Identification model for materials described by a mixture model

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1 Introduction

Subject

The development of a numerical/experimental method for the mechanical characterization of materials described by a mixture model.

Reasons

- Traditional methods are usually based on uniform stress- and strain fields, so the design of an experiment (i.e. geometry of the specimen and application of the load) must lead to uniform fields. A method is required which is not restricted to uniform fields, so it is applicable to more materials and leads to more freedom in designing an experiment.
- Due to manufacturing the structure of a specimen is often disrupted so it is no longer representative for the behaviour of the material. A method is required, which can determine material parameters in an 'in vivo' situation.

Method

Starting point is the *identification method* according to Hendriks [3], which is based on confronting experimental data with the outcome of a F.E.M. analysis. This method, which is visualized in figure 1, no longer demands a uniform stress- or strain field. The actual

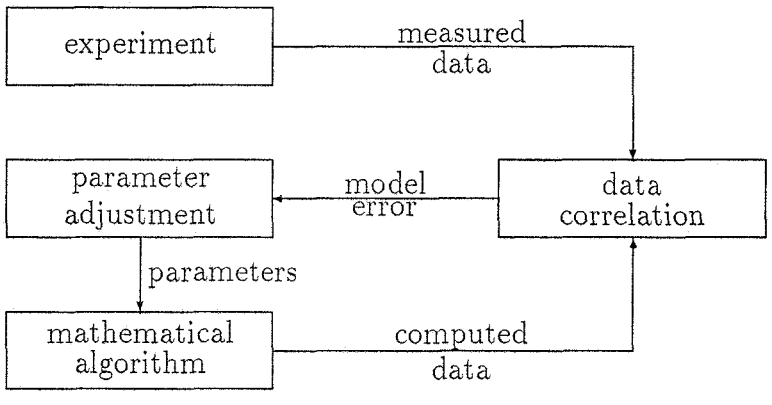

Figure 1: Diagram of the identification method

strain distribution is measured and the model strain distribution is calculated as a function of the values of the parameters. The error in the model is then used for a further adjustment of the parameters.

Remark 1 For the *identification method* a constitutive model is needed which is sufficiently accurate to describe the material under consideration. If an estimation of the variables does not look reliable, it is difficult to detect whether the algorithm failed, or the model was not sufficiently accurate, or the experiment did not contain enough information to determine all the parameters, as Hendriks' method does not distinguish between these separate causes of failure (see also van Ratingen [6]).

Remark 2 With respect to remark 1, actually 3 terms should be distinguished, namely:

material parameter identification : A method to determine material parameters which characterize the material under consideration.

model structure identification : Information, obtained from the identification process, is used to adapt the structure of the model in order to improve the material characterization.

experiment optimization : A method to adapt the experiment if it does not contain enough information to determine all the material parameters.

Object

Reformulation of the parameter estimation problem (making use of know–how from system control and identification), in order to obtain additional information about the accuracy of the constitutive model and/or the value of the experiment out of the identification process.

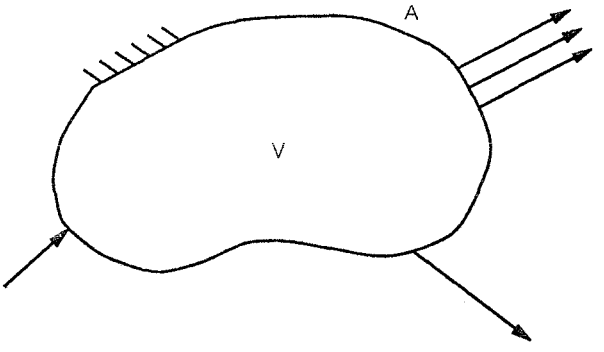

Figure 2: Model of the system

2 Problem definition

In this report the state equations and an identification model will be formulated for materials which are described by a mixture model. Here a 'simple' mixture model is considered, consisting of a purely elastic solid matrix with pores which are filled with fluid. Due to the viscosity of the fluid there will be resistance against flow of the fluid through the matrix. This makes the behavior of the bulk material time dependent, see Oomens [5]. Figure 2 shows schematically a mixture material subjected to dynamic and kinematic boundary conditions. The motion of both the solid and the fluid is governed by the laws of conservation of mass and momentum:

