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ACCONT COEFFICIENTS WIT H HOMOGENIZATION METHOD FOR COMPOSITE MATERIALS WITH SHORT FIBERS

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1.INTRODUCTION

In almost all problems of much importance, which appear in the research of some technical phenomenons governed by elliptical equations with variable coefficients.

$$Au \equiv \sum_{|a|,|ß|=1}(-1)^{|a|}D^{a}\left(a_{aß}(x)D^{ß}u\right)=f, \quad x\in V\subset R^{n} \tag{1}$$

on put the homogenization problem of equation: Determine the constant coefficients $\bar{a}_{ab}\in R$ from variable coefficients $\bar{a}_{aß}(x)$ such that (1) to the transform into an equation with constant coefficients, that, is, in homogenizated equation.
In (1) we'll suppose that A is a strong elliptical operator, $\bar{a}_{aß}(x)\in C^{1}(V)$, f sufficiently smooth in V.

$$V=\bigcup_{k=1}^{N}V_{k} \tag{2}$$

V_k are congruent parallelepipeds from V. We'll suppose that $\bar{a}_{aß}(x)$ are V_k - periodic functions, together with their derivatives until 1 order. The calculation of constant coefficients supposes [1] the usage of an asymptotic development of unknown function $u\in H^{2}(V)$, and the integration of a homogenous elliptical equation on a parallelepiped V_k, in which the boundery conditions constitute the V_k - periodicity condition of the solution. $H^{1}(V)$ is the Sobolev space.
The determination of the solution for the homogeneous problem will be realized, using a finite element type proceeding, for which we'll study the error of finite-element approximation and the qudrature's error.

The notation for D^a and $|a|,|b|$ are those usuals. This type of the problems have a large applicability in the study of composite materials with periodic structures, [1].

2.THE MICROSCOPIC AND MACROSCOPIC EQUATIONS

Suppose that the coefficients $a_{aß(y)}$, $y \in V$, are V_k - periodic function and $e > 0$ is a small parameter.

$$a^e{}_{aß}(x) = a_{aß}(y) \tag{3}$$

with $y = \frac{1}{e}x = \frac{1}{e}(x_1, x_2, ..., x_n)$

It comes aut that $a^e{}_{aß}(x)$ is eV_k - periodic.

Let $\Omega \in R^n$ be the transformed domain by the change $\frac{1}{e}x$ and $f \in C^1(\Omega)$.

We consider the following boundary value problem:

We determined $u^e \in H^2(\Omega)$, such that,

$$A^e u^e \equiv \sum_{|a|,|ß|=1} (-1)^{|a|} D^a \left(a^e_{aß} D^ß u^e(x)\right) = f \tag{4}$$

in Ω, and

$$u^e|_{\partial\Omega} = 0 \tag{5}$$

For $e > 0$ fixed, the problem (4), (5) has single solutions in $H^2(\Omega)$, because A^e is strong elliptical and $f \in C^1(\Omega)$.

Suppose that $u^e(x)$ admits an asymptotic development, when $e \to 0$ in asymptotic power series of the form:

$$u^e(x) = \Psi_0(x) + e\Psi_1(x,y) + e^2\Psi_2(x,y) + ... \tag{6}$$

where (Ψ_n) is an asymptotic base for $u^e(x)$, and $y = \frac{1}{e}x$.

We assume that the base (Ψ_n) is V_k - periodic in y variable,

If we note:

$$V_a = \sum_{|ß|=1} a_{aß} D^ß u^e = \sum_{i=1}^{n} a_{aß_i} \frac{\partial u^e}{\partial x_i}, \quad ß = (ß_1, ß_2, ..., ß_n) \tag{7}$$

$|b| = 1$, it holds

$$\sum_{|ß|=1} D^ß u^e = \sum_{i=1}^{n} \frac{\partial u^e}{\partial x_i} + \frac{1}{e}\sum_{i=1}^{n} \frac{\partial u^e}{\partial y_i} = \sum_{i=1}^{n}\left(\frac{\partial \Psi_0}{\partial x_i} + \frac{\partial \Psi_1}{\partial y_i}\right) + e\sum_{i=1}^{n}\left(\frac{\partial \Psi_1}{\partial x_i} + \frac{\partial \Psi_2}{\partial y_i}\right) + ... \tag{8}$$

