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MODELLING OF STRAIN HISTORIES FOR MEMORY INTEGRAL FLUIDS IN STEADY AXISYMMETRIC FLOWS

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Summary

A path line tracking procedure is derived which determines the strain history of infinitesimal material elements in steady axisymmetric flow. Path line tracking requires a *pointwise* knowledge of the kinematics as it is gained in numerical calculations (or may be available from measurements). Tabulated values of density as a function of position are also required. Path line tracking then interpolates spatial positions along path lines at residence times $(t-t')$, magnitude of velocity, velocity gradient normal to the path line, and slope of path line at time t. This knowledge is then condensed into the time dependent Finger strain components $C^{-1}(t',t)$ for a given material element in steady axisymmetric flow.

The tracking is applicable to compressible flows of arbitrarily large strains, since the strain history C^{-1} is determined for a material point (infinitesimal material element).

Path line tracking avoinds differentials in space, except when determining the shear strain and when interpolating between the given point values of velocity. The method is tested in a specific example (planar stagnation flow) and it is applied to modelling of processing flows.

1. Introduction

Strain histories determine the stress in polymeric material elements, the laminar mixing, and the development of molecular orientation. Process modelling therefore involves methods of determining strain histories of material elements. The integration along path lines gives detailed insight on the various contributions of the strain history at consecutive states of the process. The processing history can then be tailored to specific rheological properties or to specific physical properties of the material after processing.

The strain history between some time t' in the past and the current time t is described by a relative strain measure, such as the Finger strain tensor $C^{-1}(t',t)$ or the left Cauchy-Green strain tensor $C(t',t)$. Any other strain measures can be calculated from C. Other strain measures are therefore included in the following arguments, even if they are not mentioned further. The determination of a strain history has been called tracking since it requires to follow the upstream path of individual material elements.

Path line tracking is complicated in a three-dimensional flow. However, it simplifies considerably for steady axisymmetric flow (without circumferential velocity component). This is a class of flows which is common to many shaping operations in polymer processing. Examples are pipe extrusion, film blowing, blow molding, and sheet extrusion. This justifies the derivation of a special tracking procedure for steady axisymmetric flow including the limiting case of planar flow.

Several research groups have developed tracking techniques for studying highly elastic fluids in axisymmetric or planar flows: Court, Davies and Walters [1] calculated the strain history of material elements in two-dimensional flow. The strain tensor components were determined from spatial derivatives of the positions of material elements with respect to their preceding positions. The differentials were evaluated using a finite difference scheme of Lax-Wendroff as given by Mitchell and Griffiths [2].

Viriyayuthakorn and Caswell [3] developed a tracking technique to study axisymmetric die entry flow of memory integral fluids. Finger strain components were calculated from the displacement vector of the material element and the resulting spatial deformation gradient. Computational difficulties and methods of improvement were discussed in detail.

Bernstein and Malkus [4] developed a method to construct stream lines in a given velocity field. Transient times of a particle between two points along a stream line are calculated by means of a so-called drift function.

There are two major methods of determining the components of the Finger strain tensor and the Cauchy Green tensor: The strain of a material element is completely defined by the change of three independent material vectors e_i [5]. The material vectors are deforming affinely with the material. At time t, they are chosen to form an orthonormal system (unit length, right angles). At preceding times t', the three material vectors $e_i(t',t)$ were stretched and tilted according to the strain of the material in the flow between t' and t. Change in length and change in angle are given by the strain tensor components (left Cauchy-Green tensor)

$$(C(t',t))_{i,j} = e_i(t',t) \cdot e_j(t',t), \tag{1}$$

which easily is inverted to get C^{-1}. The components refer to the orthonormal system $e_i(t,t)$. The strain is calculated at material points, i.e. the material vectors e_i mark a material element which is small enough to make strain gradients have no influence on the components of C.

The strain tensor components can alternatively be determined by differentiating the spatial coordinates $r(t)$ of a material point at time t with respect to their previous spatial coordinates $r'(t',r)$ at an arbitrary past time t'. Bird, Armstrong and Hassager [6] list the components in different coordinate systems. The method is advantangeous in cases in which the path lines r' are known as explicit functions in end position, r. The method, however, is inconvenient for numerical calculations in which the displacements along path lines (or the velocity) are given as tables of discrete values. Other approaches have to be found which avoid the differentiation with respect to the spatial position. Such a path line tracking method will be developed in this study.

