THERMO-MECHANICAL ANALYSIS OF DEPRESSURIZATION

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SUMMARY

Pressure containing structures and their environment require investigations of phenomena resulting from a variety of hypothetical failure modes. Some of those lead to complex physical processes such as depressurization of subcooled fluids, wave propagation in fluid and solid structures, vaporization of the fluid, two phase flow and dynamic, linear and nonlinear deformation of the surrounding structures. A variational approach in Lagrangian and Eulerian or arbitrary description, used to simulate such kind of physical problems, is outlined.

The functionals representing mechanical and thermal balance are formulated in terms of deformations and temperatures in Lagrangian coordinates. The unknowns are converted to Eulerian coordinates. In Lagrangian formulation, material and geometrical nonlinearities will have an effect only on the matrix terms of the resulting system of equations. The conversion of Lagrangian to Eulerian formulation yields additional nonlinearities affecting matrix terms and unknowns of the resulting system of equations. When the relative velocity of Eulerian coordinates is considered a known parameter rather than a basic unknown, the nonlinear convective terms turn linear.

All material properties for all phases are represented by anisotropic differential material tensors. The formulation is applied to a three-dimensional finite element family which permits a variable number of nodes and Gaussian integration points per edge.

1. Introduction

Pressure containing structures and their environment require investigations of phenomena resulting from a variety of hypothetical failure modes. Some of those were approximately analysed as described in [12]. A rigorous analysis of complex physical processes such as depressurization of subcooled fluids, wave propagation in fluid and solid structures, vaporization of the fluid, two phase flow and dynamic linear and nonlinear deformation of surrounding structures requires a formulation which is capable of describing all three phases - solid, fluid, gaseous - and even phase mixtures.

Two basic sets of equations are commonly used for the description of gas-fluid-structure interaction [2], [4]:

- Equations in Lagrangian description as mainly used in solid mechanics
  - -- mechanical balance (equation of motion)
  - -- thermal balance (thermal energy equation), [7]
- Equations in Eulerian or arbitrary description as mainly used in gas-, fluid- or thermodynamics
  - -- conservation of mass
  - -- conservation of momentum
  - -- conservation of energy

Both sets of equations are equivalent and can be transformed into one another as shown in [7]. One major difference concerns the formulation of boundary conditions and solid-fluid-gas interfaces. The flexibility of both approaches has been improved with respect to boundaries and interfaces by the introduction of convected coordinates and rezoning techniques, [2], [3]. However, the two types of description appear to be almost complementary for certain classes of problems: in simulating processes associated with sudden changes in structural behaviour, Lagrangian formulations appear more useful in the early time range, when adequate resolution of shock phenomena is important, while the Eulerian methods may be more useful for the later times when large motions occur and large mass transport takes place. Here, Lagrange equations are extended to an arbitrary formulation by introduction of convective terms. This leads to an unique formulation for larger times in depressurization analysis. Analogous formulations were used in [5] with respect to thermal convection.

2. Basic Formulation

The presented approach is based on the Lagrangian incremental formulation of balance and constitutive equations. The variational principle is used to derive the mechanical and thermal balance equations, see table 3. These equations are formulated in terms of derformations and temperatures as basic unknowns. Thermal and mechanical balance equations are coupled by virtue of the constitutive relations, see table 1 and 2. Replacing the material derivative by the local derivative and the convective derivatives, table 4 eq. (23), the balance equations (20) and (21) or (18) and (19) are transformed to an arbitrary reference system in which the material points move with a relative velocity v. In this reference system, the matrices eq. (22) become a function of time, even if they are constant in the Lagrangian reference system. With respect to the numerical solution, these matrices may be expanded into Taylor series, see table 4 eq. (25).

In this formulation, the local terms remain linear with respect to the unknowns, see table 4 eq. (24). Furthermore, if the relative velocity v between the Eulerian and the Lagrangian reference system is considered a known parameter rather than a basic unknown, the nonlinear convective terms turn linear with respect to the unknowns, see eq. (24). Equation (24) can therefore be linearized, provided a good estimate for the relative velocity v can be found. Such an estimate can be taken from the preceeding time step or can be calculated by explicit schemes. The gradients of the unknowns in the convective terms can be expressed as a sum of the nodal unknowns of the discrete system, see table 4 eq. (26). By this, equation (24) representing arbitrary formulation, can be reduced to the standard form of eq. (22), which then can be solved by using standard time integration techniques.