- balance of mass:

$$\vec{\nabla} \cdot \vec{v}^s - \vec{\nabla} \cdot (\mathbf{K} \cdot \vec{\nabla} p) = 0 \tag{1}$$

- balance of momentum:

$$\vec{\nabla} \cdot (\boldsymbol{\sigma}_{eff} - p\,\mathbf{I}) = \vec{0} \tag{2}$$

where $\vec{v}^s$ is the solid velocity, p is the fluid pressure, $\boldsymbol{\sigma}_{eff}$ is the effective Cauchy stress, and $\mathbf{K}$ is the permeability tensor. The first term of the balance of mass represents the change in volume of the solid matrix, and the second term the amount of interstitial fluid which is squeezed out. $\boldsymbol{\sigma}_{eff}$ in the balance of momentum is the stress required to deform the solid matrix (with pores but without the fluid) and $p\,\mathbf{I}$ is the resulting stress beared by the interstitial fluid. In these equations the constitutive models for the fluid as well as for the mechanical interaction between solid and fluid[1] are already substituted. $\mathbf{K}$ depends on material properties. The constitutive model for the solid reads:

[1]The resistance against fluid flow through the matrix is assumed to depend linearly on the velocity of the fluid relative to the solid.

- constitutive model:

$$\boldsymbol{\sigma}_{\mathit{eff}} = \frac{1}{\det(\mathbf{F})}\,\mathbf{F}\cdot\mathbf{S}_{\mathit{eff}}\cdot\mathbf{F}^{c} \tag{3}$$

$$\mathbf{S}_{\mathit{eff}} = \mathbf{G}\{\mathbf{E}(t)\} \tag{4}$$

where $\mathbf{F}$ is the deformation tensor, $\mathbf{E}$ is the strain tensor, $\mathbf{S}_{\mathit{eff}}$ is the second Piola–Kirchhof stress, and $\mathbf{G}$ is a tensorfunction. The following assumptions are made:

- Both components are intrinsically incompressible.
- Inertia forces and external body forces are negligible.
- There is no chemical interaction between the components.

In the remainder of this report no expressions are substituted for the tensors $\mathbf{S}_{\mathit{eff}}$ and $\mathbf{K}$ to allow a more general approach.

The identification method requires an experiment on the system and a numerical analysis of this experiment. A possible experiment will be described in section 3. In section 4 the governing equations for the system will be discretized using the finite element method in preparation of the numerical analysis.

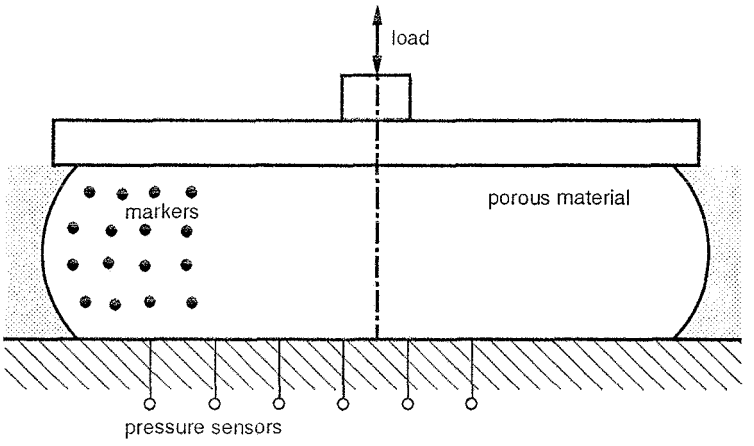

Figure 3: The proposed experiment

3 Proposed experimental set–up

In order to estimate more parameters out of one experiment, an experiment has to be designed which on the one hand contains as much information as possible and on the other hand is relatively simple. Here a bulge experiment is proposed. A circular disk of porous, permeable material, which is immersed in a fluid, is squeezed between two impermeable plates. In the first instance the material is assumed to be described sufficiently accurate by the 'simple' mixture theory. In contrast with a normal unconfined compression experiment where friction between the plates and the porous material is minimized (Armstrong e.a. [1]), in the proposed experiment the porous material is fastened to the plates (figure 3). Therefore the compressive strain in the axial direction will be inhomogeneous, which is believed to afford more information than a homogeneous strain field. The upper plate is subjected to a prescribed load or displacement which may vary in time. To increase the inhomogeneity of the strain field the upper plate may be tilted.