and

$$v_a(x,y) = v_a^0(x,y) + e\, v_a^1(x,y) + ... + e^n v_a^n(x,y) + ... \tag{9}$$

where

$$v_{\alpha}^{n}(x,y)=\sum_{i=1}^{n}a_{\alpha\beta_i}(x)\left(\frac{\partial\Psi_n}{\partial x_i}+\frac{\partial\Psi_{n+1}}{\partial y_i}\right)\quad n=0,1,2... \tag{10}$$

if we replace (9) in (4) and we identify after e we get

$$\sum\frac{\partial v_{\alpha i}^{0}}{\partial y_i}=0,\quad \alpha=(\alpha_1,\alpha_2,...,\alpha_n) \tag{11}$$

$|\alpha|=\alpha_1+\alpha_2+...+\alpha_n=1$ respectively

$$-\sum\left(\frac{\partial v_{\alpha i}^{0}(x,y)}{\partial x_i}+\frac{\partial v_{\alpha i}^{1}(x,y)}{\partial y_i}\right)=f(x) \tag{12}$$

Theorem 1. If $u^2\in H^2(V)$ is the solution of the problem (4), (5), $e>0$ fixed and $L_k:H^2(V_k)\to R$ is the meaning operator

$$L_k\left[w=\frac{1}{|D_k|}\int_{V_k}w(y)dy\right] \tag{13}$$

where V_k is one fron the parallelepipeds in the which is decomposed $V\subset R^n$, then hold:

$$-\sum_{i=1}^{n}\frac{\partial}{\partial_{x_i}}L_k\left[V_{\alpha_i}^{0}\right]=f(x),\quad in\quad \Omega \tag{14}$$

$|V_k|$ is the measure of V_k.

Proof: we apply the L_k operator in (12). Using the linearity of L_k, the derivation under the integral and effect the integration in respect of y we get:

$$-\sum_{i=1}^{n}\frac{\partial}{\partial_{x_i}}L_k\left[V_{\alpha_i}^{0}\right]-L_k\left[\sum_{i=1}^{n}\left(\frac{\partial v_{\alpha i}^{1}}{\partial y_i}\right)\right]=L_k[f(x)]\text{ but }L_k[f(x)]=\frac{1}{|V_k|}\int_{V_k}f(x)dy=f(x)$$

to obtain (14) it is enough to prove that:

$$L_k\left[\sum_{i=1}^{n}\frac{\partial v_{\alpha i}}{\partial_{y_i}}\right]=0 \tag{15}$$

if in (15) we apply the Gauss-Ostrogradski's formula we have:

$\frac{1}{|V_k|}\int_{V_k}\left(\sum_{i=1}^{n}\frac{\partial v_{\alpha i}}{\partial_{y_i}}\right)dy=\frac{1}{|V_k|}\int_{\partial V_k}<v_{\alpha},\vec{n}>_{R^n}ds$ but $v_{\alpha i}$ are V_k - periodic functions and $\vec{n}$ has contrary sign an opposite faces, therefore $<v_{\alpha},\vec{n}>_{R^n}\Big|_{\partial V_k}=0$

Thus the theorem is proved.

The equation (14) is called the macroscopic equation or the omogenized equation. Applying the L_k operator of equation (11) we get the microscopic or local equation.

In this purpose we utilize Bensoussan-Lions [1] result, loocking to existence and oneness of the solutions for the following boundary value problem:

If v is V_k periodic and g has the property $L_k[g]=0$, then, if $a_{a?} \in H_1(V_k)$ the equation $\sum_{|a|,|ß|=1}(-1)^a D^a(a_{aß}(y)D^ß v)=g(y), \forall y \in V_k$ admit a single solution $v \in H^2(V_k)$, modulo an additive constant.
Also , (11) is equivalent with the following boundary value variational problem:
Find $\Psi^1 \in H^1(V_k)$ such that

$$\int_{V_k}\left(\sum_{|a|,|b|=1} a_{ab}(y)D^a \Psi_1 D^b w\right)dy = \sum_{|a|,|b|=1} D^a \Psi_0(x)\int_{V_k} D^b a_{ab}(y)w(y)dy \tag{16}$$

