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A 3D-Numerical Thermomechanical Approach for Materials Cutting

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Abstract : Materials cutting during machining is an extremely complex thermo-mechanical problem due to the severe physical conditions associated to materials cutting mechanisms : very high elasto-viscoplastic strains and strain rates ; material passes from room temperature to the heated state in milliseconds, with the heat coming from internal dissipation and friction. Based on continuum thermomechanics and including friction and large deformations in dynamics with viscoplasticity, a materials cutting three-dimensional numerical model is briefly described. Weak forms of conservation laws are introduced in an Arbitrary Lagrangian Eulerian configuration allowing for an arbitrary surface of separation of the material, and an automatic and continuous rezoning. The Coulomb friction law is introduced to model the tool-chip and workpiece-tool contacts, and heat generation and heat transfer at these interfaces are taken into account. The flow stress including temperature and strain rate effects is based on the Johnson-Cook law proposed for high strain rate conditions. A three-dimensional example is shown when simulating the oblique cutting. Finally, some needs for the future are detailed to improve constitutive laws as well as friction, and to include more physics, for example chemical diffusion in workpiece and tool.

Keywords : Continuum thermomechanics, viscoplasticity, friction, ALE, metal cutting.

1. MACHINING AS A MULTI-SCALE PROBLEM

Despite significant technological progress in machining, today's machining operations are very difficult to model so as to predict cutting parameters, and are still

open to scientific challenge. New features on interactions between workpiece and tool materials are welcome both from an experimental and computational point of view, so as to know thermomechanical loading in dynamics accurately for both tool and workpiece. Physical and chemical properties of useful materials for machining are examined to improve performance. All these responses can then permit reaching an expected machined surface and a tool life according to production requirements. Many papers on machining are available in the literature, and a review has for instance been published recently [Ehmann et al., 1997].

Materials cutting is a very complex forming process involving (within the workpiece-tool system) high shear and friction mechanisms in dynamics, liberated as heat. Therefore, thermomechanical coupling occurs at large strains and strain rates in viscoplasticity. In addition, metallurgical and chemical transformations are often happening inside the chips and possibly near the machined surface of the workpiece, as well as dynamic phenomena produced by the cutting process. Chatter is often observed between workpiece and tool, and this has to be avoided in order to reach the expected final surface of the workpiece. Chips may be either continuous or not, or serrated. Their metallurgical analysis will bring out important features on material flow during cutting, cutting capability of a given material, as well as phase changes ; plus chemical diffusion between chip and tool. It is clear that all the above phenomena observed during the cutting process need appropriate reference scales to be properly and consistently analysed by separating physical effects with great length of variation from those with smaller length. We introduced three different scales [Touratier, 1999] to consistently study the cutting operation :

- a microscopic scale at the material grain level. In addition, a nanoscopic scale may be introduced at the material crystal level,
- a mesoscopic scale at the tool tip - workpiece material level (more often we would call this the “tool-tip – chip” level),
- a macroscopic scale either at the workpiece-tool or machine tool structure level.

The microscopic (or possibly nanoscopic) scale will be required : to analyse the material microstructure ; to construct for example a polycrystalline thermomechanical constitutive law to include grain distribution ; to take into account phase changes, chemical diffusion, damage, wear, . . . The mesoscopic scale is classic to the study of continuous chip flow, in three - dimensional form from numerical simulations in order to predict chip geometry, stresses and temperatures, as well as cutting forces. Finally, the macroscopic scale will be more appropriate to analyse dynamics of the workpiece-tool system. On the production level, a megascopic scale should be introduced to achieve corresponding studies. The main difficulty remains in some cases how to find a consistent way to pass from one scale to another, due to various

nonlinearities and also a big computational effort associated with the very different scale sizes. The physical bases of cutting models are conservation laws including phase change, diffusion ; and of course elastoviscoplasticity, friction, and damage.

