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Applications of regularized output least squares method

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Abstract

The process of numerical analysis in structural fire design comprises three main components: determination of the fire exposure, the thermal analysis and the structural analysis. The thermal analysis requires well-defined input information on thermal material properties for determining the transient temperature state of the fire-exposed structure.

This work presents a systematic methodology to treat identification of temperature dependent thermal properties from test results. This method is known as the Regularized Output Least Squares Method (ROLS). Applications of the method to identification of thermal properties in different cases are presented. For each problem, the direct problem is formulated as a system of one or several ordinary differential equations which are semi-discretized via the variational form of the general heat conduction problem. The solution of the direct problem is obtained by time-integrating the semi-discrete equations by means of numerical quadrature. The problem of identification of the parameters appearing in the formulation of the direct problem is know as an inverse problem.

A common feature of inverse problems is *instability*, that is, small changes in the data which may give rise to large changes in the solution. Small finite dimensional problems are typically stable, however, as the discretization is refined, the number of variables increases and the instability of the original problem increases. Therefore regularization is needed. Both mesh coarsing and Tikhonov-regularization have been adapted in order to achieve a stabilized solution. The available *a priori* known physical constraints on the parameters are taken into account in the minimization.

The distributed parameters are discretized. The thermal properties are approximated as piece-wise linear functions of temperature. The unknowns are found by minimizing a constrained and regularized functional which is the sum of the residual norm of the errors (data - model) plus the norm of the second derivatives of the properties with respect to the temperature. An appropriate balance between the need to describe the measurements well and the need to achieve a stable solution is reached by finding an optimal regularization parameter. Both Newton and conjugate gradient methods have been used in the minimization. The Morozov discrepancy principle is used to find a reasonable value for the regularization parameter.

Preface

The only fire resistance tests where thermal properties obtained from the test results are utilized is the NORDTEST NT FIRE 021 method in the Nordic Countries and the corresponding CEN method EN YYY5-4. However, the properties obtained are only valid to the one variable differential equation used in the design of protected steel sections. For a more complete knowledge of the temperature field, use of numerical methods based on the finite element method is necessary.

At the Technical Research Centre of Finland (VTT) and the Helsinki University of Technology the authors have conducted some preliminary studies and used the *regularized output least squares method* (ROLS) on the inverse solution of one differential equation of one variable in the case of fire protected metal structures.

In this report the method has been extended to the inverse solution of the system of ordinary differential equations obtained by variational formulation of the Finite Element Method (FEM). Regularization either by mesh coarsing or Tikhonov-regularization was used in order to acquire a more stabilized inverse solution. The finer the discretization in the FEM formulation, the closer the exact solution is to the direct problem is to as well as the inverse solution to the "real" material properties. The above-mentioned tools give us a general and systematic method for the identification of thermal properties (thermal conductivity, specific heat, convection heat transfer coefficient, emissivity) using the results of different kinds of tests.

As numerical examples the method presented is applied to different kinds of tests including furnace tests. The test results are from public projects conducted by the authors and their colleagues at VTT Building Technology and the Helsinki University of Technology. In this report the example problems have been treated as one dimensional and the number of elements have been limited to three. All the examples have been calculated using Excel-routines. Treatment of 2-D or 3-D problems of several variables would have required development of the FEM-program with an inverse solution capability and would have been too expensive for the available funding.

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Jukka Myllymäki Djebar Baroudi

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List of symbols

A_p, A_s	area of fire protect ion and metal structure, m^2
C	capacitance matrix
c	specific heat, J/(kg K)
c, c_p ,c_s	specific heat, of fire protection, of steel structure J/(kg K)
d, d_p ,d_s	thickness, thickness of fire protection, thickness of metal structure, m
e	superscript for the element number e
f	force vectors
h	convection coefficient, W/m^2
K	conductance matrix
L	latent heat per unit mass, J/kg
N_i	shape functions
Q_{ij}^p	elements of the capacity matrix of fire protection, J/ K
$Q_s = \rho_s A_s c_s d_s$	thermal capacity of the metal structure, J/ K
q	heat flux, W/m^2
T	degrees of freedom, temperature vector, K
T, T_p	temperature, temperature of protection, K
T_s, T_g	temperature of steel structure and surrounding gas, K
t	time, s
v	test function
x	space dimension, m
α	regularization parameter
$\alpha(T)$	coefficient of thermal expansion
ε	emissivity
ε_T	thermal strain
λ	thermal conductivity, W/(m K)
ρ	density, kg/m^3

Abbreviations

FEM	Finite Element Method
ODE	Ordinary Differential Equation
1-D	one dimensional (space)
3-D	three dimensional (space)
BC	Boundary Conditions
IC	Initial Conditions

1. INTRODUCTION

Easy access to reliable data on thermal properties such as thermal diffusivity, thermal conductivity and specific heat is of great importance to the advancement of numerical calculation methods for the assessment of the fire resistance of building components. To be consistent with the current fire resistance classification philosophy, material properties must be valid under conditions in the tests used for the determination of fire resistance. Increased use of more general engineering methods demands that the data be applicable under other kinds of non-standard exposure conditions.

Experimental methods for the determination of thermal properties of solids are numerous (Maglic et al. 1984). The methods suggested for use in connection with fire testing have been reviewed (Lundqvist et al. 1991). The methods used in fire technology can be divided into two categories: small scale tests (Grauers & Persson 1994) and large scale furnace methods (Kokkala & Baroudi 1993, Olafsson 1987).

Within the field of fire resistance testing it is implicitly assumed that the properties of materials and components found in a standard ISO 834 test are representative of the materials and components. Therefore, methods based on one simplified ordinary differential equation have been developed for the fire protection of steel structures (Wickström 1985, Andersen 1988, NT FIRE 021). The determination of thermal conductivity from ISO 834 tests suitable for these simple equations gives us an effective thermal conductivity that is not consistent with the assumptions in numerical methods, like the Finite Element Method (FEM), that uses a more detailed description of the temperature field. Another disadvantage with these methods is the inverse solution technique that uses the data measured directly or with some smoothing. Because inverse problems are generally very unstable, small errors in measurement may lead to large errors in calculated thermal conductivity.

Recently Dhima (1994) has used the Output Least Squares Method (OLS) with finite difference discretization (Dhima 1986, Raynaud & Bransier 1986) for the determination of thermal properties of fire protection using furnace tests according to ISO 834.

At VTT and the Helsinki University of Technology the authors (Myllymäki & Baroudi 1996) have conducted some preliminary studies and used the regularized output least squares method (ROLS), which is an improvement on the OLS-method. In this report the method has been extended to the inverse solution of a system of ordinary differential equations obtained by the variational formulation of the Finite Element Method FEM. Regularization by mesh coarsing and Tikhonov-regularization (1997) was used in order to get more stabilized inverse solutions.

The use of the above mentioned tools gives us a general and systematic method for the identification of thermal properties (thermal conductivity, specific heat, convection heat transfer coefficient, emissivity) from the results of different kinds of tests.

2. FORMULATION OF THE DIRECT PROBLEM

2.1 Heat conduction problem

The basic task is to solve the temperature field $T_i(x,t)$ in a given material region. The field equation

$$\rho\, c\, \dot{T}(x,t) = \vec{\nabla} \cdot \left(\lambda \vec{\nabla} T(\vec{x},t)\right) + r(\vec{x},T) \tag{1}$$

is the diffusion equation with $r(\vec{x},T)$ as an arbitrary source term. The 1-D form of it is

$$\rho(T)c(T)\frac{\partial T(x,t)}{\partial x} = \frac{\partial}{\partial x}\left(\lambda(T)\frac{\partial T(x,t)}{\partial x}\right) + r(x,T) \tag{2}$$

The Fourier heat conduction constitutive relation is assumed. This equation is complemented with the appropriate initial and boundary conditions to reach a well-posed problem. The boundary conditions may either be a Dirichlet type (prescribed temperature) or a Neumann type, such as the normal heat flux $q_n = h(T)(T - T_\infty) + \sigma\, \varepsilon\, (T^4 - T_\infty^4)$ with convection and radiation parts. The boundary terms, like the source terms if present, will be included into the force vector of discretized heat conduction equations. This will be a clear and systematic way to treat boundary and source terms.