Heat conduction, which is part of the thermal equation, leads to a spatial coupling of temperatures and deformations. In many depressurization problems, deformations develop much faster than heat transfer by macroscopic heat conduction. Hence, for short periods of time heat conduction may be neglected. The thermal equations then reduce to local equations and the thermal degrees of freedom become uncoupled.

3. Material Description

All material properties for all phases are represented by differential material tensors [11], see table 1. Nonlinear material behaviour as e.g. strain hardening in plasticity or the nonlinear behaviour of concrete are described by corresponding constitutive equations [6], [8], [9], [10]. The constitutive equation for fluid and gas are outlined in table 2. Energy dissipation, caused for example by viscous or damping effects, can be formulated in a similar way, table 1. Multi-phase mixtures and phase changes can be simulated by definition of geometrically coinciding subregions with source and sink terms.

4. Discretisation and Solution Technique

The formulation is applied to a three-dimensional finite element family which permits a variable number of nodes and Gaussian integration points per edge. Mass, friction and stiffness matrices are consistent. Axisymmetric and plain elements are also available. Corresponding shell elements are compatible with the three-dimensional elements in the deformation degrees of freedom. The lack of compatibility with respect to nodal rotations and temperatures, however, can be eliminated by using three-dimensional elements and subsequent condensation. Phase interfaces as well as Lagrange / Euler interfaces may be modeled by double nodes and multipoint constraints.

The linearized equations are solved by implicit schemes. Different time steps for subregions are envisaged. The relative velocity of arbitrary or Eulerian coordinates is determined by explicit schemes.

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Notation

Symbols

- p = volume force
- σ = stress tensor
- q = thermal energy
- ψ = thermal energy flux
- ρ = mass density
- r = viscosity, damping, friction,...
- h = deformation tensor
- α = thermal to mechanical coupling
- c = energy capacity
- ℓ = thermal conductivity
- β = mechanical to thermal coupling
- u = deflection
- ε = strain tensor
- t = temperature
- θ = temperature gradient
- g = base vector
- p = pressure
- v = specific volume
- t_a = absolute temperature
- $\bar{\varepsilon}$ = volume dilatation
- k = bulk modulus
- s = entropy
- v = relative velocity Euler (arbitrary)-Lagrange
- x = spatial coordinate

Differentiation

- d = differential
- $\frac{\delta}{\delta\tau}$ = local or partial derivative
- $\frac{D}{D\tau}$ = $\cdot$ = material derivative
- $,$ = spatial derivative

Indices

- o = initial value
- z = increase

Matrices

M, R, H, A, C, L, B

Table 1 : general form of constitutive relations and definition of strain, strain velocity and thermal energy flux tensors.

inertia of mass (1)	viscosity damping (2)	deformation (3)	temperature induced stress (4)	external forces (5)
$dp_i = \rho_{ij}\, d\ddot{u}_j$	$d\sigma_{ij} = r_{ijkl}\, d\dot{\varepsilon}_{kl}$ $d\dot{\varepsilon}_{kl} = \frac{1}{2}(g_k d\dot{u}_{,l} + g_l d\dot{u}_{,k} + d\dot{u}_{,k} d\dot{u}_{,l})$	$d\sigma_{ij} = h_{ijkl}\, d\varepsilon_{kl}$ $d\varepsilon_{kl} = \frac{1}{2}(g_k du_{,l} + g_l du_{,k} + du_{,k} du_{,l})$	$d\sigma_{ij} = \alpha_{ij}\, dt$	dp_i
(6)	thermal energy storage (7)	thermal energy conduction (8)	deformation induced thermal energy source (9)	external thermal energy source (10)
	$dq = c\, d\dot{t}$	$d\psi_i = l_{ij}\, d\theta_j$ $d\theta_i = g_i\, dt_{,i}$	$dq = \beta_{kl}\, d\varepsilon_{kl}$	dq