2. MATERIALS CUTTING MODELING

The modeling of chip formation is extremely complex due to the severe physical conditions associated with chip formation mechanisms : high viscoplastic strains ($\sim 10^3$) and strain rates ($\sim 10^5 s^{-1}$) ; residual state ; material passes from room temperature to the heated state (~ 700 °C) in milliseconds, with most of the heat coming from friction between tool and chip, and tool and workpiece. Considerable effort towards chip formation modeling is therefore still needed in order to bring out all thermo-metallurgico-mechanical information concerning the cutting process and to optimise it within the field of high - speed machining in turning, milling, drilling and grinding. In addition, the modeling master can help to modify features of both cutting tools and workpiece material in order to improve production.

In the past, Eulerian, Lagrangian and Arbitrary Lagrangian-Eulerian methods have been adopted, see for example [Caroll et al., 1998], [Sekhon et al., 1993], [Rakotomalala et al., 1993]. Hereafter, we will consider only predictive models which allow for an arbitrary surface of separation between workpiece and chip. Models based on a predetermined line of separation (a lot of these exist in the literature) at the tool tip in the workpiece material are not useful as they are not capable of predicting surface roughness and chip morphology, nor are they able to predict the extremely large strains encountered near the tool tip inside the workpiece material. The Arbitrary Lagrangian-Eulerian (ALE) formulation adopted in this section is an extension of both classical Lagrangian and Eulerian formulations where grid points may have an arbitrary motion. In such a description, material points are represented by a set of Lagrangian coordinates X_i , spatial points with a set of Eulerian coordinates x_i , and reference points (grid nodes) with a set of arbitrary coordinates a_i . All physical quantities are computed at points x_i occupied by grid nodes at time t . All conservation laws must be expressed taking into account the meshing evolution during the calculation.

Considering a space and time dependent quantity g , one must express all the conservation laws using the material \dot{g} , spacial g' and mixed $\overset{\circ}{g}$ time derivatives. Conservation laws are usually written using material time derivatives in an Eulerian formulation [Germain, 1986]. Therefore, we have to introduce the relationship below between material and mixed time derivatives

$$\dot{g} = \overset{\circ}{g} + g_{,i}c_i \quad (1)$$

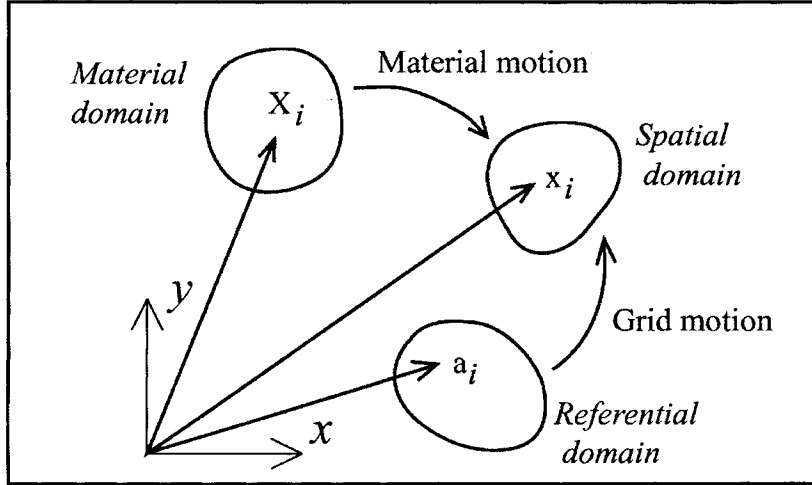


Figure 1 ; Domains and coordinates for the ALE formulation

where $c_i = v_i - \hat{v}_i$ is a convective term representing the relative velocity between the material v_i and grid \hat{v}_i velocities and $g_{,i}$ represents the space derivative of g with respect to x_i . Thus, the ALE method combines both the advantages of Eulerian and Lagrangian representations in a single description which can be considered as an automatic and continuous rezoning method. The model is ALE until the steady state conditions are reached. This permits especially free and contact surfaces to be updated. Once these conditions are obtained, then this model is equivalent to an Eulerian one.

