

# Fraction Models for Inelastic Deformation

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## 1. Validity

In the course of a fast breeder project in a period of approximately ten years a large number of experiments has been performed on tubular specimens, which were loaded in combinations of tension and compression, torsion, and internal pressure, along carefully selected stress and strain paths. During this loading the strain rate was kept nearly constant, while the experiments were restricted to strains of a few percent. The materials tested were austenitic and ferritic stainless steels. Like from earlier, but far less numerous experiments on Al-Alloy specimens it was concluded that the fraction model gives a quite accurate description for almost all loading histories considered. In particular no evidence was found in any of the tests that the yield surface may develop corners or vertices in the course of loading [3].

Much less successful has been the application of the fraction model in the creep range. In modelling creep deformation not so much the deficiencies of the mathematical model constitute the problem, however, but the large scatter that is found in experimental creep data. Tests under uniaxial stress with step loadings on Mg-Alloy specimens have shown less reproducibility than a sensible application of a complex model would require [4].

## 2. Background

In elastic deformation the distribution of the internal energy on a microscopic scale is irrelevant to the macroscopic deformation problem. Thus, the internal energy can be replaced by the internal energy of a fictitious homogeneous elastic continuum. In inelastic deformation, however, the dissipation of energy cannot in general be replaced by the dissipation in a homogeneous continuum. In the real material inelastic deformation mechanisms are initiated at certain points and will spread in subsequent loading over the whole volume in the neighborhood of a material point of the continuum. In the **fraction model** the inhomogeneous energy dissipation is discretized in a phenomenological manner by conceiving the material to be composed of a limited number of portions, which can be represented by subelements of an element of volume  $dV$ , all subjected to the deformation of the continuum, but each with its own dissipative properties. Thus the history of an inelastic deformation process is recorded in terms of fraction stresses, constituting the thermodynamic internal or hidden state variables, determining by their weighted sum the macroscopic stress tensor. From its initial formulation [1, 2] it has been stressed that the fractions are **not** to be identified as grains.

As to linear rheological models, two or more Maxwell models in parallel can be interpreted as a fraction model [5]. Also Melan's kinematic hardening model, advocated by Prager (who added the adjective kinematic to it), is contained in the fraction model. The combination of one ideally plastic or hardening fraction with one purely elastic fraction gives a kinematic hardening model with a consistent shift rule for the yield surface, as required by Ziegler [5].

## 3. Description of the model

The fraction model of a solid is based upon the concept of a so-called **natural reference state**, with respect to which changes in internal energy in thermodynamic **state space** can be defined by an invariant function of elastic strains and entropy. For a finite,

possibly very small, neighborhood of a material point of the continuum model the geometrical configuration of the elementary particles of the real material in relation to each other is assumed to differ from the configuration in the natural reference state by a linear transformation of line elements in that point:

$$d\mathbf{r} = \mathbf{F}^e d\boldsymbol{\xi}. \quad (1)$$

Here  $\mathbf{r}$  is the position vector and  $d\boldsymbol{\xi}$  is the vector of the infinitesimal line-element, that only in the case of purely elastic behavior is integrable to the position vector  $\boldsymbol{\xi}$  in the undeformed state. In case of purely elastic behavior the vector  $\boldsymbol{\xi}$  and the initial position vector  $\mathbf{r}_0$  are identical. In general the line-element  $d\boldsymbol{\xi}$  will however change its length and orientation by inelastic deformation.

The **elastic deformation tensor**, acting as objective (with respect to the material) state variable in the internal energy function, is defined by:

$$d\mathbf{r} \circ d\mathbf{r} - d\boldsymbol{\xi} \circ d\boldsymbol{\xi} = 2d\boldsymbol{\xi} \circ (\boldsymbol{\eta}^e d\boldsymbol{\xi}), \boldsymbol{\eta}^e = \frac{1}{2}(\mathbf{F}^{eT} \mathbf{F}^e - \mathbf{I}). \quad (2)$$

