. Z numerycznego punktu widzenia, procesy te są trudne do modelowania, co jest efektem występowania zjawisk charakterystycznych zarówno dla cieczy, jak i ciał stałych. Własności materiału są zależne od czasu, podobnie jak w materiałach stałych, podczas gdy odkształcenie może być bardzo duże, podobnie jak w cieczach. W artykule zaprezentowano przegląd obecnie istniejących rozwiązań numerycznych, opartych głównie na metodach dynamiki płynów, z zastosowaniem opisu kinetyki wg metody Eulera lub *Arbitrary Lagrangian Eulerian (ALE)*. Wykazana została potrzeba opracowania nowej metody symulacyjnej dla zależnych od czasu materiałów poddawanych formowaniu tiksotropowemu. Opisana została metoda konwekcji zmiennej wewnętrznej dla eulerowskiego opisu kinetyki. Przedstawiona została implementacja metody jako procedur użytkownika komercyjnego pakietu ADINA-F. Zaprezentowano przykładowe wyniki dla prostych przepływów tiksotropowych.

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