2.1 Discretised weak forms

Let $\Omega(t)$ be the domain to be considered in modeling at the current configuration and $\Gamma(t)$ its boundary. We denote by : \vec{v} the material velocity, $\vec{\hat{v}}$ the mesh (or grid) velocity, ρ the mass density, \vec{f} the external given body forces, \vec{F} the external surface forces, σ the Cauchy stress tensor, \mathbf{d} the strain rate tensor, e the specific internal energy, w the given external body heat generation, Q the external given heat and \vec{q} the heat flux. The unknowns are \vec{v} , ρ , e and constitutive laws have to be found for σ , e and \vec{q} . Supposing that $e = e(T, t)$, the final unknowns will be \vec{v} , ρ , and the temperature T . The formulation of such an intrinsic problem requires defining the following functional spaces :

$$\mathfrak{R} = \{ \rho ; \rho(x_i, t) \in H^1(\Omega(t)) ; \text{impermeable wall} \} \quad (2)$$

$$\vartheta = \{ \vec{v} / \vec{v}(x_i, t) = (v_1, v_2, v_3) ; v_i \in H^1(\Omega(t)) ; v_i = \bar{v}_i \text{ on } \Gamma_V(t) \} \quad (3)$$

$$\epsilon = \{ e ; e(T, t) \in H^1(\Omega(t)) ; T = \bar{T} \text{ on } \Gamma_T(t) \} \quad (4)$$

where H^1 is the Sobolev space of order one, and $\Gamma_v(t)$ and $\Gamma_T(t)$ are the boundary parts, respectively, where material velocity and temperature are prescribed. To achieve numerical results, we use a discretisation of the boundary value problem. We then note ρ^h , \vec{v}^h and e^h as approximated fields on ρ , \vec{v} and e respectively. The superscript h refers to the association of spaces \mathfrak{R}^h , \mathfrak{V}^h , ϵ^h containing ρ^h , \vec{v}^h , e^h with a mesh $\cup \Omega_e^h(t)$ (or discretisation) of the continuous domain $\Omega(t)$ which is classically parametrised by a characteristic length scale h , and $\Omega_e^h(t)$ refers to a finite element or a finite volume, depending on the kind of discretization chosen. We also need to introduce weighting function sets as follows :

$$\mathfrak{R}^h = \{ \rho^*{}^h ; \rho^*{}^h(x_i) \in H^1(\Omega(t)) \} \quad (5)$$

$$\mathfrak{V}^h = \{ \vec{v}^*{}^h / \vec{v}^*{}^h(x_i) = (v_1^*{}^h, v_2^*{}^h, v_3^*{}^h) ; v_i^*{}^h \in H^1(\Omega(t)) ; v_i^*{}^h = 0 \text{ on } \Gamma_V(t) \} \quad (6)$$

$$\epsilon^h = \{ e^*{}^h ; e^*{}^h(\bar{T}^h) = \bar{T}^*{}^h \in H^1(\Omega(t)) ; \bar{T}^*{}^h = 0 \text{ on } \Gamma_T(t) \} \quad (7)$$

Using both the relationship (1) between material and mixed time derivatives, and its corresponding following expression

$$\dot{K}(t) = \overset{\circ}{K}(t) + \int_{\Omega(t)} (gc_i)_{,i} d\Omega(t) \quad (8)$$

available for a volume integral of a function g , the discrete weak forms associated respectively with the mass, momentum and energy conservation laws can be expressed from classical Eulerian ones as :

i - find $\rho_e^h \in \mathfrak{R}^h$:

$$\int_{\cup \Omega_e^h(t)} \rho_e^*{}^h \left(\frac{\partial \rho_e^h}{\partial t} + \vec{c}^h \cdot \overrightarrow{\text{Grad}}_x \rho_e^h + \rho_e^h \text{div}_x \vec{v}^h \right) d(\cup \Omega_e^h) = 0, \quad \forall \rho_e^*{}^h \in \mathfrak{R}^h \quad (9)$$