2. *Path line tracking*

The starting point of this tracking procedure is a *given velocity field* of steady axisymmetric flow $v(z,r)$. The circumferential velocity component is taken to be zero. The velocity field might be known from measurements or it might be an approximate velocity field in successive numerical iteration. Path lines, $r(z)$, are equal to the stream lines ($\psi = \text{const.}$). They are given in implicit form

$$\int_{r_i}^{r(z)} \rho v_z r \, \mathrm{d}r = \psi \int_{r_i}^{r_a} \rho v_z r \, \mathrm{d}r = \text{const.}, \tag{2}$$

where r_i and r_a are the inner and the outer bounds of the flow and (z,r,θ) is the global coordinate system. The residence time on the path line

$$t - t' = \int_{z'}^{z} \frac{\mathrm{d}z}{v_z} = \int_{z'}^{z} \sqrt{1+\tan^2\alpha} \, \frac{\mathrm{d}z}{|v|} \tag{3}$$

depends on the axial displacement from z' to z. The slope of the path line

$$\tan\alpha = v_r / v_z \tag{4}$$

depends on the local velocity components.

The strain is best described by an observer which translates and rotates with material elements, when they move along their path lines. Therefore, an orthonormal coordinate frame x_i is chosen locally at each position along the

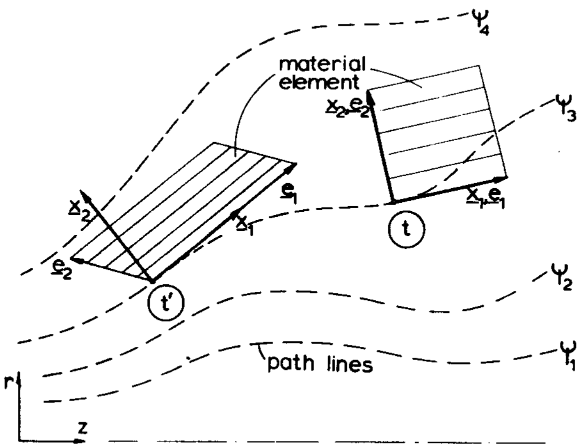


Fig. 1. Deforming material element in steady axisymmetric flow (infinitesimal element, drawn out of proportion). The material vectors $e_i(t', t)$ are defined in a cotranslating and corotating frame x_i.

path line, see Fig. 1: x_1 in flow direction (tangent to the path line), x_2 normal to an axisymmetric stream surface, and x_3 in the stream surface normal to x_1 and x_2. By definition of the path line, the velocity has the components

$$(\boldsymbol{v})_{\mathrm{p}} = (|v|, 0, 0). \tag{5}$$

The subscript p (for local) is a reminder that the components are written in the local frame on the path line.

The shear rate

$$\dot{\gamma}_{12} = \partial v_1/\partial x_2 + \partial v_2/\partial x_1 \tag{6}$$

is equal to the velocity gradient normal to the path line.

The strain tensor components in the local frame are calculated from eqn. (1). A material element is marked by three material vectors $e_i(t', t)$, see Fig. 1. One material vector is chosen to be tangent to the path line at time t and therefore remains tangent during the entire flow (by definition of path lines in steady flow). It might be worth mentioning that this is the only part of the derivation which requires the flow to be steady. In an unsteady flow, the material vector e_1 would not remain tangent to the path line.

Before defining the second material vector, it is easier to define the third one, $e_3(t', t)$. It is always directed in θ-direction of the global coordinate system of the axisymmetric flow. Vectors e_1 and e_3 are normal during the entire flow (since there is no shear in the 1–3 plane), but they change their lengths. The second material vector, $e_2(t', t)$ is normal to e_3, but it changes its angle with respect to e_1 due to shearing strains in the flow. The three material vectors are shown in Fig. 2. The components of the material vectors are

$$(e_1(t',t))_p = (L_1^{-1},0,0),$$
$$(e_2(t',t))_p = (\gamma L_2^{-1}, L_2^{-1},0),$$
$$(e_3(t',t))_p = (0,0,L_3^{-1}). \tag{7}$$

At time t, the vectors e_i become orthonormal, i.e. the material element becomes a unit cube.

