The symmetry group of the CAFFE model[*]

Sérgio H. FARIA

GZG, Department of Crystallography, University of Göttingen, Goldschmidtstrasse 1, D-37077 Göttingen, Germany
E-mail: sh.faria@geo.uni-goettingen.de

ABSTRACT. A new ice-sheet flow model called CAFFE (Continuum-mechanical Anisotropic Flow model based on an anisotropic Flow Enhancement factor) has recently become a source of considerable controversy within the glaciological community. Its main proponents (Placidi, Greve and Seddik) defend the thesis that this model can describe the effect of induced anisotropy on ice-sheet flow, while others assert that the CAFFE model is merely an isotropic model. Here I resolve this dispute by rigorously deriving the symmetry group of the CAFFE model.

INTRODUCTION

Recently, a new model of anisotropic ice-sheet flow has generated considerable debate among theoretical glaciologists. (This debate became evident during the 2nd International Workshop on Physics of Ice Core Records (PICR-2), 2–6 February 2007, convened by T. Hondoh in Sapporo, Japan, and during the European Science Foundation Exploratory Workshop on Modelling and Interpretation of Ice Microstructures (ESF–MIIM), 9–11 April 2008, convened by P.D. Bons, S.H. Faria and S. Kipfstuhl in Göttingen, Germany.) It is called the 'CAFFE model' (Placidi and Hutter, 2005; Seddik and others, 2008; Greve and others, in press), where the acronym CAFFE stands for Continuum-mechanical Anisotropic Flow model based on an anisotropic Flow Enhancement factor. (The name 'CAFFE model' should not be confused with the similar abbreviation 'CAFE model', which stands for 'Cellular Automaton – Finite Element model', used since the last decade for numerical simulations of polycrystal plasticity (e.g. Das and others, 2004).) The CAFFE model is a peculiar particularization for numerical ice-sheet simulations of the general thermodynamic theory of mixtures with continuous diversity (Faria, 2001; Faria and Hutter, 2002) applied to the creep of large polycrystalline ice masses (Faria and others, 2003, 2006; Placidi and others, 2004; Faria, 2006a,b; Placidi and Hutter, 2006).

The source of the controversy lies in the fundamental equation of the CAFFE model, which appears as a slight modification of the classical Glen's flow law:

$$\boldsymbol{D} = E(S)\,A(T)\,\sigma_{\mathrm{e}}^{n-1}\,\boldsymbol{t}^{\mathrm{D}}, \tag{1}$$

where $\boldsymbol{D}$ is the strain-rate tensor, $\boldsymbol{t}^{\mathrm{D}}$ is the deviatoric part of the Cauchy stress tensor, $\sigma_{\mathrm{e}} = \sqrt{\frac{1}{2}\mathrm{Tr}(\boldsymbol{t}^{\mathrm{D}})^2}$ is the effective stress invariant, n is the power-law exponent, T is the temperature, $A(T)$ is a temperature-dependent rate factor, and $E(S)$ plays the role of a flow enhancement factor, with S denoting the so-called 'deformability' of the polycrystal. From a continuum-mechanical point of view, S can be regarded as an internal variable used to describe the effect of crystallographic texture (also called 'fabric' by glaciologists). In particular, when the material is isotropic, it follows by definition that $S = 1$ and $E(1) = 1$ (Seddik and others, 2008; Greve and others, in press), in such a way that Equation (1) reduces to the classical version of Glen's flow law proposed by Nye (1953). Thus, the creators of the CAFFE model (Placidi, Greve and Seddik) claim that Equation (1) is an anisotropic flow law, while others assert that it is an isotropic constitutive function that cannot model anisotropy.

There is no doubt that the anisotropy of Equation (1), if it exists, must be contained in the enhancement factor, E. Therefore, all that is needed to conclude the debate is to determine whether the enhancement factor, E, is an anisotropic constitutive function or not.