ii - find $\vec{v}^h \in \mathfrak{V}^h$:

$$\int_{\cup \Omega_e^h(t)} \rho_e^h \left(\frac{\partial \vec{v}^h}{\partial t} + \mathbf{Grad}_x \vec{v}^h \cdot \vec{c}^h \right) \vec{v}^*{}^h d(\cup \Omega_e^h) = - \int_{\cup \Omega_e^h(t)} \text{tr}(\boldsymbol{\sigma}^h \mathbf{d}^*{}^h) d(\cup \Omega_e^h)$$

$$+ \int_{\cup \Omega_e^h(t)} \vec{f} \cdot \vec{v}^*{}^h d(\cup \Omega_e^h) + \int_{\cup \Gamma_{e_F}^h(t)} \vec{F} \cdot \vec{v}^*{}^h d(\cup \Gamma_e^h), \quad \forall \vec{v}^*{}^h \in \mathcal{V}^*{}^h \quad (10)$$

iii - find $T^h \in \epsilon^h$:

$$\begin{aligned} \int_{\cup \Omega_e^h(t)} \rho_e^h \left(\frac{\partial e^h}{\partial t} + \overrightarrow{\text{Grad}}_x e^h \cdot \vec{c}^h \right) \vec{T}^*{}^h d(\cup \Omega_e^h) &= \int_{\cup \Omega_e^h(t)} \text{tr}(\boldsymbol{\sigma}^h \mathbf{d}^h) \vec{T}^*{}^h d(\cup \Omega_e^h) \\ &+ \int_{\cup \Omega_e^h(t)} \vec{q}^h \cdot \overrightarrow{\text{Grad}}_x \vec{T}^*{}^h d(\cup \Omega_e^h) + \int_{\cup \Omega_e^h(t)} \rho_e^h w \vec{T}^*{}^h d(\cup \Omega_e^h) \\ &+ \int_{\cup \Gamma_{e_q}^h(t)} Q \vec{T}^*{}^h d(\cup \Gamma_e^h), \quad \forall \vec{T}^*{}^h \in \epsilon^*{}^h \end{aligned} \quad (11)$$

These functionals are strongly coupled. Thus, when the Updated Lagrangian configuration is chosen : $\vec{v}^h = \hat{\vec{v}}^h$, while if we choose the Eulerian we must take $\hat{\vec{v}}^h = \vec{0}$. Here, the suggested grid motion control algorithm has been previously proposed in [Donea et al., 1982]. If we adopt finite element approximations of equations (9) to (11), then fields \vec{v}^h and $\vec{v}^*{}^h$ will be interpolated by using the same functions. Finite volume approximations will be equivalent to taking $\vec{v}^*{}^h$ as a unitary field. Writting the boundary value problem as given above by equations (9) to (11) is very appropriate to an explicit approach that we will retain hereafter. It will be used to solve our cutting problem, being a dynamic one.

2.2 Contact and friction

The explicit integration algorithm used hereafter allows taking the contact between the bodies into account by adding an external force to the contacting nodes. This can be done by the introduction of such a force into the external surface load \vec{F} described above. Normal components of this force vector are set equal to prevent penetration, and the tangential component is set with respect to the Coulomb friction law given by :

$$\|\vec{T}_\tau^h\| < \mu \|\vec{T}_n^h\|, \quad \text{for stick ;} \quad (12)$$

$$\vec{T}_\tau^h = -\mu \|\vec{T}_n^h\| \frac{\vec{V}_\tau}{\|\vec{V}_\tau\|}, \quad \text{for slip ;} \quad (13)$$

where μ is the coefficient of friction we would prefer to assume as depending on the nature of the contacting bodies, \vec{T}_τ^h and \vec{T}_n^h are respectively the tangential and normal components of the stress vector along the interface, and \vec{V}_τ is as defined

below. Efforts to find such a coefficient from experiment associated to machining are given in [Joyot et al., 1998]. The contact algorithm must also incorporate thermal capacities. Heat generation and heat transfers at the interfaces between bodies have to be taken into account.