The rate at which locally  $d\boldsymbol{\xi}$  changes with time is characterized in the physical space by a tensor  $\mathbf{A}^p$ :

$$d\dot{\boldsymbol{\xi}} = \mathbf{A}^p d\boldsymbol{\xi} \Rightarrow d\dot{\mathbf{r}} = \dot{\mathbf{F}}^e \mathbf{F}^{e-1} d\mathbf{r} + \mathbf{F}^e \mathbf{A}^p \mathbf{F}^{e-1} d\mathbf{r} = (\mathbf{L}^e + \mathbf{L}^p) d\mathbf{r}. \quad (3)$$

The **velocity gradient tensor**  $\mathbf{L}$  has been split into an elastic and an inelastic part. Also the rate of deformation tensor  $\mathbf{D}$  and the **spin tensor**  $\boldsymbol{\Omega}$  may be split into an elastic and an inelastic part:

$$\begin{aligned} \mathbf{D}^e &= \frac{1}{2}(\mathbf{L}^e + \mathbf{L}^{eT}), \mathbf{D}^p = \frac{1}{2}(\mathbf{L}^p + \mathbf{L}^{pT}), \\ \boldsymbol{\Omega}^e &= \frac{1}{2}(\mathbf{L}^e - \mathbf{L}^{eT}), \boldsymbol{\Omega}^p = \frac{1}{2}(\mathbf{L}^p - \mathbf{L}^{pT}). \end{aligned} \quad (4)$$

We have

$$\dot{\boldsymbol{\eta}}^e = \mathbf{F}^{eT} \mathbf{D}^e \mathbf{F}^e, \mathbf{D}^e = \mathbf{D} - \mathbf{D}^p. \quad (5)$$

In the fraction model an element of volume is divided into N portions of size  $\psi^k$ , each with its own elastic deformation tensor  $\boldsymbol{\eta}^{ek}$  and its own dissipation process, leading to a  $\mathbf{D}^{pk}$ . The rate of deformation tensor  $\mathbf{D}$  remains the rate of deformation tensor of the fictitious continuum.

Denoting the temperature by T, the mass density by  $\rho$ , the internal energy per unit mass by e and the free energy per unit mass by f, we have for each fraction

$$\rho f^k = \rho e^k - T s, \rho f^k = \rho f^k(\boldsymbol{\eta}^{ek}, T). \quad (6)$$

The fraction stresses  $\boldsymbol{\sigma}^k$  are expressed in terms of the free energy by

$$\boldsymbol{\sigma}^k = \rho \left( \frac{\partial f^k}{\partial \boldsymbol{\eta}^{ek}} \right), \quad (7)$$

determining the macroscopic stress tensor  $\boldsymbol{\sigma}$  by their sum with the volume fractions  $\psi^k$  as weighting factors:

$$\boldsymbol{\sigma} = \sum_1^N \psi^k \boldsymbol{\sigma}^k, \sum_1^N \psi^k = 1. \quad (8)$$

For changes of the state variables T and  $\boldsymbol{\sigma}^k$  only rate equations can be given because of the thermodynamic irreversibility of the inelastic deformation and heat conduction processes. In the fraction model the energy dissipation per unit volume,  $\varphi$ , is the weighted sum of the dissipation functions of the N fractions:

$$\varphi = \sum_1^N \psi^k \dot{\varphi}^k(\boldsymbol{\sigma}^k, T). \quad (9)$$

In inelastic deformation the energy dissipation is the amount of work per unit volume, that is transformed into heat. For the rate of change of the temperature we then have from Fourier's law of heat conduction with  $c_v$  for the specific heat:

$$\rho c_v \dot{T} = \text{div}(\mathbf{K} \text{grad} T) + \varphi. \quad (10)$$

The scalar product of internal state variables and rates of inelastic deformation gives the rate of energy dissipation. Since the symmetric stress tensors  $\boldsymbol{\sigma}^k$  contribute to the energy dissipation solely through the symmetric inelastic deformation rates  $\mathbf{D}^{pk}$ , it would be necessary to introduce additional state variables, producing dissipation with the skew symmetric tensor  $\boldsymbol{\Omega}^p$  in order that this tensor may differ from the zero tensor.