An optical method[2] will be used to measure the displacement of a (large) number of discrete points at the outer surface of the porous disk. At this time optical methods have the disadvantage that it is only possible to measure at the outer surface. Therefore it should be verified if the surface field contains enough information for a sufficient characterization. But in addition to information of the strain field also the fluid pressure in a number of positions inside the porous disk will be measured. All measurements at time t will be stored in a column $m(t)$.

Remark An orienting numerical analysis of the experiment described in this section is one of the issues of near future research.

[2] A number of small markers is attached to the surface of the specimen. The positions of these markers are determined by a video tracking system, see Hendriks [3].

4 Numerical analysis

In this section the governing conservation laws for the mixture are discretized using the finite element method. This discretization makes it possible to reformulate the equations in terms of state, input, and output, which is very common in system control and identification (SC&I). The differential equations are rewritten in an integral form by means of the weighted residual method, introducing weighting functions g and $\vec{h}$:

$$\int_V g \left[\vec{\nabla}\cdot\vec{v^s} - \vec{\nabla}\cdot(\mathbf{K}\cdot\vec{\nabla}p)\right] dV = 0 \tag{5}$$

$$\int_V \vec{h} \cdot \left[\vec{\nabla}\cdot(\boldsymbol{\sigma}_{eff} - p\mathbf{I})\right] dV = 0 \tag{6}$$

In general the momentary volume V is unknown, since V changes in time. Calculations are simplified by transforming the equations to the reference volume V_0 with outer surface A_0. After applying Gauss' theorem the equations 5 and 6 are transformed to:

$$\int_{V_0} g\,\mathbf{F}^{-c}\cdot\vec{\nabla}_0\cdot\vec{v^s}J\,dV_0 + \int_{V_0}\vec{\nabla}_0 p\cdot\mathbf{F}^{-1}\cdot\mathbf{K}\cdot\mathbf{F}^{-c}\cdot\vec{\nabla}_0\,gJ\,dV_0 =$$

$$\int_{A_0} g\underbrace{(\vec{\nabla}_0 p\cdot\mathbf{F}^{-1}\cdot\mathbf{K})\cdot\mathbf{F}^{-c}\cdot J\vec{n}_0}_{q^f} dA_0 \tag{7}$$

$$\int_{V_0}(\vec{\nabla}_0\vec{h})^c : \left[(\mathbf{S}_{eff}\cdot\mathbf{F}^c) - pJ\mathbf{F}^{-1}\right] dV_0 = \int_{A_0}\vec{h}\cdot\underbrace{(\boldsymbol{\sigma}_{eff} - p\mathbf{I})\cdot\mathbf{F}^{-c}\cdot J\vec{n}_0}_{\vec{t}}\,dA_0 \tag{8}$$

where $\vec{n}_0$ is the outward unit normal on A_0. These equations, which are valid for each point of the continuum, are non–linear in the deformation. To solve them numerically, the equations are discretized. The mixture volume is divided in sub–volumes of a simple shape: the elements. In every element a limited number of discrete points are chosen: the nodal points. The displacement $\vec{u}$ of a material point within an element is expressed as a linear combination of the displacementvectors of the nodal points:

$$\vec{u}(t) \approx \psi^I(\gamma)\vec{u}^I(t) = \psi^I(\gamma)u_i{}^I(t)\vec{e}_i \qquad \begin{array}{rcl} I &=& 1,\ldots,N_k \\ i &=& 1,2,3 \end{array} \tag{9}$$

where ψ^I is a displacement approximation function for node I, γ is the column of material coordinates, $\vec{u}^I$ is the displacement vector of node I, $(\vec{e}_1,\vec{e}_2,\vec{e}_3)$ are the base vectors of the coordinate system, and N_k is the total number of displacement nodes. In a similar way the pressure field is approximated:

$$p(t) \approx \phi^J(\gamma)p^J(t) \qquad J = 1,\ldots,N_p \tag{10}$$

where ϕ^J is a pressure approximation function for node J, p^J is the pressure in node J, and N_p is the total number of pressure nodes. The approximation functions ψ^I and ϕ^I depend on the material coordinates and are chosen in such a way that:

$$\psi^I(\gamma^K) = \delta^{IK} \qquad ; \qquad \phi^I(\gamma^K) = \delta^{IK} \tag{11}$$

where δ^{IK} is the Kronecker–function. Following the strategy given by Galerkin the weighting functions $\vec{h}$ and g are chosen to be equal to the displacement- and pressure approximation functions respectively:

$$\vec{h} = \psi^I(\gamma)\vec{e}_i \qquad ; \qquad g = \phi^I \tag{12}$$

Substitution of the discrete forms and the weighting functions into the equations 7 and 8 gives, after some rearranging:

$$R(u)\,\dot{u} + K(u,\theta)\,p = Q(u,p,\theta) \tag{13}$$
$$S(u,\theta)\,u - R^{\mathrm{T}}(u)\,p = F(u,p,\theta) \tag{14}$$

where u is the column of node–displacements, p is the column of node–pressures, and θ is the column of material parameters. For further explanation of the matrices see the appendix. Equation 13 is a system of as many equations as the number of pressure nodes, representing the balance of mass. Equation 14 is a system of as many equations as the number of displacement degrees of freedom (DOF), representing the balance of momentum.

The number of discretized equations is equal to the total number of DOF. Since the system is subjected to boundary conditions, a number of DOF will be prescribed, which reduces the number of equations. The resulting system will be rewritten by storing known DOF in a column with index k and unknown variables in a column with index l:

$$u^{\mathrm{T}} = [\, q_l{}^{\mathrm{T}}\ q_k{}^{\mathrm{T}} \,]^{\mathrm{T}} \qquad ; \qquad p^{\mathrm{T}} = [\, p_l{}^{\mathrm{T}}\ p_k{}^{\mathrm{T}} \,]^{\mathrm{T}} \tag{15}$$

The following system of equations results (where the subscript and the superscript * denote a partition of the equally named original matrix):

$$\Longrightarrow \quad R_{ql}\,\dot{q}_l + R_{qk}\,\dot{q}_k + K_{pl}\,p_l + K_{pk}\,p_k = Q^* \tag{16}$$
$$S_{ql}\,q_l + S_{qk}\,q_k - R_{ql}{}^{\mathrm{T}}\,p_l - R_{pk}\,p_k = F^* \tag{17}$$

5 Reformulation in terms of system control

To make use of available parameter estimation techniques an appropriate mathematical model is required. The discretized balance equations 16 and 17 are therefore rewritten in a form which is common in system control:

- balance of mass:

$$A_1(q_l, t)\,\dot{q}_l + f_1(q_l, p_l, \theta, t) = 0 \tag{18}$$

- balance of momentum:

$$f_2(q_l, p_l, \theta, t) = 0 \tag{19}$$

where $A_1 \equiv R_{ql}$, f_1 contains the remaining terms of the balance of mass and f_2 represents the complete balance of momentum. In these equations the prescribed boundary conditions, which are explicit functions of time, are substituted:

$$q_k = q_k(t) \qquad ; \qquad p_k = p_k(t) \tag{20}$$

In order to estimate parameters two more equations are needed, namely an output equation and a parameter equation. The output equation determines by means of interpolation of the calculated node- positions and pressures the expected measurement data:

- output equation

$$y = g(q_l, p_l, \theta, t) \tag{21}$$

Parameters in the model are adapted on the basis of the difference between the expected measurements and the actual measurement values. The parameter equation indicates that material parameters are constant in principle:

- parameter equation

$$\dot{\theta} = 0 \tag{22}$$

The value of this equation will become evident if estimates of the parameters are considered.

Suppose it is possible to calculate estimates $\hat{q}_l$, $\hat{p}_l$ and $\hat{\theta}$. In general the model equations will not be satisfied exactly in that case. An identification model is introduced in order to find estimates which satisfy the equations as far as possible, see van de Molengraft [4]:

$$\xi_1(t) = A_1(\hat{q}_l, t)\,\dot{\hat{q}}_l + f_1(\hat{q}_l, \hat{p}_l, \hat{\theta}, t) \tag{23}$$

$$\xi_2(t) = f_2(\hat{q}_l, \hat{p}_l, \hat{\theta}, t) \tag{24}$$

$$\xi_3(t) = \dot{\hat{\theta}} \tag{25}$$

$$\zeta(t) = m(t) - g(\hat{q}_l, \hat{p}_l, \hat{\theta}, t) \tag{26}$$

where $\xi_i(t)$ and $\zeta(t)$ are residuals. The residual $\zeta(t)$ is the difference between the actual measurement data and the model predicted measurement data. The aim is to find estimates for which a functional of the residuals, like

$$J = \tfrac{1}{2} \int_{t_o}^{t_e} \{ \sum_i \xi_i^{\mathrm{T}} W_i \xi_i + \zeta^{\mathrm{T}} V \zeta \} \, d\tau \tag{27}$$

is minimized, where V_i and W are weighting matrices.