$\forall w \in H_p^1(R)$, where $H_p^1(R^n)$ denotes the Sobolev space $H^1(R^n)$ of the V_k periodic functions.
Note that (16) frames in the Bensoussan-Lions theorem. If in (15) we suppose that $\Psi_0(x)$ is know the determinations of Ψ_1 reduces to the following boundary value variational problem :
Find $h_j \in H_p^1(R^n)$ the satisfies $L_k[h_{ß j}]=0, \quad (j=1\div n)$, such that

$$\int_{V_k}\left(\sum_{|a|,|ß|=1} a_{aß}(y)D^a w\right)dy = \int_{V_k}\left(\sum_{|a|=1} D^a a_{aß j} w\right)dy, \quad \forall w \in H_p^1(R^n) \tag{17}$$

The equation (17) constitute the object of this paper, because, knowing its solution $h_{ß j}, \quad (j=1\div n)$ we are leaded [1] to the homogenized coefficients $\bar{a}_{aß}$, given by

$$\bar{a}_{a iß j} = L_k[a_{aiß j}] + \sum_{\ell=1}^{n} L_k\left[a_{ai\, ß\ell}\frac{\partial h_{ß j}}{\partial y_\ell}\right] \tag{18}$$

The extension of our results from case n=3, [1], to the general case achieves without difficulty.
In this way we come to the homogenized problem:

$$\sum_{|a|,|ß|=1}(-1)^a D^a(\bar{a}_{aß}D^ß \bar{u}) = \bar{f} \quad in\,\Omega \tag{19}$$

With

$$\bar{u}\,|_{\partial\Omega} = 0 \tag{20}$$

The equation (17) is called the macroscopic or local equation.
We have used the notation $ß = \left(0,\dots\frac{1}{j}\right) := (ß_1,\dots ß_j,\dots, ß_n) := ß_j$, putting $a_{aß j}$ in the place of $a_a\left(0,0,\dots,\frac{1}{j},0,\dots,0\right)$

3.FINITE ELEMENT FOR THE MICROSCOPIC EQUATION

Consider the equation (17) in that $a_{aß}(y)$ are V_k - periodics, search $h_{ß j} \in H_p^1(V_k)$ such that (17) holds for any $w \in H_p^1(V_k)$. The condition from Bensoussan_lions existence's theorem is satisfied, because $\int_{V_k}\left(\sum_{|a|=1} D^a a_{aß j}(y)\right)dy = 0$, since $a_{aß j}(y)$ are V_k - periodics and apply the reasoning from Theorem 1. There fore (17) is orrectly formulated boundary-value problem.

Let the Δ_M - discretization in $M \in N$ simplexes of V_k, we note with k one of the simplexes of Δ_M, $\overset{(e)}{k} = conv\left(\overrightarrow{e_1}, \overrightarrow{e_2}, ..., \overrightarrow{e_{n+1}}\right)$, where $\vec{e_k}$, $(k = 1 \div n+1)$ are the position-vectors of the k – simplexes vertexes. Denote with $\hat{k}$ the Standard-simples in wich is transformed each of k therefore $\hat{e}_k = (0,0,...,0,1,0,...,0)$, $(k = 1 \div n)$ and $\hat{e}_{n+1} = (0,0,...,0)$

The transformation T: $\overset{(e)}{k} \longrightarrow \hat{k}$ achieves by

$$x_k = \overset{(1)}{x}_k + \sum_{j=1}^{n} (\overset{(j+1)}{x_k} - \overset{(1)}{x_k}) \hat{x}_k \quad , \quad (k = 1 \div n) \tag{21}$$

where $\vec{e}_j = \left(\overset{(j)}{x_1}, \overset{(j)}{x_2}, ..., \overset{(j)}{x_n}\right)$ $(j = 1 \div n+1)$. Using (21) it is sufficient to know the finite-element local base on the standard element $\hat{k}$, that is:

$\left\{\hat{}_k(x)\right\}_{k=1}^{n+1}$ given by

$$\hat{}\left(\hat{x}\right) = \hat{x}_k, \quad (k = 1 \div n), \ \hat{}_{n+1}\left(\hat{x}\right) = I - \sum_{k=1}^{n} \hat{x} \tag{22}$$

the geometry of V_k allows such a simple choise.