Scalar multiplication of the material vectors, eqn. (1), gives the Cauchy-Green tensor

$$(C(t',t))_p = \begin{pmatrix} L_1^{-2} & \gamma L_1^{-1}L_2^{-1} & 0 \\ \gamma L_1^{-1}L_2^{-1} & (1+\gamma^2)L_2^{-2} & 0 \\ 0 & 0 & L_3^{-2} \end{pmatrix} \tag{8}$$

and its inverse, the Finger strain tensor

$$(C^{-1}(t',t))_p = \begin{pmatrix} (1+\gamma^2)L_1^2 & -\gamma L_1 L_2 & 0 \\ -\gamma L_1 L_2 & L_2^2 & 0 \\ 0 & 0 & L_3^2 \end{pmatrix}. \tag{9}$$

The shear γ and the change of length in the three directions, L_i, depend on the kinematics along path lines. The stretches L_i are specifically determined from the local values of velocity, radial position, and density.

The stretch in path line direction, L_1, changes the cross section, A, of a stream tube around the path line, see Fig. 3. The mass flow rate is constant in the stream tube

$$\rho(t')v_1(t')A(t') = \rho(t)v_1(t)A(t). \tag{10}$$

A mass element along the tube changes its length l_1 during the motion from t' to t:

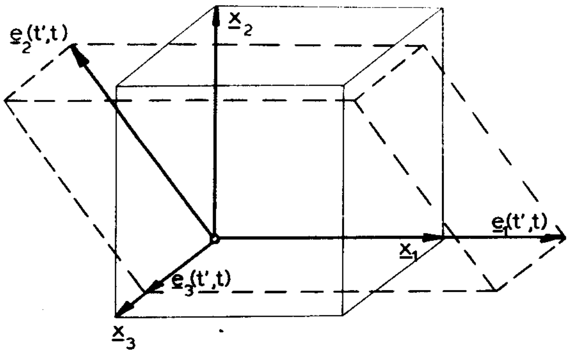
$$\rho(t')l_1(t')A(t') = \rho(t)l_1(t)A(t). \tag{11}$$

Combination of the two equations gives the stretch of a length in 1-direction

$$L_1(t',t) = \frac{l_1(t)}{l_1(t')} = \frac{v_1(t)}{v_1(t')}. \tag{12}$$

The material element in Fig. 1 is part of a ring-shaped element around the axis of the axisymmetric flow. A change in radial position is therefore associated with a change in circumference and hence with a stretch of a length in 3-direction:

$$L_3(t',t) = r(t)/r(t'). \tag{13}$$



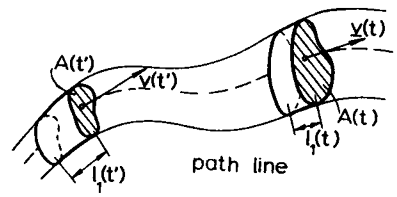


Fig. 2. Strain of infinitesimal material element between t' and t (using $L_1 = 0.65$, $L_2 = 1.35$; $L_3 = 1.15$, $\gamma = 0.85$).

Fig. 3. Path line and stream tube of infinitesimal cross section $A(t)$. Change of length of incremental material element during flow between t' and t.

Planar flow requires $L_3(t', t) = 1$ during the entire strain history. The mass of the material element is conserved between t' and t. The change of separation of a neighbouring stream surface becomes

$$L_2(t', t) = \frac{\rho(t')}{\rho(t) L_1 L_3}. \tag{14}$$

The tangent of the shear angle, $\gamma(t', t)$, is the fourth quantity to be known for a complete description of the strain between t' and t. We may temporarily call the components of the second material vector $(a(t'), b(t'), 0)$. Then the tangent of the shear angle is defined as

$$\gamma(t', t) = a(t')/b(t'). \tag{15}$$

We consider an intermediate state t'', with $t' < t'' < t$. During the short time interval $\mathrm{d}t''$, an infinitesimal displacement

$$\mathrm{d}a'' = \dot{\gamma}_{12}(t'') b(t'')\, \mathrm{d}t'' \tag{16}$$

is imposed on the endpoint of material vector $\boldsymbol{e}_2(t'')$. This displacement in 1-direction is stretched between state t'' and state t', according to the stretch of material vector $\boldsymbol{e}_1(t')$:

$$\begin{aligned} \mathrm{d}a' &= \mathrm{d}a'' \frac{e_1(t')}{e_1(t'')} \\ &= \dot{\gamma}_{12}(t'') b(t'') \frac{L_1(t'', t)}{L_1(t', t)}. \end{aligned} \tag{17}$$

The total displacement in 1-direction integrates to

$$a(t') = \frac{1}{L_1(t',t)} \int_t^{t'} \dot{\gamma}_{12}(t'') b(t'') L_1(t'',t) \, \mathrm{d}t''. \tag{18}$$

Recall that $b(t'') = 1/L_2(t'',t)$. The tangent of the shear angle, eqn. (15), is therefore calculated as

$$\gamma(t',t) = -\frac{L_2(t',t)}{L_1(t',t)} \int_{t'}^{t} \frac{L_1(t'',t)}{L_2(t'',t)} \dot{\gamma}_{12}(t'') \, \mathrm{d}t''. \tag{19}$$

It is an interesting result that the shear $\gamma(t',t)$ not only depends on the shear rate $\dot{\gamma}_{12}$ but also on the stretches between t' and t.