ON ANISOTROPIC FUNCTIONS

Succinctly, in continuum physics (cf. Truesdell and Noll, 1965; Hutter, 1983; Nye, 1985; Liu, 2002, and references therein) a material is said to be isotropic in a given reference configuration if its response is invariant with respect to any orthogonal transformation (viz. rotation, reflection or inversion) of the body, otherwise it is called anisotropic. (When defining isotropy, some authors consider only rotations (i.e. proper orthogonal transformations), since only these are usually feasible in practice. However, this approach would be unsuitable, for example, for optically active materials (hemitropic media) and is therefore not adopted here. As remarked by Nye (1985): 'if we are to link physics to the mathematical theory of symmetry it is difficult to avoid the use of such unperformable operations'.) The set of transformations that render the material response invariant is called the 'symmetry group' of the material in the given configuration.

Simple applications of this fundamental notion may, at first sight, give the impression that any anisotropic constitutive function must be defined as a vector- or tensor-valued function possessing tensorial transport coefficients. These tensors (of compliance, viscosity, conductivity, etc.) provide distinct scalar coefficients for different directions, known as 'directional properties'. Based on these simple concepts it becomes hopeless to conceive any anisotropic effect in the enhancement factor, $E(S)$, since it is a scalar function of a single scalar variable and consequently does not allow the introduction of directional properties. Thus, from this point of view the opposers of the CAFFE model seem to be correct.

It should be remarked, however, that scalar-valued anisotropic functions do exist (cf. Spencer, 1971; Boehler, 1975; Liu, 1982; Xiao, 1996). In constitutive theory such functions are often constructed with the help of certain vectors and tensors that define particular directions, lines and planes of symmetry in the material. Evidently, not all material anisotropies can be described in this manner, but many of them

[*]To the memory of Prof. Tony Spencer, FRS.

can be, including the most common symmetries (e.g. transverse isotropy, orthotropy) and several crystal classes. For such materials, we propose the following:

Theorem 1 (e.g. Liu, 2002) *Let*

$$\mathcal{G} = \left\{ \boldsymbol{H} \in \mathcal{H}, \; \boldsymbol{H}\boldsymbol{n}_\alpha = \boldsymbol{n}_\alpha, \; \boldsymbol{H}\boldsymbol{M}_\beta\boldsymbol{H}^{\mathsf{T}} = \boldsymbol{M}_\beta \right\} \quad (2)$$

be the symmetry group of a certain anisotropic material. The set, $\mathcal{H}$, denotes an appropriate group of transformations, while the matrix, $\boldsymbol{H}$, stands for a transformation that preserves the directions, lines and planes of material symmetry defined by the directors, $\boldsymbol{n}_\alpha$ (with $\alpha = 1, 2, \ldots$), and the tensors, $\boldsymbol{M}_\beta$ (with $\beta = 1, 2, \ldots$). Let $\hat{F}(\boldsymbol{X})$ be a scalar function of the tensor variable $\boldsymbol{X}$. Thus, $\hat{F}(\boldsymbol{X})$ is invariant relative to $\mathcal{G}$ – and is therefore called an anisotropic scalar function – if and only if it can be represented by

$$\hat{F}(\boldsymbol{X}) = \tilde{F}(\boldsymbol{X}, \boldsymbol{n}_\alpha, \boldsymbol{M}_\beta) , \quad (3)$$

where $\tilde{F}(\boldsymbol{X}, \boldsymbol{n}_\alpha, \boldsymbol{M}_\beta)$ is invariant relative to $\mathcal{H}$.