The heat generation in the slipping contact surfaces is given by

$$dQ_{friction}^h = \|\vec{T}_\tau^h\| \cdot \|\vec{V}_\tau^h\| dt \quad (14)$$

where \vec{V}_τ^h is the tangential slip relative velocity between contacting bodies. According to the explicit scheme, calculated heat flux is then re-introduced as an external thermal flux for each contacting node. Generated heat flux is shared among bodies in contact in a ratio depending on their thermal and geometric features, but this point of view is not sufficient since sliding motion occurs at the interface. In addition, we may introduce a thermal resistance in order to represent the thermal discontinuity at the interfaces, but the reality is as above with the shared coefficient. Because of motion between contacting bodies, sharing thermal coefficient and thermal resistance are very difficult to identify separately from the experiment. We will come back later to this essential difficulty.

2.3 Constitutive laws

For the heat flux \vec{q}^h , the Fourier conduction law is generally appropriate :

$$\vec{q}^h = - \underline{k}(T^h) \overrightarrow{Grad}_x T^h \quad (15)$$

where \underline{k} is the conduction matrix available for an anisotropic material. It may depend on temperature. Otherwise, the specific internal energy e^h is usually linked to the temperature T^h by the following relationship (state law) :

$$de^h = C_v(T^h) dT^h \quad (16)$$

where C_v is the specific heat which may depend on temperature. Today, the material constitutive law used in cutting modeling takes into account elasto-viscoplasticity, temperature and strain rates within a standard plasticity formulation. In large strains, the well known strain rate decomposition is allowed if elastic strains are small ($< 2\%$) as we will suppose below. The material constitutive law is then written as :

$$\mathbf{s}^h = \mathbf{C}^h : \mathbf{d}^h \quad \text{and} \quad \boldsymbol{\sigma}^{Jh} = \frac{dp^h}{dt} \mathbf{I} + \mathbf{s}^{Jh} \quad (17)$$

where \mathbf{s}^h is the deviatoric part of the Cauchy stress tensor $\boldsymbol{\sigma}^h$, \mathbf{s}^{Jh} is the Jaumann derivative of the \mathbf{s}^h stress tensor which depends on the spin tensor and on a convective term in ALE. Otherwise, p^h is the hydrostatic pressure which is determined from a polynomial expression. \mathbf{I} is the second order identity tensor and \mathbf{C}^h is the constitutive tensor defined as in [Soua et al., 1999]. Then, introducing the yield function as

$$f^h = \bar{\sigma}^h - R^h \quad (18)$$

where $\bar{\sigma}^h$ is the Von-Mises equivalent stress and R^h the flow stress, according to the author's knowledge, two different choices have been made in the past for R^h so as to simulate numerically chip formation within the above thermo-mechanical requirements.

i- Johnson-Cook [Johnson et al., 1983] flow stress in [Joyot et al., 1998], [Rakotomalala et al., 1993], [Pantalé et al., 1998] :

$$R^h = [A + B(\bar{\varepsilon}^h)^{\frac{1}{n}}][1 + C \text{Log}(\dot{\bar{\varepsilon}}^h/\dot{\bar{\varepsilon}}_0)][1 - (T^h - T_0)^m/(T_{melt} - T_0)^m] \quad (19)$$

where $\bar{\varepsilon}^h$ is the equivalent plastic strain, $\dot{\bar{\varepsilon}}^h$ is the equivalent plastic strain rate, T^h is the current temperature, T_0 is a reference temperature ; and A, B, C, T_{melt} , are material characteristics, while $\dot{\bar{\varepsilon}}_0 = 10^3 s^{-1}$ in order to normalise equation (19). Note also that n is the hardening exponent, and m is the softening exponent.

ii- Lemonds-Needleman [Lemonds et al., 1986] hardening rule in [Marusich et al., 1995] :

$$R^h = [1 - \alpha(T^h - T_0)][1 + (\varepsilon^{ph}/\varepsilon_0^p)]^{\frac{1}{n}} \sigma_0 \quad (20)$$

where α is a softening coefficient, σ_0 the yield stress at T_0 , ε_0^p a reference plastic strain, and ε^{ph} the accumulated plastic strain.