2.2 Semi-discretization of the field equations

Using the standard FEM-approach (Eriksson et al. 1996) one obtains the variational form of the problem (1) as

$$\int_\Omega \rho c \dot{T}\, v\, d\Omega + \int_\Omega \lambda\, \vec{\nabla} T \cdot \vec{\nabla} v\, d\Omega = \int_\Omega r\, v\, d\Omega - \int_{\partial\Omega_q} \vec{q} \cdot \vec{n}\, v\, d\Gamma \tag{3}$$

that reads in 1-D as follows

$$\int_0^L \rho c \frac{\partial T}{\partial t} v dx + \int_0^L \lambda \frac{\partial T}{\partial x}\frac{\partial v}{\partial x} dx = \int_0^L r v dx - \left[q_{\infty n} v \right]_0^L \tag{4}$$

The temperature field is approximated by $T^e(x,t) = \mathbf{N}^e(x)\mathbf{T}^e(t)$, where the test and the basis functions are in a linear 1-D element

$$N_1(\xi) = \frac{1-\xi}{2}; N_2(\xi) = \frac{1+\xi}{2} \tag{5}$$

The semi-discretization of the heat conduction equation (3) produces the non-linear initial value problem

$$\mathbf{C}(t,\mathbf{T})\dot{\mathbf{T}}(t) = \mathbf{f}(t,\mathbf{T}) - \mathbf{K}(t,\mathbf{T})\mathbf{T}(t), \quad t > 0 \tag{6}$$

$$\mathbf{T}(0) = \overline{\mathbf{T}}_0, \quad t = 0 \tag{7}$$

where $\mathrm{T}(t) = \begin{pmatrix} T_1(t) & T_2(t) & \dots & T_m(t) & T_{m+1}(t) & \dots & T_n(t) \end{pmatrix}^T$ is the global vector for the unknown temperatures.

Equation (6) is a set of *n x 1*-non-linear ordinary differential equations. Notice that the right hand in equation (3) corresponds to the force vector $\mathbf{f}(t,\mathbf{T})$, which contains the boundary terms as well as all possible source terms. Equation (6) is complemented with appropriate initial conditions (7). Natural boundary conditions are already included in the variational forms (3) and (4). The essential boundary conditions will be taken into account during the solution process of the initial value problem. The global matrices and vectors are assembled using standard FE-assembling techniques. The elementary conductivity matrix

$$K_{ij}^e = \int_{\Omega^e} \lambda\big(T(\mathrm{x})\big)\, \vec{\nabla}\mathrm{N}_\mathrm{i}(\mathrm{x}) \cdot \vec{\nabla}\mathrm{N}_\mathrm{j}(\mathrm{x}) \quad d\Omega \tag{8}$$

the elementary capacity matrix

$$C_{ij}^{e} = \int_{\Omega^e} \rho\big(T(\mathbf{x})\big)\; c\big(T(\mathbf{x})\big)\; \mathrm{N_i}(\mathbf{x})\; \mathrm{N_j}(\mathbf{x})\;\; d\Omega \tag{9}$$

and the force vector

$$f_i^{\,e} = \int_{\Omega^e} r\big(T(\mathbf{x})\big)\; \mathrm{N_i}(\mathbf{x})\; d\Omega - \int_{\partial\Omega_q} \vec{q}\cdot\vec{n}\; \mathrm{N_i}(\mathbf{x})\; d\Gamma \tag{10}$$

are obtained. For instance, in 1-D cases using basis functions (5) these matrices look like:

$$K_{ij}^{e} = 2/l^{e}\int_{-1}^{1}\lambda(T(\xi))\;\; N_{i,\xi}(\xi)N_{j,\xi}(\xi)\; d\xi\,,$$

$$C_{ij}^{e} = \frac{l^{e}}{2}\int_{-1}^{1}\rho(T(\xi))c(T(\xi))N_i(\xi)N_j(\xi)\; d\xi \text{ and}$$

$$f_i^{\,e} = \frac{l^{e}}{2}\int_{-1}^{+1} r(T(\xi))N_i(\xi)\; d\xi - \big[q_n N_i(\xi)\big]_{-1}^{+1}, \text{ respectively.}$$

The elementary matrices and vectors are integrated numerically using the Gauss-Legendre integration scheme with as many integration points as needed to accurately integrate their expressions. For example, the contribution of the source term to the force vector source term is space-integrated as $f_{r,i}^{\,e} \approx \frac{2}{l^{e}}\sum_{K=1}^{NG} r(T(\xi_K))N_i(\xi_K)w(\xi_K)$. The elementary matrices and vectors may depend on the unknown temperature.

The above mentioned integration scheme leads to a consistent capacity matrix, where the non-diagonal terms $C_{i\,j}^{e}\;(i \neq j)$ are non-zero. In some cases it is useful to use a diagonal capacity matrix ($C_{i\,j}^{e}\;(i \neq j)$=0), especially when we use a Dirichlet type boundary condition. Using the Newton-Cote integration scheme where the nodal points are used as integration points and the weights of the integration are calculated from the equation $w_i = \int_0^l N_i N_i dx$ we always get a diagonal capacity matrix.

2.3 Time-integration of the ODE-system

Let us consider an initial value problem in type (11). The problem here is treated more generally because, in the numerical examples, y may be temperature T in a heat conduction problem or thermal strain ε_T in a problem of thermal elongation.

$$\dot{y} = a(y)y + f(y), \quad y(0) = y_o \quad , \quad y = y(t) \tag{11}$$

We may interpret this in terms of a coefficient-to-solution operator

$$\mathbf{F(a)} = \mathbf{y} \tag{12}$$

where the operator F is defined by

$$F(a, y; t) = y(0) + \int_0^t \{ay + f(y)\}\, d\tau = y(t), \ with\ a = a(y) \tag{13}$$

Depending on the integration scheme used in equation (13) we get explicit or implicit methods (Eriksson et al. 1996). In order to avoid iterations during optimization, the explicit Euler scheme has been used. Now, instead of the exact equation (3), we solve discretized equations

$$\tilde{\mathbf{F}}(\tilde{\mathbf{a}}) = \mathbf{Y}^n = Y^{n-1} + \{a(Y^{n-1})Y^{n-1} + f(Y^{n-1})\}\Delta t_n \tag{14}$$

$$where\ \tilde{\mathbf{a}} = \tilde{\mathbf{a}}(\mathbf{Y})\ and\ Y \approx y\ and\ \Delta tn = tn - tn - 1$$

In a case of a heat conduction problem $(y \equiv T)$ the time-integration of equation (6) provides us with the nonlinear system of equations

$$\mathbf{A}(t_{n-1}, \mathbf{T}_{n-1})\mathbf{T}(t_n) - \mathbf{g}(t_{n-1}, \mathbf{T}_{n-1}) = \mathbf{0} \tag{15}$$

The solution **T**(t) is solved from equation (15) at each time step. The matrix in equation (15) is calculated as

$$\mathbf{A}(t_{n-1}, \mathbf{T}_{n-1}) = \mathbf{C}(t_{n-1}, \mathbf{T}_{n-1}) \tag{16}$$

and the vector

$$\mathbf{g}(t_{n-1}, \mathbf{T}_{n-1}) = \mathbf{C}(t_{n-1}, \mathbf{T}_{n-1})\mathbf{T}(t_{n-1}) + \Delta t_n \mathbf{f}(t_{n-1}, \mathbf{T}_{n-1}) + \Delta t_n K(t_{n-1}, T_{n-7}) \tag{17}$$

3. GENERAL FORMULATION OF THE INVERSE PROBLEM

Consider a coefficient determination problem, i.e. the problem of determining a non-constant coefficient $a(y)$ in an initial value problem (11) based on the existing data of solution y. The non-linear inverse problem has been solved using the *regularized output least squares method* (ROLS**).** We have to discretize the distributed unknown parameter $a(y)$ into a certain number of sub-intervals $[y_i, y_{i+1}]$ of arbitrary length $y_{i+1} - y_i$ using suitable almost orthogonal basis functions. The goal is to find the regularized least squares solution for the vector of the nodal values $\vec{a}_i^{\,*}$ of (11).

Since the *inverse problem is ill-posed* it has to be *regularized*. Here, in the regularized output least squares method (ROLS) the regularization of the problem is achieved by *mesh coarsing* and by *use of the available a priori known physical constraints* on the parameters. Another alternative is to perform the regularization using the *penalized least squares* method (Groetsch 1993) regarded as a *Tikhonov regularization* of non-linear problems (Groetsch 1993, Hansen 1990). One seeks unknowns $\vec{a}_i^{\,*}$ such that

$$\left\| \widetilde{F}(\vec{a}^{\,*}) - \vec{y}^{\,\delta} \right\|^2 + \alpha \left\| L\vec{a}^{\,*} \right\|^2 \tag{18}$$

is minimized with respect to $\vec{a}_i^{\,*}$. The constraints set D is the set of physically admissible parameters. Unfortunately the data vector $\vec{y}$ is known only within a certain tolerance δ. This approximation $\vec{y}^{\,\delta}$ satisfying the condition $\left\| \vec{y} - \vec{y}^{\,\delta} \right\| \le \delta$ is known (for example due to the scatter/data errors in the experimental measurements) and one therefore seeks an $\vec{a}^{\,*}$ minimizing (18) using data infected with noise. Here $\vec{y}_k^{\,\delta}$ is the vector of measured data. The minimization problem (18) is non-linear. Here either Newton or Conjugate Gradient methods are used.