Although it is unusual in continuum mechanics, a residual has been allowed on the parameter equation 25. In other words, it is made possible that the estimation procedure finds an estimate $\hat{\theta}_{n+1}$ at time t_{n+1} which slightly deviates from the estimate $\hat{\theta}_n$ at time t_n. When the residual on the parameter equation is not heavily weighted, the parameter estimate as a function of time may strongly vary as a result of model errors (e.g. the assumption that parameters are constant will in general not be correct). In this way information is gained about the accuracy of the model or about the region in which the model and thus the estimated parameters are valid.

Minimizing J is equivalent to minimizing an alternative functional J_2 defined by:

$$\begin{aligned} J_2 = \int_{t_o}^{t_e} \{ & \tfrac{1}{2} \hat{f}_2^{\mathrm{T}} W_2 \hat{f}_2 + \tfrac{1}{2} [m(t) - \hat{g}]^{\mathrm{T}} V [m(t) - \hat{g}] + \\ & \tfrac{1}{2} \xi_1^T W_1 \xi_1 + \tfrac{1}{2} \xi_3^T W_3 \xi_3 + \lambda^{\mathrm{T}} \left[\hat{A}_1 \dot{\hat{q}}_l + \hat{f}_1 - \xi_1 \right] + \mu^{\mathrm{T}} \left[\dot{\hat{\theta}} - \xi_3 \right] \} \, d\tau \end{aligned} \tag{28}$$

where λ and μ are columns with Lagrange multipliers. For simple notation, the function arguments have been omitted. In this formulation ξ_1 and ξ_3 can be treated as independent variables [4]. A necessary, but not sufficient condition for J_2 to be minimal is $\delta J_2 = 0$ for all variations δq_l, δp_l, $\delta\theta$, $\delta\xi_1$, $\delta\xi_3$, $\delta\lambda$ and $\delta\mu$. The following result is obtained:

$$W_1^{-1} \lambda = \hat{A}_1 \dot{\hat{q}}_l + \hat{f}_1 \tag{29}$$

$$W_3^{-1} \mu = \dot{\hat{\theta}} \tag{30}$$

$$\dot{\mu} = \left(\frac{\partial f_1}{\partial \theta} \right)^{\mathrm{T}} \lambda - \left(\frac{\partial g}{\partial \theta} \right)^{\mathrm{T}} V^{\mathrm{T}} (m - \hat{g}) + \left(\frac{\partial f_2}{\partial \theta} \right)^{\mathrm{T}} W_2^{\mathrm{T}} \hat{f}_2 \tag{31}$$

$$0 = \left(\frac{\partial f_1}{\partial p_l} \right)^{\mathrm{T}} \lambda - \left(\frac{\partial g}{\partial p_l} \right)^{\mathrm{T}} V^{\mathrm{T}} (m - \hat{g}) + \left(\frac{\partial f_2}{\partial p_l} \right)^{\mathrm{T}} W_2^{\mathrm{T}} \hat{f}_2 \tag{32}$$

$$\dot{(\hat{A}_1 \lambda)} = \left(\frac{\partial (f_1 + A_1 \dot{\lambda})}{\partial q_l} \right)^{\mathrm{T}} \lambda - \left(\frac{\partial g}{\partial q_l} \right)^{\mathrm{T}} V^{\mathrm{T}} (m - \hat{g}) + \left(\frac{\partial f_2}{\partial q_l} \right)^{\mathrm{T}} W_2^{\mathrm{T}} \hat{f}_2 \tag{33}$$

where $\dim(q_l) = nq$, $\dim(p_l) = \dim(\lambda) = np$, $\dim(\theta) = \dim(\mu) = n\theta$. nq and np are the number of variable displacement- and pressure- DOF respectively. By solving this system of equations, determination of the deformation and pressure field is integrated with the estimation of material parameters.