It has to be noted, that the components of the strain tensor are calculated in a coordinate system which is tilted by angle

$$\alpha = \tan^{-1}(v_r/v_z) \tag{20}$$

with respect of the axis of the flow, taken at the position on the stream line which corresponds to time t.

3. Example of the tracking procedure

The tracking procedure can be demonstrated in a flow with *curved path lines* and with *known* Finger strain components. A convenient example of such a flow is planar stagnation flow with uniform rate of deformation and constant density, see for instance ref. [7]. The velocity components in a principal coordinate system (x,y,z) are given as

$$(\boldsymbol{v}) = (\dot{\epsilon}x, -\dot{\epsilon}y, 0) \tag{21}$$

with a uniform extension rate $\dot{\epsilon}$. The Finger strain components in the principal coordinate system (x,y,z)

$$(\boldsymbol{C}^{-1}) = \begin{bmatrix} (x/x')^2 & 0 & 0 \\ 0 & (x'/x)^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{22}$$

describe the strain of a material element which moves from x' to x along the path line $xy = B$ (see left side of Fig. 4). For testing the tracking procedure the same Finger strain components are calculated by choosing a material element with a material vector $\boldsymbol{e}_1(t')$ which is tangent to the path line (see right side of Fig. 4). The curved path lines follow

$$xy = B = \text{const.}, \tag{23}$$

and the normal vector has the components

$$(\boldsymbol{n}) = \frac{(y,x,0)}{\sqrt{x^2+y^2}}. \tag{24}$$

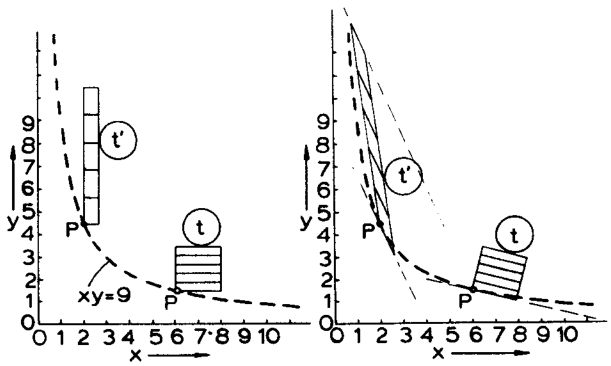


Fig. 4. Infinitesimal material element in plane stagnation flow, eqn. (18); strain between $x(t')$ and $x(t)$ (using $xy=9, x(t')=2, x(t)=6$). The material element on the left hand side has edges parellel to x and y. The material element on the right hand side has one edge tangent to the path line $xy=B$. The path line tracking procedure is tested by showing that the Finger strain $C(t',t)$ is independent of the choice of material element.

The shear rate in the local coordinates (x_1, x_2, x_3) becomes

$$\dot{\gamma}_{12} = \frac{4xy\,\dot{\varepsilon}}{x^2+y^2}. \tag{25}$$

The shear and the stretches between positions x' and x on a path line are calculated from equations (12), (13), (14), (19):

$$\gamma = \frac{B}{x'^2}\left\{\frac{x'^4/B^2 - x^4/B^2}{x^4/B^2+1}\right\}, \tag{26}$$

$$L_1 = \frac{x}{x'}\sqrt{\frac{1+(B/x^2)^2}{1+(B/x'^2)^2}}, \tag{27}$$

$$L_2 = L_1^{-1}, \tag{28}$$

$$L_3 = 1. \tag{29}$$

Finger strain components in the tilted frame in the Fig. 4, right side, are determined by introducing γ, L_1, L_2, L_3 into eqn. (9). Rotation of the coordinate system gives the components of eqn. (22), i.e. the tracking method passes this test application. The rotation tensor between the local coordinate frame (x_1, x_2, x_3) and the global frame is

$$(Q) = \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{30}$$

with $\cos\alpha = (1 + B^2/x^4)^{-1/2}$.