The coefficient $\alpha(>0)$ is a regularization parameter depending on the noise level of the data and $L = I$ or some other suitable differential operator (D^1 or D = Laplace) depending on the needed *regularity* of the solution. The first term in equation (18) enforces the consistency of the solution while the second term

enforces its stability. An appropriate balance between the need to describe the measurements well and the need to achieve a stable solution is reached by finding an optimal regularization parameter.

In a heat conduction problem $(y \equiv \mathbf{T})$ the overall procedure of determination of the thermal properties (and other relevant parameters) may be condensed schematically as follows:

Discretize the unknown vector **a** with respect to the temperature (if necessary) using piece-wise linear basis functions. Estimate a 'realistic' initial value for **a** and choose a value for α. Then ***Solve*** **a** from the minimization problem

- $\min_{\vec{a}\in D} \left\| T_{FE}(\vec{a};\vec{x};t) - T_{data}(\vec{x},t) \right\|^{\hat{}} + \alpha \left\| \mathbf{L}\ \vec{a} \right\|^2$ with respect to **a,**

  where the model is $T_{FE}(\vec{a};\vec{x};t) = \mathbf{N}(\vec{x})\mathbf{T}(t)$

  and the data is $T_{data}(\vec{x};t)$ with **T**(t) the solution of the initial value problem:

  $$\mathbf{C}\left(\vec{a}(\mathbf{T})\right)\ \dot{\mathbf{T}}(t) = \mathbf{f}\left(\vec{a}(\mathbf{T})\right) - \mathbf{K}\left(\vec{a}(\mathbf{T})\right)\ \mathbf{T}(t)$$ & BC and IC

- The unknown parameter vector is: $\vec{a}(\mathbf{T}) = \left(\lambda(T) \quad c_p(T) \quad \vec{b}\right)$ with the vector

  $\vec{b} = \left(\varepsilon \quad h(T) \quad Q_{loss} \quad etc...\right)$ containing the remaining relevant additional parameters we want to estimate. The norms (Euclidean) are taken with respect to the collocation points **x** at collocation time *t* as $\left\| \mathrm{f}(\vec{\mathrm{x}};\mathrm{t}) \right\|^2 = \sum_{\mathrm{i}} \sum_{\mathrm{j}} \left| \mathrm{f}(\vec{\mathrm{x}}_{\mathrm{i}};\mathrm{t}_{\mathrm{j}}) \right|^2$ $(\mathrm{i},\mathrm{j}) \in \left\{ \text{collocation index set} \right\}$. **L** is a regularization operator (depending on the degree of regularization we want), usually the identity **I** matrix or a discrete version of the Laplacian with respect to the temperature.

3.1 The use of Morozov discrepancy principle and the L-curve

In equation (18) parameter α controls how much weight is given to the minimization of $\left\| L\vec{a}^* \right\|^2$ relative to the minimization of the residual norm $\left\| \tilde{F}(\vec{a}^*) - \vec{y}^{\delta} \right\|^2$. The problem considered here is the appropriate choice of

parameter α so that we can distinguish the real signal from measurements with noise.

Perhaps the simplest rule to define the regularization parameter is to set the residual norm equal to some upper bound for the norm $\left\|\tilde{F}(\vec{a}^{*})-\vec{y}^{\delta}\right\|^{2}$ of the errors, i.e. find α such that (Groetsch 1993)

$$\left\|\tilde{F}(\vec{a}^{*})-\vec{y}^{\delta}\right\| \leq R\ \delta \tag{19}$$

where δ is the measure of the error during the time considered $\delta^{2}=\int_{0}^{t}\left|\partial\right|^{2}dt$ and ∂ is the error at a certain time. An appropriate value for the coefficient is $R \approx 1.6-1.7$. In connection with discrete ill-posed problems, this is called *Morozov discrepancy principle* (Hansen 1990).

Another, more recent alternative is to base the regularization parameter on a so-called *L-curve* (Hansen 1990), (Hansen and O´Leary 1991). The L-curve is a parametric plot of measure of the size of the regularized solution and the corresponding residual. The underlying idea is that a good method for choosing the regularization parameter for discrete ill-posed problems must incorporate information about the solution size in addition to using information about the residual size. The L-curve has a distinct L-shaped corner located where the solution changes in nature from being dominated by regularization errors to being dominated by the errors on the right side of equation (18). According to Hansen (1990) the corner of the L-curve corresponds to a good balance between the minimization of the sizes; the corresponding regularization parameter α is optimal. In their experiments Hansen and O´Leary have found that in many cases it is advantageous to consider the L-curve at a log-log scale.

When the norms of unknown parameters differ considerably, the vector of unknowns may be divided into more than one vector: $\vec{a}_{1}(\mathbf{T})=(\lambda(T))$, $\vec{a}_{2}(\mathbf{T})=(c_{p}(T)\quad\vec{b})$ and different α parameters may be used

$$\left\| \tilde{F}(\vec{a}^{*}) - \vec{y}^{\delta} \right\|^{2} + \alpha_{1} \left\| L\vec{a}_{1}^{*} \right\|^{2} + \alpha_{2} \left\| L\vec{a}_{2}^{*} \right\|^{2} \tag{20}$$

In this case the L-curve is actually a surface and use of it is not practical. In cases where the same α parameter was used the optimum of the L-curve corner was seldom seen, so Morozov discrepancy principle was preferred.

Since the functional to be minimized is generally non-linear it may have several solutions that fulfil the Morozov discrepancy principle. In order to find the physically admissible solution we must have preliminary test information on the values of the material properties at a constant temperature (for example thermal conductivity at 20 ^{o}C).

4. DETERMINATION OF THE COEFFICIENT OF THERMAL EXPANSION

4.1 General

In the following Chapter the problem of determination of the coefficient of thermal expansion is considered. Results are from tests conducted in the project "Aluminium properties at elevated temperatures" at the Helsinki University of Technology (Myllymäki 1998) where the specimen of aluminium alloy AA6063-T6 was heated at a constant rate and thermal strain $\varepsilon_T(T) = \Delta l / l$ was measured as a function of time. The problem is not actually a heat conduction problem but can be considered in a broader sense the determination of a thermal property. The reason for the presentation of the case is that it shows the generality of the ROLS-method and its applicability to other systems of ODE as well as those obtained from the semi-discretized partial differential equation of heat conduction. The second reason for the presentation is the simplicity of the differential equation which allows us to show the application of different stopping criteria such as Morozov discrepancy principle and the L-curve method in a rather trivial but hopefully illustrative way.

The ROLS method is also compared to the traditional polynomial approximation method applied in such cases in Eurocodes.

4.2 Polynomial approximation

There are two alternative ways to present the thermal strain. It can be given as a state function of temperature as in the polynomial approximation

$$\varepsilon_T(T) = \frac{\Delta l}{l} = \sum \beta_i T^i \tag{21}$$

In the Eurocodes, the following parabolic function has been given for the thermal strain

$$\varepsilon_T = \frac{\Delta l}{l} = \beta_2 T^2 + \beta_1 T + \beta_0 \tag{22}$$

In the transient heating tests we have measured the strain ε_T in a test where the stress has been 3 N/mm^2. One can solve the coefficients of the polynomial by minimizing function (23) with respect to polynomial coefficients β_i.

$$F(\beta_i) = \min_{\beta_i} \left\| \varepsilon_T - \varepsilon_T^{\delta} \right\|^2 \tag{23}$$

where ε_T^{υ} is the measured strain and ε_T is the calculated strain. This technique is the so-called Output Least Squares Method.

Traditionally and also more generally thermal strain has been presented in rate form, where no assumption of the recovery of the thermal strain need not have to be made;

$$\dot{\varepsilon}_T = \alpha(T)\ \dot{T} \tag{24}$$

In equation (24), $\alpha(T)$ is the coefficient of thermal expansion. Equation (21) can be presented in rate form as

$$\dot{\varepsilon}_T = 2\beta_2 T \dot{T} + \beta_1 \dot{T} = (2\beta_2 T + \beta_1)\ \dot{T} \tag{25}$$

where the coefficient of thermal expansion is

$$\alpha(T) = 2\beta_2 T + \beta_1 \tag{26}$$

If we use a series of polynomials, (as in equation (22)), the rate form is

$$\dot{\varepsilon}_T(T) = \sum_{i=0}^{n} \beta_i\ i\ T^{\ i-1} \dot{T} \tag{27}$$

where the coefficient of the thermal expansion is

$$\alpha(T) = \sum_{i=0}^{n} \beta_i \, i \, T^{\,i-1} \tag{28}$$

4.3 Piece-wise linear approximation

A more sophisticated way is to use a piece-wise linear approximation for the coefficient of thermal expansion $\alpha(T) = (1-\xi)\,\alpha_i + \xi\alpha_{i+1}$ for each temperature interval $T \in [T_i, T_{i+1}]$, $\xi = T/(T_{i+1} - T_i)$, separately. Using the explicit Euler scheme

$$\varepsilon_T^{\,j+1} = \alpha\,(T^j)\Delta T_j + \varepsilon_T^{\,j} \tag{29}$$

we can calculate the thermal strain. In equation (29), ΔT_j is the temperature step for each time step $\Delta\, t_j$. The unknown parameters can be sought to minimize the functional, (30) with the Tikhonov regularization method

$$\left\| \vec{\varepsilon}_T - \vec{\varepsilon}_{\delta\,T} \right\|^2 + \beta \left\| \partial^2 \vec{a} \;/\, \partial T^2 \right\|^2 \tag{30}$$

where $\vec{\varepsilon}_T$ is the vector of the calculated strain and $\vec{\varepsilon}_{\delta\,T}$ is the vector of the measured stress dependent strain and β > 0 is a regularization parameter, depending on the noise level of the data. Vector $\vec{a}$ consists of the coefficients of thermal expansion α_i at each nodal point T_i.