In usual cases, which include creeping polycrystalline media like natural ice, we may assume $\mathcal{H} = \mathcal{O}$, where $\mathcal{O}$ is the group of all orthogonal transformations. This implies that $\tilde{F}(\boldsymbol{X}, \boldsymbol{n}_\alpha, \boldsymbol{M}_\beta)$ is an *isotropic function* of $\boldsymbol{X}$, $\boldsymbol{n}_\alpha$ and $\boldsymbol{M}_\beta$, since it is invariant relative to $\mathcal{H} = \mathcal{O}$, while $\hat{F}(\boldsymbol{X})$ is an *anisotropic function* of $\boldsymbol{X}$, because it is invariant with respect to $\mathcal{G}$ only. Obviously, in the particular case of an isotropic material with no preferred symmetry directions and planes (i.e. no directors, $\boldsymbol{n}_\alpha$, and no tensors, $\boldsymbol{M}_\beta$), we have simply $\mathcal{G}_{\text{iso}} = \mathcal{H} = \mathcal{O}$.

THE CAFFE SYMMETRY GROUP

We can now try to apply these concepts to the CAFFE equation (1). As already mentioned, all we need to do is analyze the symmetry properties of the enhancement factor function, E. This is rather trivial, since E is, by assumption, a simple polynomial function of the deformability, S (Seddik and others, 2008; Greve and others, in press). Therefore, we conclude immediately that E is an isotropic function of S and consequently the CAFFE equation (1) is indeed an *isotropic constitutive function* of the variables T, $\boldsymbol{t}^{\mathrm{D}}$ and S. These are independent variables determined, respectively, through the balance equation of internal energy (first law of thermodynamics), the balance equation of linear momentum (equation of motion) and the following integral equation (cf. Seddik and others, 2008; Greve and others, in press):

$$S = \int_{\mathcal{S}^2} f^* S^* \mathrm{d}^2 n ,$$

with

$$S^* = \frac{5}{2\sigma_{\mathrm{e}}^2} \left[\boldsymbol{n} \cdot \left(\boldsymbol{t}^{\mathrm{D}} \right)^2 \boldsymbol{n} - \left(\boldsymbol{n} \cdot \boldsymbol{t}^{\mathrm{D}} \boldsymbol{n} \right)^2 \right] . \quad (4)$$

It is through Equation (4) that the notion of a mixture with continuous diversity is introduced. Roughly (for more details see Faria, 2001, 2006a; Faria and others, 2003; Placidi and others, 2004), we visualize the polycrystal as a mixture of lattice orientations, in such a manner that the orientation vector $\boldsymbol{n} \in \mathcal{S}^2$ denotes the normal to a plane of material symmetry (more precisely the basal plane of the ice lattice), with the unit sphere, $\mathcal{S}^2$, describing the space in which this continuous diversity of lattice orientations (more generically called 'species') is defined. Accordingly, $\mathrm{d}^2 n$ denotes an infinitesimal solid angle of $\mathcal{S}^2$, while the orientational mass fraction,

$f^*(\boldsymbol{n}, \boldsymbol{x}, t)$, stands for the fraction of crystalline matter in position $\boldsymbol{x}$ at time t with basal planes normal to $\boldsymbol{n}$. (In materials science (e.g. Kumar and Dawson, 1996; Raabe and Roters, 2004) the orientational mass fraction, $f^*(\boldsymbol{n}, \boldsymbol{x}, t)$, would be called 'orientational distribution function' (ODF). I refrain from using this name here because glaciologists frequently use it with a different connotation (for historical reasons), as the *relative number* (instead of the mass fraction) of grains with a given lattice orientation.) Thus, the integral in Equation (4) represents a weighted average of the function S^* over all species of the mixture, i.e. over all orientations.

We can now identify the source of polemic about the anisotropy of the CAFFE model: the internal variable, S, makes Equation (1) seem very simple, but it does not provide any clue about the symmetry of the material, because all the information about material symmetry is hidden within the integral of Equation (4). Luckily, it is straightforward to overcome this problem because the integrand of Equation (4) is such that the integral can be solved directly. Solving Equation (4) is straightforward: we need first notice that neither σ_{e} nor $\boldsymbol{t}^{\mathrm{D}}$ are dependent on $\boldsymbol{n}$.