6 Discussion

In this report a parameter estimation procedure is proposed for a material which is described by a mixture model. The method is based on finite element discretization and system identification techniques. An identification model is introduced which includes the discretized system equations, the parameter equation, and the output equation. The parameter equation states that material parameters are in principle constant and the output equation determines the expected measurement data on the basis of the material parameters and the node- displacements and pressures. From this model a system of equations is deduced whose solution minimizes a quadratic norm of the residuals on the model equations and the difference between actual and predicted measurement data. This approach has the following *advantages*:

- Residuals can be weighted separately.
- Determination of the strain and pressure field is integrated with the identification proces.
- Common techniques are used from both continuum mechanics and system control.

Important *disadvantages* are:

- The elaboration depends on the chosen model.
- The method may be time consuming and laborious.

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A Appendix

In the equations 13 and 14 matrices are used which will be given in this appendix. The same notation is used as by Bovendeerd [2].

$$R = \begin{bmatrix} R_1^{11} & R_2^{11} & R_3^{11} & R_1^{12} & \dots & R_3^{1N_k} \\ R_1^{21} & R_2^{21} & & & & \\ \vdots & & \ddots & & & \vdots \\ & & & & & \\ R_1^{N_p 1} & \dots & & & & R_3^{N_p N_k} \end{bmatrix} \tag{34}$$

$$R_i^{IJ} = \int_{V_0} (\vec{e}_i \vec{\nabla}_0 \psi^J) : \mathbf{F}^{-1} \phi^I J \, dV_0 \qquad \begin{aligned} I &= 1, \dots, N_p \\ J &= 1, \dots, N_k \\ i &= 1, 2, 3 \end{aligned} \tag{35}$$

$$K = \begin{bmatrix} K^{11} & K^{12} & \dots & K^{1N_p} \\ K^{21} & & & \\ \vdots & & \ddots & \vdots \\ & & & \\ K^{N_p 1} & & \dots & K^{N_p N_p} \end{bmatrix} \tag{36}$$

$$K^{IJ} = \int_{V_0} \vec{\nabla}_0 \phi^J \cdot \mathbf{F}^{-1} \cdot \mathbf{K} \cdot \mathbf{F}^{-c} \cdot \vec{\nabla}_0 \phi^I J \, dV_0 \qquad \begin{array}{rcl} I & = & 1, \ldots, N_p \\ J & = & 1, \ldots, N_p \end{array} \tag{37}$$

$$Q = \left[\begin{array}{cccc} Q^1 & \ldots & Q^{N_p} \end{array} \right]^{\mathrm{T}} \tag{38}$$

$$Q^I = \int_{A_0} \phi^I q^f \, dA_0 \qquad I = 1, \ldots, N_p \tag{39}$$

$$S = \left[\begin{array}{cccccc} S_{11}^{11} & S_{12}^{11} & S_{13}^{11} & S_{11}^{12} & \ldots & S_{13}^{1N_k} \\ S_{21}^{11} & S_{22}^{11} & S_{23}^{11} & S_{21}^{12} & & \\ S_{31}^{11} & S_{32}^{11} & S_{33}^{11} & S_{31}^{12} & & \\ S_{11}^{21} & S_{12}^{21} & S_{13}^{21} & S_{11}^{22} & & \\ \vdots & & & & \ddots & \vdots \\ S_{31}^{N_k 1} & & & & \ldots & S_{33}^{N_k N_k} \end{array} \right] \tag{40}$$

$$S_{ij}^{IJ} = \int_{V_0} (\vec{e}_i \vec{\nabla}_0 \psi^I) : (\mathbf{S}_{\mathit{eff}} \cdot \vec{\nabla}_0 \psi^J \vec{e}_j) \, dV_0 \qquad \begin{array}{rcl} I & = & 1, \ldots, N_k \\ J & = & 1, \ldots, N_k \\ i & = & 1, 2, 3 \\ j & = & 1, 2, 3 \end{array} \tag{41}$$

$$F = \left[\begin{array}{ccccc} F_1^1 & F_2^1 & F_3^1 & \ldots & F_3^{N_p} \end{array} \right]^{\mathrm{T}} \tag{42}$$

$$F_i^I = -\int_{V_0} (\vec{e}_i \vec{\nabla}_0 \psi^I) : \mathbf{S}_{\mathit{eff}} \, dV_0 + \int_{A_0} \psi^I \vec{e}_i \cdot \vec{t} \, dA_0 \qquad \begin{array}{rcl} I & = & 1, \ldots, N_k \\ i & = & 1, 2, 3 \end{array} \tag{43}$$