4.4 Numerical examples of the calculation of the coefficient of thermal expansion

In this chapter we show how the solutions of the coefficients of thermal expansion methods differ from each other. Some comparisons to the values in literature are given. Figure 1 shows the calculated coefficients of thermal expansion from transient tests of temperature rate 10 K/min.

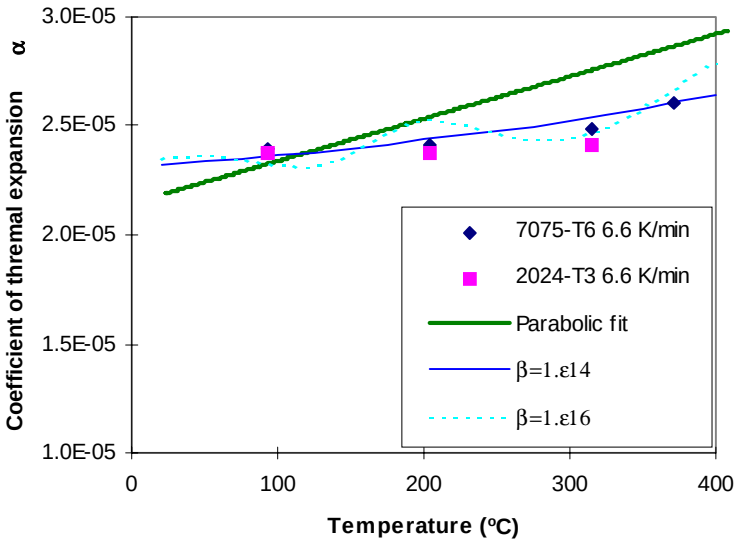

Figure 1. The coefficient of thermal expansion calculated from transient tests, where the oven temperature rate was 10 K/min. Results of alloys 7075-T6 and 2024-T3 (markers) are from Heimerl and Inge (1955).

Figure 1 shows both the parabolic fit (22) of Eurocodes for thermal strain that gives a line function (26) for the thermal expansion coefficient. Two solutions, each with a different regularization parameter β are given. The Eurocode type of parabolic fit for thermal strain tends to overestimate the thermal expansion coefficient at high temperatures and underestimate the thermal exponent at lower temperatures. It can be seen that the solutions with regularization have solutions that are nearer the values given in literature.

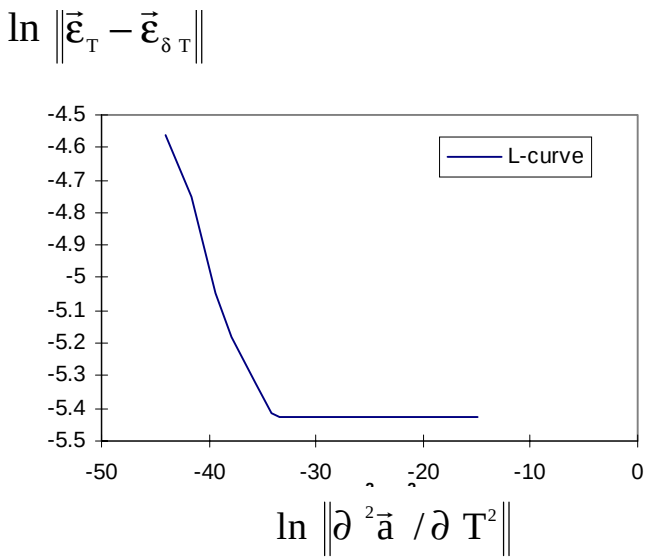

Figure 2. The L-curve of the thermal expansion problem. The solution with regularization parameter β =1.e14 corresponds to ln (Residual)=-5.04 while regularization parameter β =1.e16 corresponds to ln (Residual)=-4.56, which is the same as a 0.004 % error in the strain measurements.

Figure 2 shows the L-curve of the problem, i.e. the parametric plot of the measure of the size of the regularized solution (in this case Laplacian) and the corresponding residual. Here each point of the curve corresponds to a certain value of the regularization parameter β. The L-curve has a distinct L-shaped corner located where the solution changes in nature from being dominated by regularization errors to the errors in the size of the solution. According to Hansen (1990) the corner of the L-curve corresponds to a good balance between the minimization of the sizes, and the corresponding regularization parameter β is an optimal one. In this case, however, the Morozov discrepancy principle with its estimated measurement error of 0.004 % provides a more reasonable result that matches test results in literature.

5. DETERMINATION OF SPECIFIC HEAT

5.1 Determination using the heat flux boundary condition

Consider a board specimen of volume V, with surface A_1 under the effect of heat flux $\vec{q}$. The temperature of the specimen $\tilde{T}^{\delta}(t)$ is measured. The specific heat is discretized using piece-wise linear basis functions with respect to the temperature $c(T) = \sum N_j a_j(T)$. The conservation of energy in the board specimen can be written as

$$\int_V \rho c \dot{T} dV = -\int_{\partial V} \vec{q} \cdot \vec{n} d\Gamma + \int_V \rho r dV \tag{31}$$

The source term in the equation is incorporated into the effective specific heat. Equation (31) after semi-discretization reads as

$$\dot{\tilde{T}}(t) = +q \frac{A_1}{\rho c(\tilde{T})V} \equiv f(T(x;t),t) \tag{32}$$

where function $\tilde{f}$ is defined by $f(t) = 1/d \int_d f(x;t)dx$. ODE (32) is integrated numerically using an explicit Euler scheme:

$$\tilde{T}(t_{k+1}) = \tilde{T}(t_k) + \int_{t_k}^{t_{k+1}} f(\tilde{T}(\tau),\tau)d\tau \approx \tilde{T}(t_k) + f(\tilde{T}(t_k),t_k)\Delta t_k \tag{33}$$

The specific heat capacity *c(T)* is the regularized solution of the constrained minimization problem

$$\min\left(\left\| \tilde{T}(t) - \tilde{T}_{calc.}(\vec{a};t) \right\|^2 + \alpha \left\| \mathrm{L}\vec{a} \right\|^2 \right), \qquad with\ a_j \in D(\vec{a}) \tag{34}$$

The solution is found from the domain of physically admissible functions which take into account the possible range of the unknown parameters a_j . Equation (34) is non-linear for which a solution is found using Newton method.

5.1.1 Numerical example: Gypsum board at cone calorimeter

The cone calorimeter test in the horizontal configuration at a heat flux level of q_{cone} = 25 kW/m^2 was performed. The test specimen consisted of a 13 mm thick gypsum board (density 721 kg/m^3) laying on a 30 mm thick layer of mineral wool (Fig. 3). The surface area exposed to the heat flux was A_1=100 mm x 100 mm. The temperature of the upper surface of the gypsum board was measured using an infrared temperature measuring device The temperature profile inside the specimen as a function of time was measured.

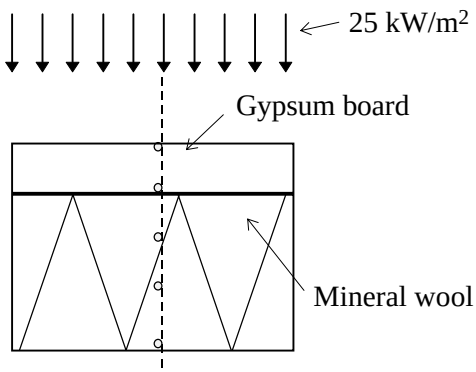

Figure 3. Idealized test arrangements in cone calorimeter.