Theorem 2. Let (17) be the boundary-value variational problem; if $h^*_{ßj}$ its finite-element solution, generated by the base (22) then there is a constant c>0 independent of h and $h^*_{ßj}$ such that $\left\| h^*_{ßj} - \tilde{h}_{ßj} \right\|_{H^1(V_k)} < c.h^2$, where h denotes the finite-element discretization norm of V_k, $(j = 1 \div n)$. The proof of this theorem founds in [3]. Generally, the calculation of the coefficients from the finite-element local system obtain approximating the integrals which appear by the quadrature's formula. We'll use the C.Kalik's formula in [2], which frames this theory. If $\hat{k}$ is the standard simplex, $\left\{\hat{}\left(\hat{x}\right)\right\}_{k=1}^{n}$ is the base given by (22) and $g : \hat{k} \longrightarrow R$ is the function to be integrated, then it holds [2],

$$\int_{\hat{k}} g\left(\hat{x}\right) d\hat{x} = Q_{\hat{k}} + R_n[g], \tag{23}$$

where $Q^1_{\hat{k}}(g) = \sum g\left(\overset{(k)}{x}\right) \int \hat{}_k\left(\hat{x}\right) d\hat{x}$, $R_n[g]$ is the remainder of the formula, that for $n \le 3$ allows the estimation

$$\left|R_n[g]\right| \le c(\hat{k}).\left[mess\left(\hat{k}\right)\right]^{1/2} h^2 |g|_{H^2\left(\hat{k}\right)} \tag{24}$$

where $|g|^2_{H^2\left(\hat{k}\right)} = \sum \left\| D^{a} g \right\|^2_{L_2\left(\hat{k}\right)}$. In our case, if $\hat{a}_{aß} \in C^2\left(\hat{k}\right)_2$ the conditions in which this formula may be applied are satisfied.
Denote by:

$$a\left(h_{ß\,j}, w\right) = \int_{V_k} \left(\sum_{|a|,|ß|=1} a_{aß}(y) D^{a} h_{ß\,j} D^{ß} w \right) dy \tag{25}$$

$$\tilde{a}\left(\tilde{h}_{ß\,j}, w\right) = \sum_{|a|,|ß|=1} Q_{V_k}\left(a_{aß}(y) D^{a} h_{ß\,j} D^{ß} w\right) \tag{26}$$

$$\ell(w) = \int_{V_k} \left(\sum_{|a|=1} D^{a} a_{aß\,j}(y) w(y) \right) dy \tag{27}$$

$\tilde{\ell}(w) = \sum Q_{V_k}\left(D^{a} a_{aß\,j} w\right)$, and

$$S_h(V_k) = span\{\ _k(x)\}_{k=1}^{n} \tag{28}$$

where $\{\ _k\}_{k=1}^{n}$ is the global base, generated by the local base (22).
Holds the following quadrature error estimation result:

Theorem 3. Supose that the bilinear from $\tilde{a}(u,v)$ satisfies the conditions: there are the positive contents $\tilde{M}_0$ and $\tilde{M}_1$ such that,

(i) $\tilde{a}(u,u) \geq \tilde{M}_0 \|u\|^2_{H^1(V_k)}$, $\forall u \in S_h(V_k)$

(ii) $\left| \tilde{a}\left(\tilde{h}_{ß\,j}, w\right) - a\left(\tilde{h}_{ß\,j}, w\right) \right| + \left| \tilde{\ell}(w) - \ell(w) \right| \leq \tilde{M}_1 \|w\|_{H^2(V_k)}$ $\forall w \in S_h(v_k)$, <u>where</u> $S_h(V_k)$ <u>has the</u> inverse property. Then the error due to quadrature is given by

$\left\| \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j} \right\|_{H^1(V_k)} \leq \tilde{M} h^2$, $(j = 1 \div n)$, $\tilde{M} = \dfrac{\tilde{M}_1}{\tilde{M}_0}$, where $\tilde{h}_{ß\,j}$ is the finite element solution for (17) and $\tilde{\tilde{h}}_{ß\,j}$ is the finit element solution applying (23).

Proof. The condition (i) results from the fact that operator A defined in (17) is strong-elliptic, therefore the are associated bilinear from coercive.

The finite-dimensional $S_h(V_k)$ generated by the local-bases $\left\{ {}^{(e)}_{\ k} \right\}_{k=1}^{n+1}$ satisfies [2] the invers property. For n>3 use the same formula (23) with the local base functions, polynomial of high degree [2].