Table 2 : constitutive equations for gas and fluid phase

equation of state

$$p = f_p(v,t_a) \longrightarrow s = f_s(v,t_a) \qquad (11)$$

total differentiation with $dv = v\, d\bar{\varepsilon}$

$$dp = \underbrace{\left(\frac{\delta f_p}{\delta v}\right)_t}_{\bar{k}} v\, d\bar{\varepsilon} + \underbrace{\left(\frac{\delta f_p}{\delta t}\right)_v}_{\alpha} dt \qquad (12)$$

$$dq = t_a d_s \qquad (13)$$

$$dq = \underbrace{t_a \left(\frac{\delta f_s}{\delta v}\right)_t}_{\beta} v\, d\bar{\varepsilon} + \underbrace{t_a \left(\frac{\delta f_s}{\delta t}\right)_v}_{c} dt \qquad (14)$$

change in volume expressed by strain tensor

$$d\bar{\varepsilon} = f_1(\varepsilon)\, d\varepsilon_{11} + f_2(\varepsilon)\, d\varepsilon_{22} + f_3(\varepsilon)\, d\varepsilon_{33} \qquad (15)$$

bulk modulus

$$\bar{k}\,(v) = dp\, /\, d\bar{\varepsilon} \qquad (16)$$

deformation tensor, using (15) and (16)

$$h_{ijkl} = k(v,\varepsilon) \quad \text{for} \quad i = j \quad \text{and} \quad k = l \qquad (17)$$

$$h_{ijkl} = 0 \quad \text{for all other components}$$

similar evaluations lead to α_{ij}, β_{kl}, c

Table 3 : lagrange formulation of mechanical and thermal balance equations using variational principle :

mechanical balance :

$$\begin{matrix} +\int u_z \rho \ddot{u}_z & +\int \varepsilon_z r \dot{\varepsilon}_z & +\tfrac{1}{2}\int \varepsilon_z h \varepsilon_z & +\int \varepsilon_z \alpha t_z & -\int u_z p_z \\ +\int u_z p_0^{\rho} & +\int \varepsilon_z \sigma_0^{r} & +\int \varepsilon_z \sigma_0^{h} & +\int \varepsilon_z \sigma_0^{E} & -\int u_z p_0 \end{matrix} \overset{!}{=} \text{Min} \qquad (18)$$

thermal balance :

$$\begin{matrix} +\int t_z c \dot{t} & +\tfrac{1}{2}\int \tau_z \ell \tau_z & +\int t_z \beta \varepsilon_z & -\int t_z q_z \\ +\int t_z q_0^{c} & +\int \tau_z \psi_0^{\ell} & +\int t_z q_0^{E} & -\int t_z q_0 \end{matrix} \overset{!}{=} \text{Min} \qquad (19)$$

using discretisation techniques, this yields a set of coupled thermal and mechanical equations :

$$\begin{matrix} + M\ddot{u}_z & + R\dot{u}_z & + Hu_z & + At_z & - p_z \\ + p_0^{M} & + p_0^{R} & + p_0^{H} & + p_0^{E} & - p_z \end{matrix} = 0 \qquad (20)$$

$$\begin{matrix} + C\dot{t}_z & + Lt_z & + Bu_z & - q_z \\ + q_0^{C} & + q_0^{L} & + q_0^{E} & - q_0 \end{matrix} = 0 \qquad (21)$$

Table 4 : transformations from Lagrangian to Eulerian formulation

equation (20) and (21) may be represented by

$$M \frac{D^2 u}{D\tau^2} + C \frac{Du}{D\tau} + Ku = s \tag{22}$$

using the definition of material derivative

$$\frac{Du}{D\tau} = \frac{\delta u}{\delta \tau} + \sum_{j=1}^{3} V_j \frac{\delta u}{\delta x_j}$$

$$\frac{D^2 u}{D\tau^2} = \frac{D}{D\tau}\left[\frac{\delta u}{\delta \tau} + \sum_{j=1}^{3} V_j \frac{\delta u}{\delta x_j}\right] \tag{23}$$

in (20) :

$$+ M(\tau) \quad \frac{D}{D\tau}\left[\frac{\delta u}{\delta \tau} + \sum_{j=1}^{3} V_j \frac{\delta u}{\delta x_j}\right]$$

$$+ C(\tau) \quad \left[\frac{\delta u}{\delta \tau} + \sum_{j=1}^{3} V_j \frac{\delta u}{\delta x_j}\right]$$

$$+ K(\tau) \quad u \qquad = s(\tau) \tag{24}$$

the matrices M, C, K and the vector s may be e.g. expanded into Taylor series

$$M(t) = M_o + \frac{DM}{D\tau}\tau + \ldots \text{with } \frac{DM}{D\tau} = \frac{\delta M}{\delta \tau} + \sum_{j=1}^{3} V_j \frac{\delta M}{\delta x_j} \tag{25}$$

spatial derivatives $\delta u / \delta x_j$ may be expressed by a sum of values of u^k in the points of discretisation :

$$\frac{\delta u}{\delta x_j} = \sum_k u^k \tag{26}$$