The results of the calculations are shown in Figure 4. A reasonable degree of regularization (the value of the regularization parameter α is found using Morozov discrepancy principle $\left\| \tilde{T}^{\delta}(t) - \tilde{T}_{calc.}(\vec{a}^{\delta}_{\alpha(n)};t) \right\| \approx R\delta$ (R = 1.6 and α = 0.00001). The accuracy of the temperature measurements in these tests was estimated to be

$$\left\| \tilde{T}^{\delta}(t) - \tilde{T}(t) \right\| \le \delta \approx \int_{t_\infty} 2^o C \, dt \approx 98^o Cs.$$

An average of the measured temperatures at the top and bottom of the board was

used as $\tilde{T}^{\delta}(t)$. The relative amount of humidity (mass of water / total mass of gypsum) in the gypsum board was calculated from the peak of the specific heat and was found to be equal to 21 %. Experimental results show that the water content of gypsum boards is about 18 % in the temperature range < 200 ^{o}C.

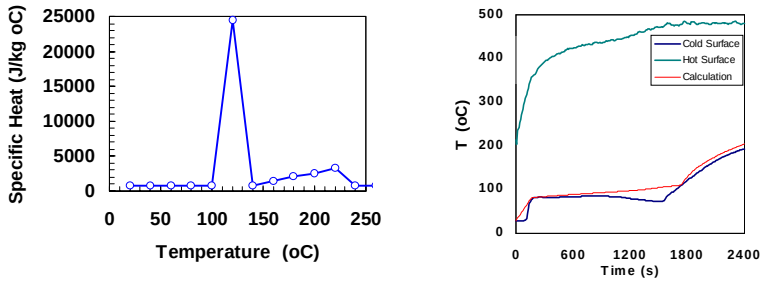

Figure 4. a) Calculated specific heat of the gypsum board measured in a cone calorimeter experiment at 25 kW/m^2. b) Measured surface temperature in bold, and the calculated as a thin line.

5.2 Determination using the heat flux boundary condition with convection and radiation parts

Consider a bare metal structure without fire protection (Fig. 5). We use only one finite element with one basis function $N_1 = 1$ which is the same as assuming the temperature to be constant in the solution domain. Applying the Galerkin method ($\nu = 1$) the variational formulation is the following:

$$\int_0^{d_s} c_s(T_s)\ \rho_s(T_s) A_s dx\ \dot{T} = q_n(0)\ A_{\Gamma 0} - q_n(d_s)\ A_{\Gamma d_s} \tag{35}$$

where $q_n(0)$ and $A_{\Gamma 0}$ are the heat flux and boundary area on the fire unexposed surface and $q_n(d_s)$ and $A_{\Gamma d_s}$ are the same on the exposed surface.

Assume the radiative and convective boundary conditions at the boundary x=d$_s$.: $q_n = 0\ q_n(d_s) = h_c(T_s - T_g) + \varepsilon\ \Phi\sigma\ (T_s^4 - T_g^4)$. The structure and gas are assumed to be two infinitely long parallel plates, for which the following

relation applies: $\varepsilon\ \Phi_{1-2} = \varepsilon_r = (1/\varepsilon + 1/\varepsilon_g - 1)^{-1}$. Here ε is the emissivity of the structure, ε_g is the emissivity of the gas and ε_r is the resultant emissivity. We also combine the two boundary conditions thus: $\tilde{h}(T, T_c) = h_c + \varepsilon_r\ \sigma(T^2 + T_c^2)(T + T_c)$ and finally get the equation:

$$\dot{T}_s = \frac{\tilde{h}\ A_{\Gamma L}(T_g - T_s)}{c_s(T_s)\ \rho_s(T_s) A_s\ d_s} + \frac{q_n(0)\ A_{\Gamma 0}}{c_s(T_s)\ \rho_s(T_s) A_s\ d_s} \tag{36}$$

We may now assume that the heat flow through the boundary is a function of the temperature of the metal structure $q_n = q_n(0, T_s)$. If the heat flow through the boundary is not taken into account (adiabatic boundary condition $q_n = 0$), equation (36) will take on the traditional form used in the fire safety design of unprotected steel structures (Note that $A_s\ d_s = V_s$)

$$\dot{T}_s = \frac{\tilde{h}\ A_{\Gamma d_s}(T_g - T_s)}{c_s(T_s)\ \rho_s(T_s)\ V_s} \tag{37}$$

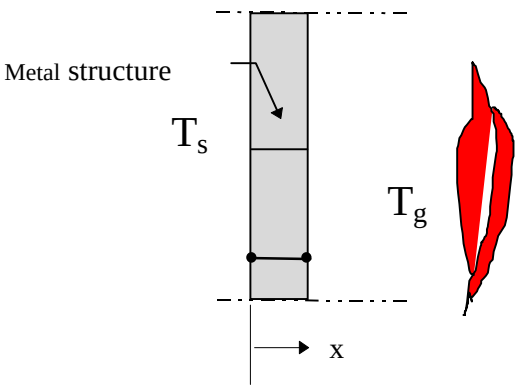

Figure 5. One dimensional idealization of an unprotected metal structure on fire.

The inverse solution of equation (37) is achieved by minimizing equation (18), where $y^{\delta}(t)\ \left(\equiv T_s^{\delta}(t)\right)$ is the measured and $y\ (t)\ \left(\equiv T_s\ (t)\right)$ the solved temperature of the aluminium structure. In this case the discrete coefficient-solution operator is:

$$\tilde{F}(T_s^{n-1}, \Delta t_n) = T_s^{n-1} + \frac{\tilde{h}(T_g^{n-1}, T_s^{n-1})\, A_{\Gamma d_s} (T_g^{n-1} - T_s^{n-1})}{c_s \rho_s A_s d_s} \Delta t_n + \frac{q_n(T_s^{n-1}, 0)\, A_{\Gamma 0}}{c_s \rho_s A_s d_s} \Delta t_n \quad (38)$$

5.2.1 Numerical example: Aluminium specimen in heating oven

Let us consider a case where an uninsulated aluminium specimen, a bar, (2700 kg/m^3) is placed in an oven in order to be tested at high temperatures. The specimen is surrounded by the oven, but the ends of the specimen are clamped into steel rods so part of the heat flow escapes through the ends of the specimen. The heat conduction problem is treated as one dimensional where it has been assumed that heat loss through the clamped ends of the specimen $Q_{loss} = q_n A_{\Gamma_0} / c_{Al} \rho_{Al} A_{Al}\, d_{Al}$ is constant. Here Ar_0 is the tottal area of the ends of the specimen.

The inverse problem, given the measured temperatures, is to find the effective heat losses Q_{loss} (from the aluminium specimen to the surrounding), the effective heat convection coefficient *h* (between the specimen and the heater), the resultant emissivity ε of the aluminium alloy and the thermal capacity $c_p(T)$ of the aluminium alloy. This last one is temperature dependent (discretized with respect to the temperature by linear basis functions). Therefore the unknown vector of parameters in this problem is **a** = ($c_p(T)$, h, ε, Q_{loss}).

Tests have been conducted at the Helsinki University of Technology in a project dealing with the high temperature properties of aluminium (Myllymäki 1998). Oven temperature is controlled in order to ensure a constant temperature or of the specimen or certain rate of specimen temperature, Figures 6b and 7.

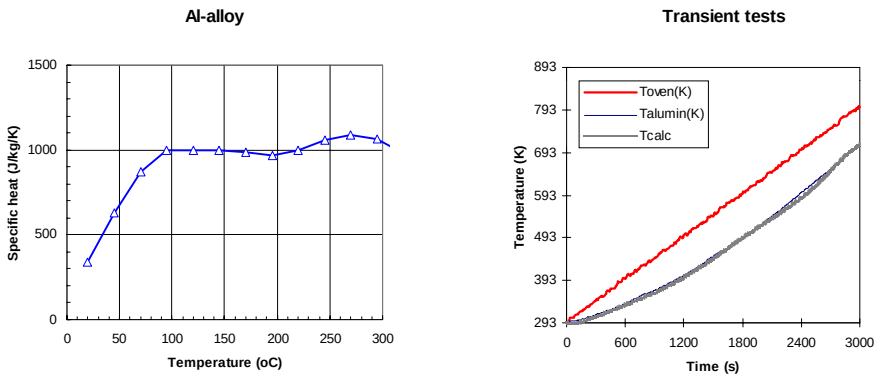

Figure 6 a) Calculated heat capacity of the aluminium alloy. b) Measured and calculated temperatures of the aluminium specimen in heated oven, transient test. The upper curve represents the temperature of the oven.