Using the bilinearity of $\tilde{a}$, hold:

$$\tilde{a}\left(\tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}, \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right) = \tilde{a}\left(\tilde{h}_{ß\,j}, \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right) - \tilde{a}\left(\tilde{\tilde{h}}_{ß\,j}, \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right) = \tilde{a}\left(\tilde{h}_{ß\,j}, \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right)$$

$$\tilde{\ell}\left(\tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right) - \tilde{a}\left(\tilde{h}_{ß\,j}, \tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right) + \tilde{\ell}\left(\tilde{h}_{ß\,j} - \tilde{\tilde{h}}_{ß\,j}\right)$$

If in the condition (i) we take $u = \tilde{h}_{bj} - \tilde{\tilde{h}}_{bj}$, we can write

$$\left\| \tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right\|_{H^1(V_k)} \le \frac{1}{\tilde{M}_0} \left| \tilde{a}\left(\tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j}, \tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) \right| = \frac{1}{\tilde{M}_0} \left| \tilde{a}\left(\tilde{h}_{\beta j}, \tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) - a\left(\tilde{\tilde{h}}_{\beta j}, \tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) + \ell\left(\tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) \right|$$

$$\le \frac{1}{\tilde{M}_0} \left[\left| \tilde{a}\left(\tilde{h}_{\beta j}, \tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) - a\left(\tilde{\tilde{h}}_{\beta j}, h_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) \right| + \left| \ell\left(\tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) - \tilde{\ell}\left(\tilde{h}_{\beta j} - \tilde{\tilde{h}}_{\beta j} \right) \right| \right]$$

Using now the condition (ii) we obtain the theorem's assertion.

4.SIMULATION OF THE DISCONTINUOUS COMPOSITE FLUID FLOW

The analyses of the melt plastic material in injection molded cam be of the type:

- Full flow
- Filling only
- Runner balance
- Molding window
- Gate location

In this paper we used only the first and the second option analysis. In order to analyze the flow of plastic material during it's injection in the mold it's necessary to cover several stages;(fig 2)

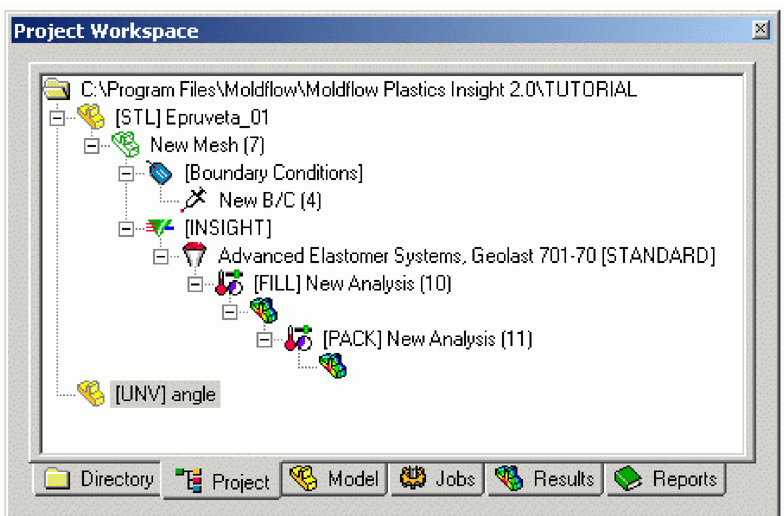

Fig.1. Program files / moldflow plastics

1. The import of 3D models of the piece(test tube)

The geometrical model of the piece (fig.2) to be analyzed can be realized directly in Mold flow, using the module MPI/Modeler or in the CAD 3D program , afterwards imported in MDI/STUDIO module as a file STL or IGES.

2. The discretization of geometrical model (New Mesh)

It's a very important stage of the simulating process, because it can appear various deficiencies of the mash, for example: breaches , superposition of the elements, unorientated elements. This deficiencies doesn't permit the realization of the simulating and appear messages of errors.

3. The selection of the boundary conditions

In this stage we choose the point of the injection. The place will be represented by a yellow knot on model surface.

4. Stualysis Preparation Wizard

In this stage take place the choice of the material for the piece from the data base of the soft, the choice of the analysis type (Flow , Gptinum profile analysis, Cool, Warp or Stress)
Choosing the Flow option, further will choose the oprion Filling only and the necessary parameters for the injection.