Thus, after introducing the orientation tensors

$$\begin{aligned} A_{ij} &= \int_{\mathcal{S}^2} f^* \, n_i n_j \, \mathrm{d}^2 n , \\ B_{ijkl} &= \int_{\mathcal{S}^2} f^* \, n_i n_j n_k n_l \, \mathrm{d}^2 n , \end{aligned} \quad (5)$$

we can immediately integrate Equation (4), obtaining

$$S = \frac{5}{2\sigma_{\mathrm{e}}^2} \, t_{ij}^{\mathrm{D}} \, t_{kl}^{\mathrm{D}} \left(\delta_{ik} A_{jl} - B_{ijkl} \right) . \quad (6)$$

The orientation tensors, Equation (5), are closely related to the moments of the distribution, f^*. Strictly, the moments of f^* are the irreducible versions of Equation (5), i.e. the traceless parts of A_{ij} and B_{ijkl} (see, for example, Ehrentraut and Muschik, 1998). These tensors can be called by a variety of names, such as structure or alignment tensors.

Thus, we may use Equation (6) to perform a change of variables $S \to \{\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B}\}$ such that

$$E(S) = \tilde{E}(\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B}) . \quad (7)$$

With this change of variables we can now derive the new form of the CAFFE equation (1):

$$\boldsymbol{D} = \tilde{E}(\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B}) \, A(T) \, \sigma_{\mathrm{e}}^{n-1} \, \boldsymbol{t}^{\mathrm{D}} , \quad (8)$$

where $\tilde{E}(\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B})$ is the enhancement factor as a function of the deviatoric stress, $\boldsymbol{t}^{\mathrm{D}}$, and the orientation tensors, $\boldsymbol{A}$ and $\boldsymbol{B}$, defined in Equation (5).

Equation (8) is the desired anisotropic representation of the CAFFE model. Indeed, from Theorem 1 we recognize that there exists an anisotropic scalar function of the deviatoric stress, $\hat{E}(\boldsymbol{t}^{\mathrm{D}})$, such that (cf. Equation (3))

$$\hat{E}(\boldsymbol{t}^{\mathrm{D}}) = \tilde{E}(\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B}) , \quad (9)$$

where $\tilde{E}$ is an isotropic function of $\boldsymbol{t}^{\mathrm{D}}$, $\boldsymbol{A}$ and $\boldsymbol{B}$.

At last, using Theorem 1 we can finally derive the symmetry group of the CAFFE model (cf. Equation (2))

$$\begin{aligned} \mathcal{G}_{\text{CAFFE}} = \{ \, \boldsymbol{H} \in \mathcal{O}, \\ H_{ij} A_{jk} H_{lk} = A_{il} \, , \, H_{ij} H_{lk} B_{jkrs} H_{pr} H_{qs} = B_{ilpq} \} , \end{aligned} \quad (10)$$

from which we readily recognize that $\tilde{E}(\boldsymbol{t}^{\mathrm{D}}, \boldsymbol{A}, \boldsymbol{B})$ is invariant relative to $\mathcal{O}$, while $\hat{E}(\boldsymbol{t}^{\mathrm{D}})$ is invariant with respect to $\mathcal{G}_{\text{CAFFE}}$ only.

FINAL REMARKS

It should be emphasized that Equation (8) is *not* an approximation of Equation (1). It is the *exact result* of a suitable change of variables. Likewise, Equation (10) is a complete and rigorous description of the anisotropy of the CAFFE model valid in all possible situations, that is, for any crystallographic texture ('fabric'). Evidently, the symmetry of the crystallographic texture is, in general, not precisely described by the CAFFE symmetry group, Equation (10), which simply reflects the fact that the CAFFE model has its limitations (or, more precisely, the integral in Equation (4) filters out any symmetry element of the crystallographic texture that is not included in Equation (10).) These are, however, not severe limitations in the case of ice-sheet modelling, since most natural crystallographic textures ('fabrics') observed in ice-core samples possess symmetries that are reasonably compatible with Equation (10).

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