In the fraction model the tensor  $\boldsymbol{\Omega}^p$  is taken to be the zero tensor and the constitutive equations for the tensors  $\mathbf{D}^{pk}$  are formulated in terms of energy dissipation functions  $\varphi^k$ :

$$\varphi^k = \langle \mathbf{T}^k, \mathbf{D}^{pk} \rangle = \langle \mathbf{F}^{ek} \boldsymbol{\sigma}^k \mathbf{F}^{ekT}, \mathbf{D}^{pk} \rangle = \langle \boldsymbol{\sigma}^k, \dot{\boldsymbol{\eta}}^{pk} \rangle, \mathbf{D}^{pk} = \mathbf{F}^{ekT-l} \dot{\boldsymbol{\eta}}^{pk} \mathbf{F}^{ek-l}. \quad (11)$$

Here the weighted sum of the tensors  $\mathbf{T}^k$  determines the stress tensor of Cauchy,  $\mathbf{T}$ , that occurs in the equations of motion of the continuum. The tensors  $\mathbf{T}^k$  are state variables in state space, not subjected to the equations of motion that apply in the physical space.

$$\mathbf{T} = \sum_l^N \psi^k \mathbf{T}^k = \sum_l^N \psi^k \mathbf{F}^{ek} \boldsymbol{\sigma}^k \mathbf{F}^{ekT}. \quad (12)$$

For a solid, that permits a thermodynamic description, change of volume is according to experiments a purely elastic phenomenon. Hence  $\text{tr} \mathbf{D}^{pk} = \text{tr} \dot{\boldsymbol{\eta}}^{pk} = 0$  and only the deviator of the stress tensors,

$$\mathbf{T}^d = \mathbf{T} - (\frac{1}{3} \text{tr} \mathbf{T}) \mathbf{I}, \boldsymbol{\sigma}^d = \boldsymbol{\sigma} - (\text{tr} \boldsymbol{\sigma}) \mathbf{I}, \quad (13)$$

contributes to the energy dissipation. Then  $\mathbf{D}^{pk}$  and  $\dot{\boldsymbol{\eta}}^{pk}$  must be proper duals of  $\mathbf{T}^{dk}$  and  $\boldsymbol{\sigma}^{dk}$ . If the fraction has an isotropic behavior the function  $\varphi^k$  is a function of the stresses through the invariants of the stress tensor and has thereby the required invariance with respect to rotation. Then we have in

$$\mathbf{D}^{pk} = \varphi^k \langle \mathbf{T}^{dk}, \frac{\partial \varphi^k}{\partial \mathbf{T}^{dk}} \rangle^{-1} \frac{\partial \varphi^k}{\partial \mathbf{T}^{dk}} \quad (14)$$

a tensor with the required duality properties. In case a fraction would have anisotropic behavior the energy dissipation must be considered to be a function of the objective stresses  $\boldsymbol{\sigma}^k$  and the derivatives of  $\varphi^k$  with respect to  $\boldsymbol{\sigma}^{dk}$  provide the proper duality for the tensor  $\dot{\boldsymbol{\eta}}^{pk}$ .

The constitutive equations for the inelastic deformation of one fraction are presented for the general case. The superscript k, denoting the fraction, will be omitted.

In terms of a yield function  $\Phi$  with a yield stress  $\sigma_F$ ,

$$\Phi = \Phi(\boldsymbol{\sigma}, \sigma_F), \quad (15)$$

the dissipation function is defined by

$$\varphi = \varphi(\Phi + \beta, \mathbf{T}). \quad (16)$$

It determines the creep rate  $\dot{\boldsymbol{\eta}}^c$  by

$$\dot{\boldsymbol{\eta}}^c = \varphi \langle \boldsymbol{\sigma}^d, \frac{\partial \varphi}{\partial \boldsymbol{\sigma}^d} \rangle^{-1} \frac{\partial \varphi}{\partial \boldsymbol{\sigma}^d}. \quad (17)$$

Experiments with metal specimens show that at a certain stress level the dissipation rate starts to increase very rapidly, such that very high rates of strain have to be imposed for a small increase of stress. This implies a high nonlinearity of the dissipation function at these stresslevels. A dissipation function with this type of high nonlinearity leads to

great difficulties in numerical simulations of the inelastic deformation process. From the start of the theory of plasticity a discontinuity in the constitutive description in the form of a yield surface has been introduced, by which these difficulties are overcome.