3. MATERIALS CUTTING SIMULATIONS. AN EXAMPLE

In this section, results from an ALE model are represented to simulate three-dimensional steady metal cutting allowing to take into account lateral expansion of the chip and to represent oblique cutting avoiding any assumption on the chip separation at the tool tip. The thermomechanical equations above discretised by finite elements (momentum)/finite volumes (mass and energy) are kept strongly

coupled. The Johnson-Cook hardening rule is used, contact conditions with friction are included between chip and tool, and also workpiece and tool. Material properties are given Reference [Pantalé et al., 1998] for a 42 CD-4 steel workpiece material, and a tungsten carbide for the assumed rigid tool (SECO TPGN-160302 P10). The quite coarse mesh created involves 5200 three-dimensional eight node finite elements (same mesh for the finite volume discretization). Cutting conditions are given in Reference [Pantalé et al., 1998] as well as thermomechanical boundary conditions. The time integration of the above discretised equations is accomplished from an explicit central difference scheme of the third order. The time increment Δt is subject to the Courant stability criterion defined by $\Delta t \leq \Delta t_{crit.}$ where $\Delta t_{crit.}$ is usually a function of the sound and convective speeds. The ALE method also requires the use of an appropriate grid (mesh) motion algorithm controlled by both space and time criteria, coming here from [Donea et al., 1982]. Knowledge of the grid speed allow us to compute the convective speed. Thus, integrating successively equations (9) to (11) gives the unknown values of $\vec{v}^h(t+\Delta t)$, $\rho^h(t+\Delta t)$ and $e^h(t+\Delta t)$. Finally, integrating the material constitutive law given by equation (17) allow one to determine the Cauchy stress tensor $\sigma^h(t+\Delta t)$ using an explicit elastic prediction and a radial return algorithm. Of course, we also needed to take into account the Fourier conduction law, the state law for internal energy and contact with friction as given above. We assumed k , c , and m as constant. Figures 2 and 3 give results on three-dimensional chip flow within oblique cutting conditions (angle between the edge of the tool and the cutting speed direction equal to 75°), [Pantalé et al., 1998].

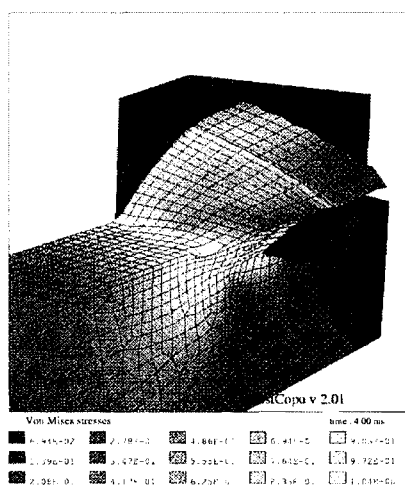


Figure 2 ; Von Mises stress contour plot

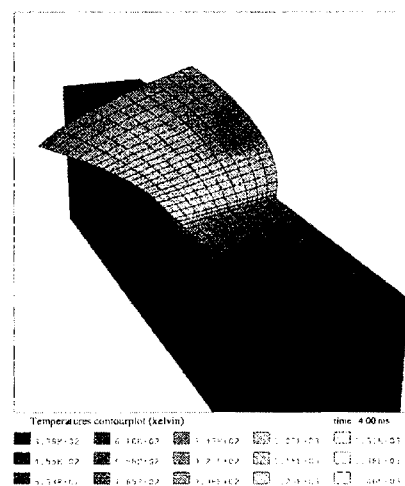


Figure 3 ; Temperature distribution in the chip and workpiece

Comparing oblique and orthogonal chip flow based on a three-dimensional ap-

proach, temperature distributions are found quite similar, but cutting forces and advancing forces have been reduced by the obliquity while lateral forces increase in a wide range. A very good agreement on forces are found for orthogonal chip flow when comparing with available experimental results [Pantalé et al., 1998].