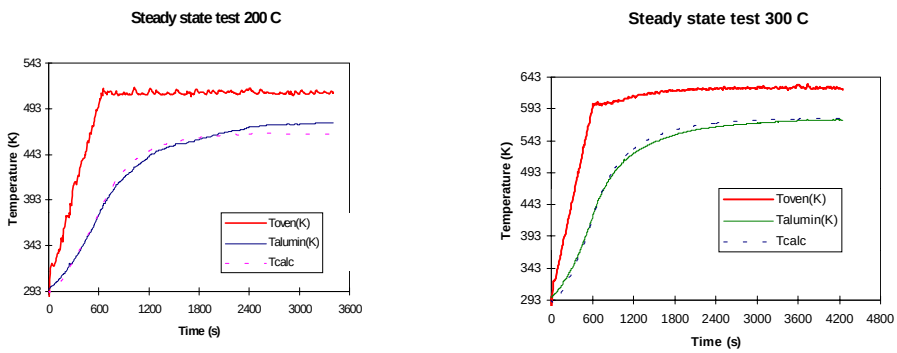

Figure 7 a) and b) Measured and calculated temperatures of the aluminium specimen in heating oven in two different tests, # 2 and # 3. The upper curves are the temperatures of the oven. The lower curves are those of the aluminium specimen (calculated and measured).

The unknown parameter vector **a** has been solved using all three tests simultaneously. It was found that h = 10.4 W/m^2 K, ε = 0.11 and Q_{loss} = -0.74 W. The calculated specific heat capacity of the aluminium alloy is shown in Fig 6a as a function of the specimen temperature. These calculated values seem to be near the pure Al values of c_p = 900 J/kg K at 20 ^{o}C are cited in literature. The measured temperatures of the oven and specimen and also the calculated temperatures of the aluminium specimens are shown in Figures 6b - 7.

6. DETERMINATION OF THERMAL CONDUCTIVITY AND SPECIFIC HEAT

6.1 Determination using one ODE

In the design codes of metal structures the temperature of the structure is calculated by using only one approximate differential equation usually presented as a difference equation.

Effective conductivity of fire protection materials of steel structures is studied in Nordic countries according to the NORDTEST method NT FIRE 021 (1980). In this method, the protected steel column is placed in the horizontal furnace. The temperature of the steel and the gas temperature near the protected section are measured by thermocouples. The thermal conductivity of the protection material is calculated as a function of time using one simple differential equation and the derivatives of the measured steel temperature. The calculated thermal conductivity is then not a real but an effective one that can be used in the design procedure of steel structures.

In this chapter the variational formulation of the Finite Element Method has been used in its simplest form using just one or two linear elements in the case of steel structures. It is shown that this trivial derivation gives us most of the simple one variable ODEs developed for temperature calculation of protected steel structures. The thermal properties obtained by the application of the Regularized Output Least Squares Method to these *one variable equations* gives us *effective* values that are not consistent with the assumptions of FEM calculations, but can be used when designing steel structures with the same simple ODEs.

Consider an insulated steel structure. The problem can be treated as a one dimensional problem using two finite elements (Fig 1). One element is used for the steel part and one element for the insulation part. For the steel part it is assumed that the temperature is uniform (one basis function $N_1 = 1$, one trial function $v = 1$). For the insulation one element with linear interpolation polynomials is used.

If only linear interpolation functions N_1 and N_2 are used the elementary conductivity matrix will have the form

$$\mathbf{K}^{(k)} = \frac{1}{l_k}\int_{-1}^{1} \lambda(T(\xi))A(\xi)\ d\xi \begin{bmatrix} +1/2 & -1/2 \\ -1/2 & +1/2 \end{bmatrix} \tag{39}$$

and the elements of the elementary capacity matrix are

$$c_{ij}^{(k)} = \frac{l_k}{2}\int_{-1}^{1} \rho(T(\xi))c(T(\xi))N_i(\xi)N_j(\xi)A^{(k)}(\xi)\ d\xi \tag{40}$$

With the linear basis functions matrix and, assuming that c and ρ are constants and assuming area of perimeter of the protection to be constant $A^{(k)}(\xi) = A^{(k)}$, the consistent elementary capacity will have a form

$$\mathbf{C}^{(k)} = \frac{l_k}{2}\rho_0 c_0 A^{(k)} \begin{bmatrix} +2/3 & +1/3 \\ +1/3 & +2/3 \end{bmatrix} \tag{41}$$

We divide the solution domain into two elements, one for the metal part of the domain and one for the insulation. We also assume that the temperature of the metal part is uniform (Figure 8).

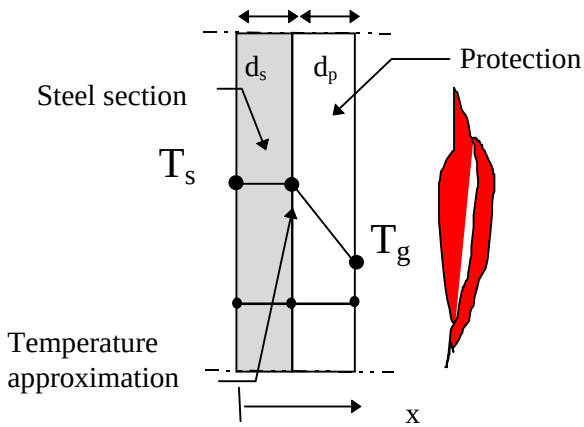

Figure 8a. One dimensional idealization of insulated steel structure in a fire. 8b. Two dimensional real case of insulated stell structure.

We get the following initial value problem:

$$\mathbf{C}\dot{\mathbf{T}} = \mathbf{f} - \mathbf{K}(t,\mathbf{T})\mathbf{T} \tag{42}$$

where the global capacity matrix is

$$\mathbf{C} = \begin{bmatrix} C_s + C_{11}^p & C_{12}^p \\ + C_{21}^p & + C_{22}^p \end{bmatrix} \tag{43}$$

where $C_s = \rho_s A_s c_s(T_s) d_s$

and $C_{ij}^p = \dfrac{d_p}{2} \int_{-1}^{1} \rho_p(T(\xi)) c_p(T(\xi)) N_i(\xi) N_j(\xi) A_p(\xi) \; d\xi$

and the global conductivity matrix is

$$\mathbf{K} = \frac{1}{d_p} \int_{-1}^{1} \lambda_p(T(\xi)) A_p(\xi) \; d\xi \begin{bmatrix} +1/2 & -1/2 \\ -1/2 & +1/2 \end{bmatrix} \tag{44}$$

and the unknown temperature vector is

$$\mathbf{T} = \begin{bmatrix} T_s \\ T_{pb} \end{bmatrix} \tag{45}$$

were T_s is steel temperature and T_{pd} is temperature at the boundary of the insulation.

If we assume that, at the boundary x=0, we have an adiabatic boundary condition $q_n = 0$ and at the boundary x=L=d_s+d_p we have a prescribed Dirichlet boundary condition $T_{pb} = T_g$ which means that the temperature at the boundary of the insulation is the temperature of the convective medium (=gas temperature of the surrounding fire), we get only one equation:

$$\dot{T}_s + \frac{\tilde{\lambda}_p \tilde{A}_p / d_p}{C_s + C_{11}^p}(T_s - T_g) = -\frac{C_{12}^p}{C_s + C_{11}^p}\dot{T}_g \tag{46}$$

where the following notation has been used: $\tilde{\lambda}\ \tilde{A}_p = \frac{1}{2}\int_{-1}^{1} \lambda_p(T(\xi))A_p(\xi)d\xi$,

$C_s = \rho_s A_s c_s(T_s)d_s$ and $C_{ij}^p = \frac{d_p}{2}\int_{-1}^{1} \rho_p(T(\xi))c_p(T(\xi))N_i(\xi)N_j(\xi)A_p(\xi)\ d\xi$.

Let us assume that the thermal conductivity depends on temperature and the specific heat of the protection is constant. Insulation is assumed to be so thin that the area of the perimeter of the protection can be considered constant, $A_p(\xi) = A_p$ (see Fig 8b). Then equation (46) will have the form:

$$\dot{T}_s + \frac{\tilde{\lambda}_p A_p / d_p}{C_s + C_p / 3}(T_s - T_g) = -\frac{C_p / 6}{C_s + C_p / 3}\dot{T}_g \tag{47}$$

where $\tilde{\lambda} = \lambda_p(T(\xi = 1/2)) = \lambda_p((T_s + T_g)/2)$ is calculated at the midpoint of the element (protection) when one point Gauss integration is used. Dividing by $C_s = c_s \rho_s V_s$ we finally get the equation:

$$\dot{T}_s = \frac{\tilde{\lambda}_p A_p / d_p}{c_s \rho_s V_s (1+\phi/3)} (T_g - T_s) - \frac{\phi/6}{1+\phi/3} \dot{T}_g \tag{48}$$

where notations $\phi = C_p / C_s$ and $\mathrm{C_p} = d_p \rho_p c_p A_p$ have been used

This equation is the same as the equation derived by Melinek and Thomas (1987) in a case when material properties are constant. They considered this equation to be the best one when $C_p / C_s << 1$. The equation is nearly the same as the equation proposed by Wickström (1985):

$$\dot{T}_s = \frac{\lambda_p A_p / d_p}{c_s \rho_s V_s (1+\phi/3)} (T_g - T_s) - [\exp(\phi/10) - 1]\ \dot{T}_g \tag{49}$$

The coefficients of $\dot{T}_g$ are also quite near each other, when $C_p / C_s < 1{,}7$ as can be seen in Figure 9. The equation by Wickström is the one that is used in design codes for metal structures: Eurocode 3 for steel structures and Eurocode 9 (1995) for aluminium structures.