The yield function defines a closed surface in stress deviator space, limiting the stress states that can be reached,

$$0 \geq \Phi \geq -1. \quad (18)$$

The value -1 for  $\Phi$  corresponds to zero stress. The energy dissipation must be positive and the dissipation function is defined such that it is equal to zero for  $\Phi + \beta = 0$ . The parameter  $\beta$  introduces a threshold for the stresses, below which no energy dissipation takes place. For  $\beta = 1$  this is the state of zero stress. We have

$$0 \leq \beta \leq 1, \quad \varphi > 0 \text{ for } \Phi + \beta > 0, \text{ else } \varphi = 0.$$

With the aid of the fourth order tensors

$$\mathbf{L} = \frac{\partial^2 f}{\partial \eta^e \partial \eta^e}, \quad \mathbf{Y} = \left\langle \frac{\partial \Phi}{\partial \sigma^d}, \mathbf{L} \frac{\partial \Phi}{\partial \sigma^d} \right\rangle^{-1} \left( \mathbf{L} \frac{\partial \Phi}{\partial \sigma^d} \right) \otimes \left( \mathbf{L} \frac{\partial \Phi}{\partial \sigma^d} \right), \quad (20)$$

and the compression modulus  $C$  and the coefficient of cubic thermal expansion  $\alpha$  the rates of stress are defined by:

$$\begin{aligned} \text{if } \Phi = 0 \text{ and } \dot{\Phi} = 0 : \dot{\sigma} &= (\mathbf{L} - (1-h)\mathbf{Y})\dot{\eta} - h\mathbf{L}\dot{\eta}^c - C\alpha\dot{T}\mathbf{I}, \\ \text{else if } \Phi + \beta > 0 : \dot{\sigma} &= \mathbf{L}(\dot{\eta} - \dot{\eta}^c) - C\alpha\dot{T}\mathbf{I}, \\ \text{else} & \dot{\sigma} = \mathbf{L}\dot{\eta} - C\alpha\dot{T}\mathbf{I}. \end{aligned} \quad (21)$$

Here  $h$  is a small positive or negative hardening coefficient, that determines the change of the yield stress in plastic deformation. From the consistency condition  $\dot{\Phi} = 0$  follows:

$$h \left\langle \frac{\partial \Phi}{\partial \sigma^d}, \mathbf{L}\dot{\eta} \right\rangle + \frac{\partial \Phi}{\partial \sigma_F} \dot{\sigma}_F = 0. \quad (22)$$

When the material behavior is simulated by a number of fractions with different values for the yield stresses  $\sigma_F$ , with different values for the threshold values  $\beta$ , and possibly with different values for the hardening coefficients  $h$ , the typical anisotropic, memory sensitive characteristics of inelastic deformation are described by the model.

#### 4. Determination of the model parameters

The validation experiments have mainly been restricted to materials, which in their annealed state could be considered to have isotropic properties. Furthermore these experiments did encompass strains not larger than a few percent in nearly time-independent plastic deformation. Here the determination of the model parameters will be discussed for this particular application.

For small strains the stresses  $\mathbf{T}^k$  and  $\sigma^k$  are related by the orthogonal transformation  $\mathbf{R}$ . It represents the rotation of the neighborhood of the material point of the continuum with respect to the initial configuration:

$$\mathbf{T}^k = \mathbf{R}\sigma^k\mathbf{R}^T.$$

Because of the isotropic properties of the fractions, the fourth order tensors  $\mathbf{L}$  and  $\mathbf{Y}$ , as well as the yield function  $\Phi$  and thereby the dissipation function  $\varphi$ , are invariant under rotation. Von Mises' yield condition is based upon the stress invariant

$$J_2 = \frac{1}{2} \text{tr}(\sigma^d)^2.$$

We have with the shear modulus  $G$ :

$$\Phi = \frac{3J_2}{\sigma_F^2} - 1, \quad \sigma = G\eta^{\text{ed}} + C(\frac{1}{3}\text{tr}\eta - \alpha(T - T_0))\mathbf{I}. \quad (23)$$

In view of its limited significance in the envisioned applications a simple dissipation function suffices:

$$\varphi = \gamma(T) \cdot \sinh\left(0.88137 \frac{\Phi + \beta}{\beta}\right). \quad (24)$$

In this expression  $\gamma(T)$  contains the temperature dependence of the creep process. Since  $\sinh 0.88137 = 1.0000$  the dissipation rate of a fraction upon reaching the yield surface is equal to  $\gamma(T)$ . Because of the linear term in the series expansion of this function it proves to be much more suitable for the description of stress relaxation effects than the well-known power law of creep. For the higher power values the relaxation rate decreases too rapidly with the value of the excess stress  $\Phi + \beta$ .