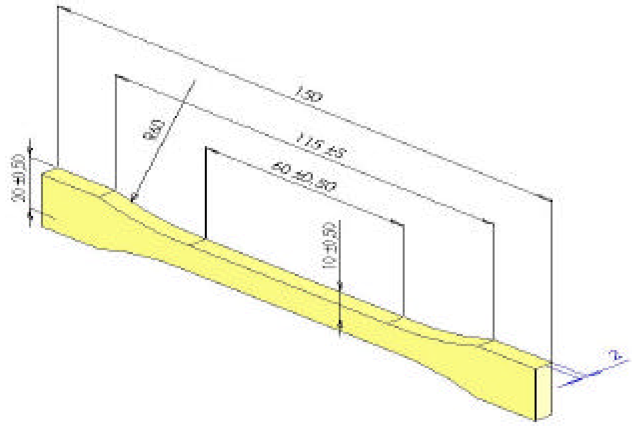

Fig. 2. Test tube from plastic material, the model to be studied

In this simulating we'll obtain the following results:

1. Fill time
2. Fill pressure
3. The flow front temperature
4. The cooling time
5. Bulk shear rate
6. Bulk stress
7. The diagram of the volume filled with discontinuous composite

The diagram of fill time shows the flow front position at regular time intervals during the mold fill.
The outlines represented by the same colour show the part of the mold filled in the same time. At the beginning of injection the result it's red and at the end is navy blue. If the injection time is too short, the part of the piece unfilled isn't coloured.
In a piece with balance fill time:

- the material flow in every directon is fil\nished in the same time, i.e the flow front reaches the extremities at the same time. This means that all the fronts of of flow ends with navy blue colour.
- The outlines are simmetrically disposed.

The disposition of the outlines shows the speed of the flow. The largest spaces between the outlines shows a fast flow while the deuse spaces show that the piece is filled slowly.

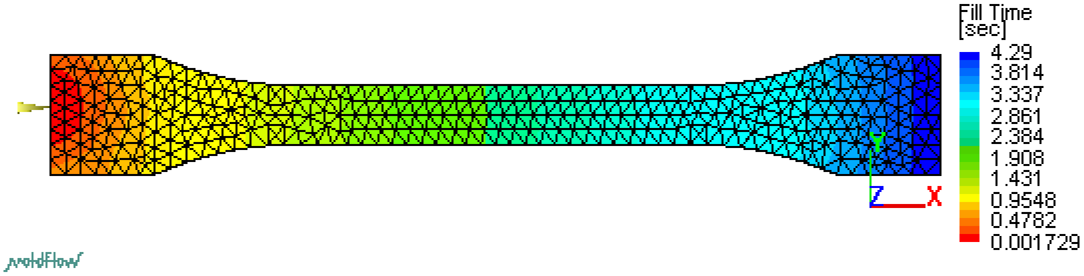

Fig. 3. The fill time diagram

The fill pressure (fig.4) presents the pressure distribution during the material flow. The pressure must be zero at the end of any flow trajectories and at the end of flow. Usually, the maximum pressure of injection is approximate 200 Mpa.

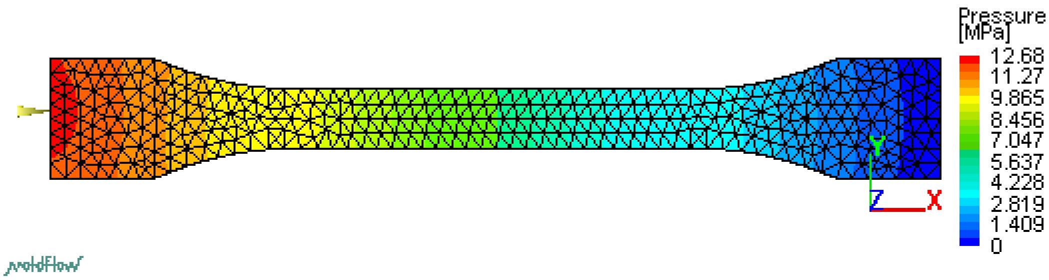

Fig. 4. The fill pressure diagram

The diagram of the flow fronts temperature(fig.5) presents the temperature distribution when the flow front reaches a specified point. The graple can be obtaind at the end of the analysis ar at a specified time during the analysis. Ts recomanded a small variation of the flow fronts temperature from the first point of the cavity until the last filled point.