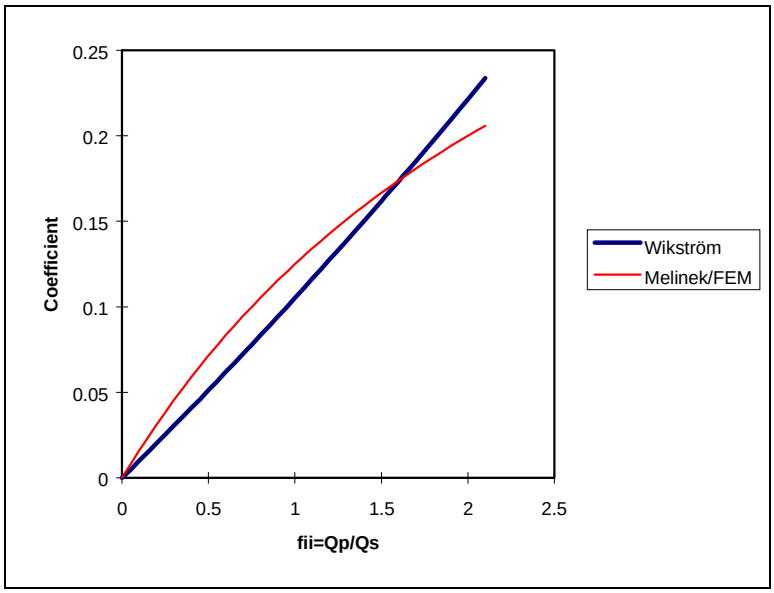

Figure 9. The coefficent of $\dot{T}_g$ as a function of parameterϕ, Wickström´s coefficient (bold line) coefficient of FEM solution (thin line).

If we had used the diagonal capacity matrix instead of the consistent capacity matrix: $C_{11}^p = C_{22}^p = C_p / 2 \quad ; \quad C_{12}^p = C_{21}^p = 0$, we would have obtained the equation:

$$\dot{T}_s = \frac{\tilde{\lambda}_p A_p / d_p}{c_s \rho_s V_s (1 + \phi / 2)} (T_g - T_s) \tag{50}$$

which is the equation derived by McGuire et al. (1975).

Actually, equations (48) and (50) above are valid when the *specific heat of the protection is constant and insulation is so thin that the protection area can be considered constant.* Otherwise, equation (47) should be used. If the one point Gauss integration scheme is used the equation (47) will have the form:

$$\dot{T}_s = \frac{\tilde{\lambda}_p\ (T_p)\tilde{A}_p / d_p}{c_s \rho_s V_s\ (1+\tilde{\phi}(T_p)/4)}(T_g - T_s) + \frac{\tilde{\phi}(T_p)/4}{1\ +\tilde{\phi}(T_p)/4}\dot{T}_g \tag{51}$$

where $\tilde{\phi}(T_p, T_s) = C_p / C_s = \frac{\tilde{A}_p d_p \rho_p c_p(T_p)}{A_s d_s \rho_s c_s(T_s)}$, $T_p = (T_s + T_g)/2$ and $\tilde{A}_p(T_p)$ is the area of the perimeter of the insulation calculated at the midpoint of the insulation. This is also one of the alternative equations proposed by Melinek and Thomas (1987).

The inverse solution of an equation of the type

$$\dot{T}_s = A\,(T)(T_g - T_s) + B(T)\ \dot{T}_g \tag{52}$$

is achieved by minimizing equation (18) , where $y^o(t)\ \ (\equiv T_s^o(t))$ is the measured temperature of the metal structure, and $y\ \ (t)\ \ (\equiv T_s\ (t))$ is the solved temperature of the metal structure. The discrete coefficient-solution operator is in this case

$$\tilde{F}(T_s^{n-1}, \Delta t_n) = T_s^n = T_s^{n-1} + A^{n-1}(T_g^{n-1} - T_s^{n-1})\Delta t_n + B^{n-1}T_g^{n-1} \tag{53}$$

when the explicit Euler scheme is used.

6.1.1 Numerical example: Steel section protected with intumescent paint

Fire protection materials for steel structures are studied according to the NORDTEST method NT FIRE 021 (1980) in the Nordic countries. In this method, the protected steel column is placed in the horizontal furnace. The temperature of the steel and the gas temperature near the protected section are measured by thermocouples. The thermal conductivity of the protection material is calculated as a function of time using the equation and the derivatives $\dot{T}_s$ of the measured steel temperature. Small deviations in the measured temperature data may cause large differences in the calculated thermal conductivity. The measured temperature is thus smoothed.

The method is also applied to intumescent paints that expand during testing and for which the equation is not actually valid. The thermal conductivity is calculated assuming that the material does not expand and maintains its original thickness. The calculated thermal conductivity is not real but effective which can then be used in the design procedure of steel structures.

Figure 10b shows the thermal conductivities calculated using ROLS. The discrete operator (27) and test results of a commercially available intumescent paint are used. Figure 10a shows the furnace temperature and the measured and calculated temperatures in the steel specimen.

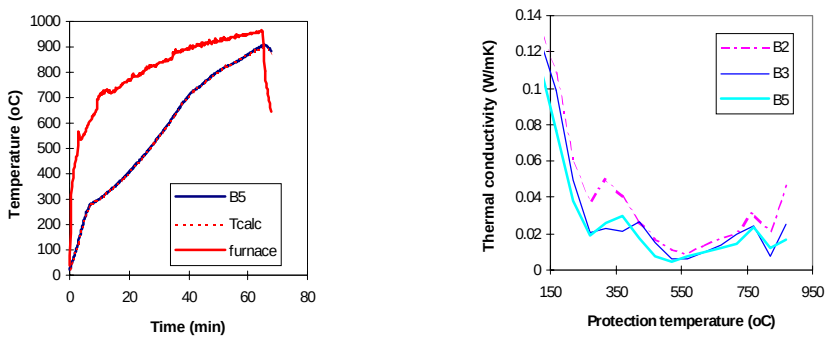

Figure 10 a) Furnace temperature, and measured and calculated temperatures of the steel specimen, b) thermal conductivities of the intumescent paint as a result of the inverse solution. B2, B3 and B5 are the identification numbers of test specimens.

6.1.2 Numerical example: Aluminium plate protected by gypsum board

The cone calorimeter test in a horizontal configuration at a heat flux level of q_{cone} = 25 kW/m^2 was performed. The test specimen consisted of a 13 mm thick gypsum board (density 721 kg/m^3) laying on a 30 mm thick layer of mineral wool (Fig. 11). The surface area exposed to the heat flux was A_1=100 mm x 100 mm. There was a 10 mm thick aluminium plate under the gypsum board. The temperature of the upper surface of the gypsum board was measured using an infrared temperature measuring device.

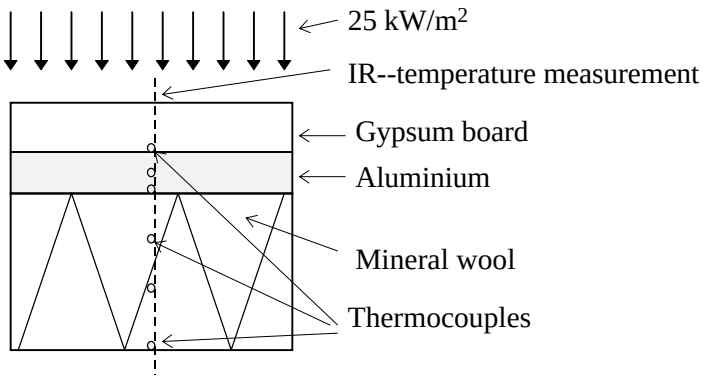

Figure 11. Idealized test arrangements in the cone calorimeter test with aluminium plate.

The temperature distribution inside the gypsum board was approximated to be linear and the aluminium temperature was assumd as a constant. Equation (51) with discretization (53) was used in modelling the direct problem. Here both the specific heat and the thermal conductivity were discretized using piece-wise linear basis functions with respect to the temperature. Figure 12 shows the results. The thermal conductivity of gypsum according to Pettersson and Ödeen (1978) is shown for comparison.