There remains the determination of the number  $N$  of fractions, their weighting factors  $\psi^k$ , the values of their yield stresses  $\sigma_F^k$ , the hardening coefficients  $h^k$ , and the values of their threshold values  $\beta^k$ .

Simple tests on tensile specimens may provide the necessary data. If more than four fractions are taken, a smoother representation of the stress-strain diagram is obtained, but the accuracy of the simulation of complex stress histories will not be greatly enhanced in terms of predicted stress values. Furthermore the model is not very sensitive to the precise location of the breakpoints on the model stress-strain diagram, that mark the onset of yielding of one more fraction. This is of course a property, that is essential for the usefulness of the model.

The determination of the model parameters for time-independent plasticity is best illustrated for an experimental stress-strain diagram, approximated by the Ramberg-Osgood formula with material parameters  $E$ ,  $\sigma_3$ ,  $m$ .

$$\frac{E\eta}{\sigma_3} = \frac{\sigma}{\sigma_3} + \frac{3}{7} \left(\frac{\sigma}{\sigma_3}\right)^m. \quad (25)$$

We specify the breakpoints by their values for the secant modulus  $E_s$ , denoting the breakpoints with subscript  $p$ . For  $\sigma_p = E_s^p \eta_p$  we have

$$\frac{\sigma_p}{\sigma_3} = \left[ \frac{7}{3} \left( \frac{E}{E_s^p} - 1 \right) \right]^{\frac{1}{m-1}}. \quad (26)$$

The value of  $\sigma_3$  corresponds to the secant modulus, which has a value of  $0.7E$ . Usually a good choice for the breakpoints is given by the following values of the secant moduli:

$$\frac{E_s}{E} = 0.98, 0.85, 0.7, 0.4, 0.1. \quad (27)$$

**Table 1** Determination of fraction parameters from Ramberg-Osgood diagram with  $m = 10$  and  $\nu = 0.3$

P	$E_s^p/E$	$\sigma_p/\sigma_3$	$E\eta_p/\sigma_3$	$\Delta\sigma/(E\Delta\eta)$	k	$\sum_{n=1}^k \psi^n$	$\psi^k$	$\sigma_y^k/\sigma_3$
1	0.98	0.713	(0.728)	0.547	1		0.498	0.713
2	0.85	0.906	1.066	0.259	2	0.498	0.285	1.091
3	0.7	1	1.429	0.103	3	0.783	0.144	1.495
4	0.4	1.140	2.873	0.023 $\Rightarrow h = 0.020$	4	0.927	0.073	3.139
5	0.1	1.403	14.025		4	1		

Table 1 shows the successive determination of the breakpoints and of the values for  $\psi^k$  and  $\sigma_y^k$ . The yield stresses  $\sigma_y^k$  are the initial values of the flow stresses  $\sigma_F^k$  of the various fractions, which are subject to change because of isotropic hardening. This isotropic hardening may, in a first estimate, be described by the same value  $h$  for all fractions. The values of  $h^k$  do not greatly affect the values of  $\psi^k$  and  $\sigma_y^k$ , but they are essential because of the cumulative effect of the isotropic hardening. An estimate for  $h$  is needed for the determination of the values of  $\psi^k$ . A further refinement of the model with different values for  $h^k$  is mainly of value for cyclic loading.