4. Application to processing flows

The path line tracking is a first step to the study of strain histories of individual material elements in processing flows. The strain tensor components are needed to evaluate memory integrals of the stress and of the distribution function. Typical memory integral equations for the stress are the rubberlike liquid equation of Lodge [5] and its modifications. Recent molecular theories by Doi and Edwards [8] and by Curtiss and Bird [9] give the distribution function of macromolecular materials as a memory integral of the strain.

Modelling studies most commonly prescribe the kinematics in some simplified way. The two-dimensional flow field is made one-dimensional by choosing a representative stream line or by averaging over the cross section. Examples for representive stream lines are the center line in injection molding [10,11] and the center line in the spinning process [12]. An average strain history was used for modelling the spinning process [13] and the film blowing process [14]. A distribution of strain histories has been studied by assuming shear flow in an injection mold [11,15] and by superimposing shear and extension in axisymmetric flows [16–18]. These studies, however, are restricted to path lines which are nearly parallel to the flow axis. The current tracking procedure is derived for path lines with arbitrary curvature as long as the flow is steady and axisymmetric (or planar, as a limiting case). Density changes are also permitted.

Path line tracking is currently applied to the modelling of processing flows. The modelling basically consists of three steps.

(a) Approximate determination of the kinematics and the temperatures by means of conventional modelling techniques.

(b) Tracking of material elements along their paths in a processing device. The time dependent strain components are determined from the kinematics (strain history) and the temperature change with time is calculated from the temperatures along the path.

(c) Calculation of the stress for the strain- and temperature-history using a rheological constitutive equation. Molecular orientation can be determined by calculating distribution functions from molecular theory.

Most polymer processing flows are complex in nature. The flows are unsteady from a Lagrangian point of view and/or shear and extension are superimposed onto each other. The kinematics (not the dynamics), of these flows, however, can often be determined approximately by simple calculations. The kinematics of contained flow in channels (for example in extrusion dies) can be *locally modelled by steady shear flow*, i.e. one assumes that the flow in a specific cross-section of a *tapered* flow channel is essentially equal to the velocity field in a *parallel* channel of the same cross section. This assumption is equivalent to the classical "lubrication approximation"

$$\partial\tau/\partial x_2 \gg \partial\tau/\partial x_1, \partial\tau/\partial x_3; \quad p = p(x_1), \tag{31}$$

(with x_1 being the normal to the channel cross section) together with an assumption that the shear stress locally can be determined from the local shear rate and the corresponding shear viscosity. The rheological constitutive equation then simplifies significantly. These are good assumptions for two reasons:

(1) Flow channels in polymer processing are designed such that changes in cross sectional area occur only gradually. Step changes in cross section are avoided.

(2) Any steady flow near a rigid surface (no slip assumed) reduces to shear flow. This can be easily checked using an arbitrary velocity field:

Near a wall of normal x_2, the velocity gradients can be ordered

$$\frac{\partial \boldsymbol{v}}{\partial x_2} \gg \frac{\partial \boldsymbol{v}}{\partial x_1}, \frac{\partial \boldsymbol{v}}{\partial x_3} \tag{32}$$

if the fluid does not slip. Conservation of mass then requires $\partial v_2/\partial x_2 = 0$ near the wall. With these conditions, an arbitrary flow reduces to shear flow. For a detailed analysis of flow near a wall see ref. [19]. The rheological behavior near the wall is completely described by the three visometric functions. Note that if the fluid slips along the wall, extensional components are introduced into the flow and the rheological behavior becomes more complex.

In the next modelling steps (tracking and calculation of stress), the kinematics are taken to be known. Later, one might want to return to these initial calculations and improve the velocity with the calculated stress. This complicated step has not yet been attempted in this approach. Methods for iterative numerical determination of the velocity field are given by Court, Davis, and Walters [1] and Viriyayuthakorn and Caswell [3]. The developing temperatures should be taken from measurements or they may be calculated using established numerical techniques, see for instance ref. [20].

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Notation

A	area, m^2
B	constant, m^2, xy in planar stagnation flow
$C^{-1}(t',t)$	relative Finger strain tensor, $-$,
e_i	material vectors
L_i	stretch of material element in i-direction, $-$,
n	vector normal to path line
r	coordinate, path line $r(z)$
t	time, s
v	velocity, m/s
x_1, x_2, x_3	local coordinate system on path line
z	axial coordinate
α	angle of path line with respect to z
γ	shear
$\dot{\gamma}$	shear rate, s^{-1}
ρ	density, kg m^{-3}
ψ	stram function, $\psi =$ const. is path line in steady flow

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