4. NEEDS FOR THE FUTURE

Chip formation and chip morphology during machining is mainly dependent on very intense shear inside the chip in the so-called primary shear zone where shear banding occurs. Crystal plasticity employing the fundamental principle of sliding in crystalline slip systems can provide a better approach to model the phenomena inside the primary shear zone and to capture shear band localisation. In addition, this makes it easier to include induced plastic anisotropy which appears when material is being machined. Finally, this seems to be the only way to reach an accurate description of the material microstructure evolution and to control it during machining to improve product performance. The combination of the crystal plasticity theory, techniques for measurement of texture, quantitative texture analysis and the finite element method enables the study of gradients in deformation which follows from the interplay of the material state and the boundary conditions. It is even possible in this way to introduce inhomogeneous material if the number of grains is not large or as soon as computational means will be adequate. Finally, a crystal plasticity constitutive law provides a way to consistently pass from the microscopic scale to the mesoscopic defined in the above Section 1.

The chip formation and morphology, as well as temperatures, cutting forces and tool-chip contact length are found numerically very dependent on friction from a friction sensitivity analysis. Recently, a paper has been published [Oancea et al., 1997] on a thermodynamically consistent formulation of thermomechanical rate-dependant frictional sliding, within large deformations. A constitutive relationship has been proposed for frictional traction including thermal softening of frictional response, rate dependence, pressure dependent for contact thermal resistance across the interface, and heat sinks on the interfaces created by trapped wear debris. Then, the coefficient of friction is depending on the maximum temperature on the two surfaces at the current point. To this coefficient of friction is surimposed a function which controls the evolution of the frictional stress and which depends on a new state variable to be determined from a supplementary equation derived from thermodynamics. This state variable allow us to govern transitions of response between a viscous dependence of frictional traction on sliding velocity and a dependence of the coefficient of friction upon the sliding velocity. Finally, another quantity is surimposed to the coefficient of friction : it is a parameter which might be associated with the viscoplastic shearing effects of the asperities tips.

Several microstructural experiments have been done for 32CDV 13 martensitic iron machined either by ceramic or cermet tools. Machining conditions may lead to a white thin layer in the chip on the chip-tool side, not seen on many other tested steels, among them stainless steel. This thin white layer of thickness near $5\mu\text{m}$, is attributed to phase transformations and contains austenite (γ -phase), as shown from XR diffraction analysis. From a secondary ion mass spectrometry analysis, chemical diffusion of titanium and nitrogen elements has been observed, both from tool to chip, and tool to workpiece. To include chemical diffusion capability analysis into the boundary value problem shown above one conservation equation has to be added for the mass concentration. The main differences between mass conservation and mass concentration laws are now that we need to express the diffusion flux of the diffusing phase coming out the diffusing boundary, as a function of the concentration. A typical constitutive law for the diffusion flux may be expressed as a Fick law. The diffusion between chip and tool changes the mechanical strength of the tool, resulting in wear. Keeping all the above discretised weak forms and adding a damage law to produce crack initiation, then crack propagation should be an efficient way to study tool wear. Wear mechanisms during cutting may come from mechanical effects : adhesion, abrasion, sliding/delamination, erosion, fretting, ... and from chemical effects : solution, diffusion, oxidation, corrosion, ... Wear is a very important and difficult subject that we have to pursue in order to master cutting, especially concerning tool wear which is an economic as well as a workpiece surface quality challenge. Finally, metallurgical effects have also to be included into the formulation of the boundary value problem to take into account phase transformations. These will involve supplementary coupling when deriving the corresponding discrete boundary value problem in order to simulate chip formation. Corresponding features of the metallurgical model will include proportions of metallurgical constituents and dilatations of various phases as functions of temperature. Then, as above for friction and diffusion, new state variables have to be introduced according to thermodynamic requirements.

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