With the aid of the well-known relations

$$G = \frac{E}{2(1+\nu)}, C = \frac{E}{3(1-2\nu)},$$

we derive the following expressions:

$$\frac{\sigma_y^k}{\sigma_3} = \frac{3}{2(1+\nu)} \left( \frac{E\eta^k}{\sigma_3} - \frac{1-2\nu}{3} \frac{\sigma^k}{\sigma_3} \right), \quad (28)$$

$$(1-h) \sum_l^k \psi^i = \left( \frac{1 - \Delta\sigma / (E\Delta\eta)}{1 - \frac{1}{3}(1-2\nu) \Delta\sigma / (E\Delta\eta)} \right).$$

These expressions show that in the case of incompressibility ( $\nu = 1/2$ ) the volume fractions follow directly from the slope of the stress-strain curve between breakpoints, while the initial yield stresses of the fractions are given by the strain at the breakpoints, multiplied by the elastic modulus. Note that for the slope of the curve from  $p=1$  to  $p=2$  the line is taken to start on the elastic part of the diagram. The value of  $E\eta_l/\sigma_3$  is not used.

Even far below the true creep range of temperatures, inelastic material behavior may be accompanied by strong strain rates effects (differences in predicted stress values of the order of 10%). In the tensile test a considerable drop in stress can occur if the loading of a specimen is interrupted at constant strain for several minutes. In a first approximation the drop in stress in such a relaxation period turns out to be more or less constant for the whole range of stress over the inelastic part of the tensile curve. Based upon this observation the threshold stress value for each fraction may put equal to the yield stress, diminished by this drop of stress,  $\Delta\sigma$ . The values of  $\beta$  then follow from

$$1 - \beta^k = \frac{(\sigma_y^k - \Delta\sigma)^2}{(\sigma_y^k)^2}.$$

Usually, for a good correspondence between the experimental curves for cyclic loading and the curves according to the fraction model, an adjustment of the hardening coefficients  $h^k$  for the various fractions is needed. This adjustment is best carried out if the values are chosen such that the curve for the first reversed loading is well represented. Often good results are obtained with values for  $h^k$  which are proportional to the difference between the yield limit  $\sigma_y^k$  of the fraction  $k$  and the yield limit of the first fraction. Obviously this implies  $h^1 = 0$  and as a result the initial yield surface does not expand, leading to a pronounced Bauschinger effect, followed by a rapidly increasing hardening.

For unequal values of  $h^k$  the determination of their values is best solved by an iterative process. For the data from the Ramberg-Osgood formula, considered in table 1, this

iterative process is illustrated in table 2. The values of  $\psi^k(I-h^k)$  remain constant in the iteration process, since they determine the slope between breakpoints. Their values are given by  $\psi^k(I-h)$  in accordance with the values of table 1. After the values of  $h^k$  have been calculated by running down the first column and up the second column of each iteration, the new values for  $\psi^k$  follow from the known values of  $\psi^k(I-h^k)$ . Sufficient accuracy was obtained in two steps.

**Table 2** Iterative determination of hardening coefficients

k	$\psi^k(I-h^k)$	$h^k/h^4$	$\sum_{n=1}^k \psi^n h^n / h^4$	$h^k$	$\psi^k$	$\sum_{n=1}^k \psi^n h^n / h^4$	$h^k$	$\psi^k$
1	0.489	0	0	0	0.489	0	0	0.489
2	0.279	0.1557	0.044	0.019	0.285	0.044	0.018	0.284
3	0.141	0.322	0.091	0.039	0.147	0.092	0.037	0.147
4	0.072	1	0.163	0.120	0.081	0.173	0.115	0.080
					1.002			1.000

## 5. How to use it

Any finite element analysis of inelastic deformation problems will introduce the constitutive equations of the material in sampling (or integration) points of the elements. If these points are material points of the continuum, as they in case of small strains usually will be, the fraction model equations may be directly applied. Of course, for each sampling point, in which inelastic deformation has occurred, the history of the internal state variables must be recorded. The history of the variables of all fractions that have contributed to inelastic deformation must be traced by storing the values of the fraction stresses with the model parameters. In the case of large deformations the mesh of finite elements has to be redefined in a continuous or discontinuous process, but in either case the problem of keeping track of the material points of the continuum with their history arises.

In order to facilitate the comparison between laboratory tests and the simulation of these tests by the fraction model a JAVA-computer program was developed, based upon an earlier PASCAL-version, used at the time of writing the book [1]. This program TESTTUBE provides a finite element simulation of tests on circular bars and tubes under tension/compression, torsion, and in the case of tubes, internal and external pressure. Also the heat production and conduction may be taken into account.

## 6. References

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