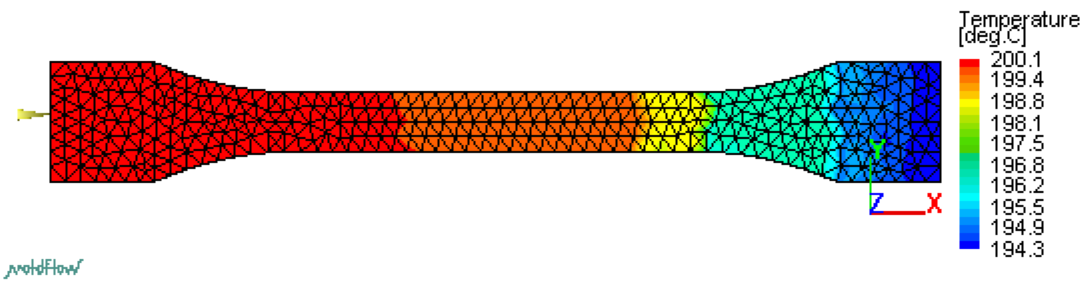

Fig. 5. The flow fronts temperature diagram

The cooling time diagram (fig 6) presents the additional time needed after finishing the fill (fill analysis) or after compacting (compacting analysis) for cooling the plastic.
The cooling time can offer a clue about the total time of the cycle.
In a part with good cooling time:

- The total cooling time is minimal. This lowers the costs associated to long cycle times.
- The intervals between the fill times are minimal. The difference between the longest and the shortest cooling time have to be minimized, because it determines contractions in the part material.
- The longest cooling time is necessary for the material around the injection point. It is necessary to ensure that the injection point will stay open allowing part compacting.

In order to reduce the cooling time, any of the following measures can be taken:

- Avoiding very thick walls of parts;
- Decreasing the temperature of the mold or of the melt;
- Modifying the injection position, in order to standardize flowing.

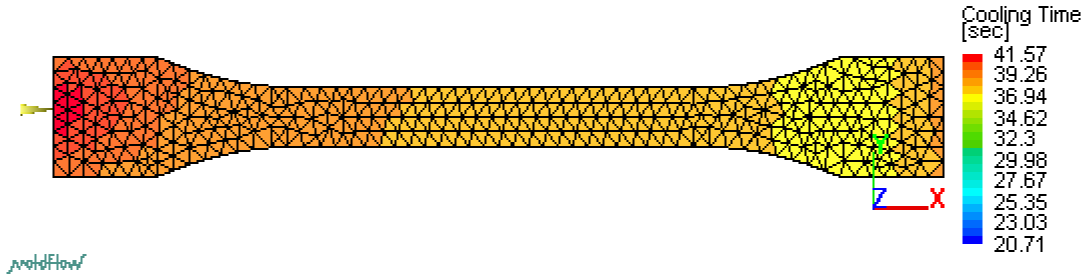

Fig.6 The cooling time diagram

The bulk shear rate (fig. 7.)should have a value as small as possible and less than the maximal permissible value of the chosen plastic.The chart of the maximal bulk shear rate indicates, for each elements of the model, the value of the maximal bulk shear rate that appears during the injection cycle and can be directly compared to the value stored in the material database. In this example, the maximal bulk shear rate recommended for the used material is 40,000 1/s.

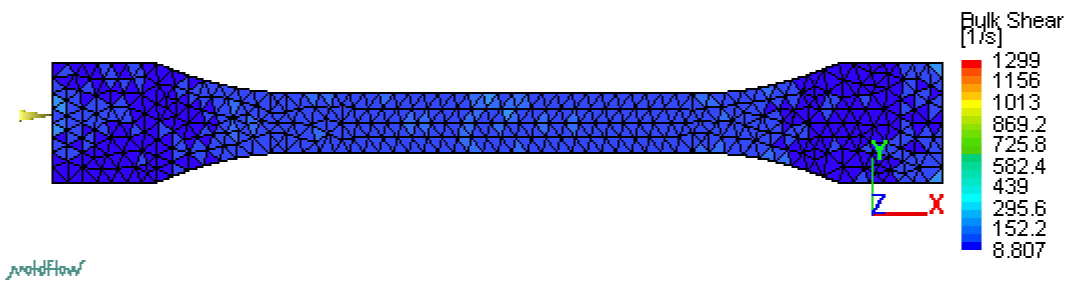

Fig. 7. The bulk shear rate diagram

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