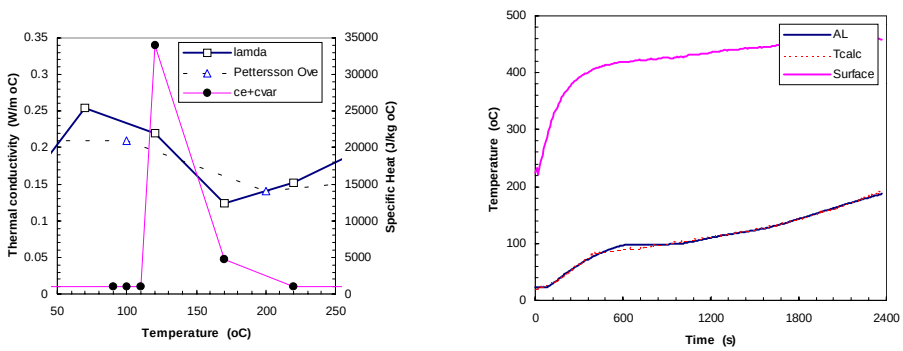

Figure 12. a) Calculated specific heat and thermal conductivity of the gypsum board measured in a cone calorimeter experiment at 25 kW/m². Test data for the thermal conductivity according to Pettersson and Ödeen (1978) is shown for comparison. b) Measured surface temperatures and the temperature of the aluminium plate, in bold and the calculated in a thin dotted line.

6.2 Determination using two ODEs

Consider once again an insulated steel structure. The problem is now treated as a one dimensional problem using three elements (Fig 13). One element is used for the steel part and two elements for the insulation part. For the steel part it is assumed that the temperature is uniform (one basis function $N_1 = 1$, one trial function $v = 1$). For the insulation, two elements with linear interpolation polynomials are used.

We get a following initial value problem:

$$\mathbf{C}\dot{\mathbf{T}} = \mathbf{f} - \mathbf{K}(t, \mathbf{T})\mathbf{T} \tag{54}$$

If integration is conducted using one Gauss integration point at the centre of the finite elements we get the following formula for the calculation of the terms of the element capacity matrix;

$$C_{\mathrm{ij}}^{(\mathrm{e})} = \frac{d_p}{2} \int_{-1}^{1} \rho^{(e)}{}_p(T(\xi)) c^{(e)}{}_p(T(\xi)) N_i(\xi) N_j(\xi) A_p{}^{(e)} \, d\xi \tag{55}$$

$$= \frac{1}{4} \, (\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(e)}$$

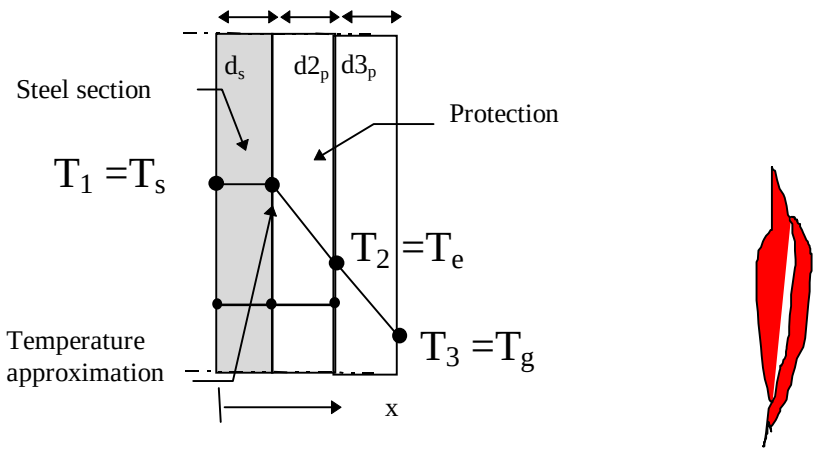

Figure 13. One dimensional idealization of an insulated steel structure on fire, with two linear elements for fire protection.

The terms of the element conductivity matrix are

$$K_{ij}^{(e)} = \frac{1}{2d_p^{(e)}} \int_{-1}^{1} \lambda_p(T(\xi)) A_p d\xi = \frac{\tilde{\lambda}_p \tilde{A}_p}{d_p}$$

where the thermal properties f_p as well as the area have been calculated at the centre of the element using equations $\tilde{f}_p^{(e)} \equiv f_p(\frac{T_1^{(e)} + T_2^{(e)}}{2})$, $\tilde{A}_p = A_p(\frac{x_1^{(e)} + x_2^{(e)}}{2})$ where superscript $^{(e)}$ refers to the number of element.

When the Dirichlet type of boundary condition $T_3 = T_g$ (surface temperature of the fire protection is the same as the gas temperature) is used, and the corresponding variable is eliminated from equation (54), we get the following matrix equation with two unknowns, steel temperature $T_s = T_1$ and fire protection temperature $T_e = T_2$;

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{pmatrix} \dot{T}_1 \\ \dot{T}_2 \end{pmatrix} + \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = -\begin{pmatrix} K_{13}T_g + C_{13}\dot{T}_g \\ K_{23}T_g + C_{23}\dot{T}_g \end{pmatrix} \tag{56}$$

where the conductivity matrix is

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} = \begin{bmatrix} (\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(2)} & -(\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(2)} \\ -(\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(2)} & (\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(2)} + (\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(3)} \end{bmatrix} \tag{57}$$

the capacity matrix is

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} \tilde{\rho}_s \tilde{c}_s d_s \tilde{A}_s + \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(2)} & \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(2)} \\ \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(2)} & \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(2)} + \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(3)} \end{bmatrix} \tag{58}$$

and the “force” vector is

$$--\begin{pmatrix} K_{13}T_g + C_{13}\dot{T}_g \\ K_{23}T_g + C_{23}\dot{T}_g \end{pmatrix} = -\begin{pmatrix} 0 \\ -(\frac{\tilde{\lambda}_p \tilde{A}_p}{d_p})^{(3)} T_g + \frac{1}{4}(\tilde{\rho}_p \tilde{c}_p d_p \tilde{A}_p)^{(3)} \dot{T}_g \end{pmatrix} \tag{59}$$

Equation (56) is solved by using the explicit Euler scheme.

$$\begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{pmatrix} T_1^n \\ T_2^n \end{pmatrix} = -\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}^{n-1} \begin{pmatrix} T_1^{n-1} \\ T_2^{n-1} \end{pmatrix} - \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}^{n-1} \begin{pmatrix} T_1^{n-1} \\ T_2^{n-1} \end{pmatrix} \Delta t - \begin{pmatrix} K_{13}T_g + C_{13}\dot{T}_g \\ K_{23}T_g + C_{23}\dot{T}_g \end{pmatrix}^{n-1} \Delta t_n \tag{60}$$

6.2.1 Thermal conductivity of rock wool determined from fire resistance tests

Fire resistance tests on steel columns were performed at VTT (Ala-Outinen and Oksanen 1997). The columns were rectangular hollow sections with a cross-sectional dimension of RHS 40x40x4. The length of each column was 900 mm with the end plates. The columns were protected with 20 mm thick rock wool

(density 220 kg/m^3). Rock wool sheets were attached to each other with a fixing system consisting of spirals and screws.

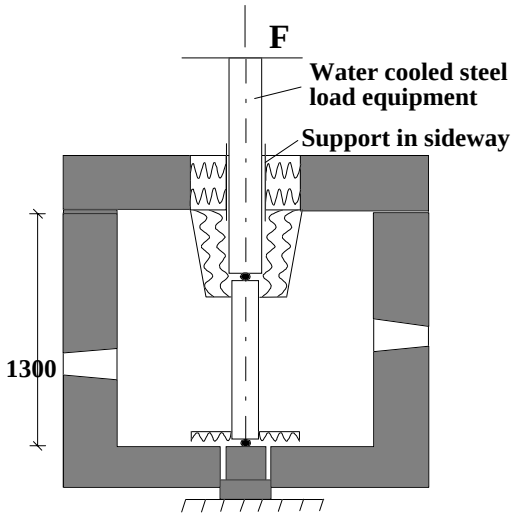

Figure 14. Set-up in furnace tests.

A preliminary test was performed before the actual test series in order to find the right temperature rise in the furnace and to collect data on the behaviour of rock wool as well as the fixing system. The preliminary specimen tested was a rectangular hollow section (50x50x5) with rock wool as fire protection. The specimen was applied to a fire exposure of 15 ^{o}C/min for 65 min. On the basis of the temperatures measured, the temperature field of the steel section (40x40x4) was calculated as a function of time with a different gas temperature rate in the furnace. As a result, it was decided to control the temperatur from 20 ^{o}C to 300 ^{o}C within 3 min and subsequently by 5 ^{o}C/min. All columns were tested in the vertical position. The steel columns were heated in a model furnace specially built for testing loaded columns and beams.

The temperatures of each column were measured at three cross-sections using a total of 12 Chromel-Alumel thermocouples of the K-Type, 2 x 0.5 mm. Furnace gas temperatures 100 mm from the columns were measured with 12 Chromel-Alumel thermocouples of the K-type, ∅ 3 mm stainless steel sheathed, at the

same levels as for the steel temperatures. Figure 15. shows the location and numbering of thermocouples in the steel sections.

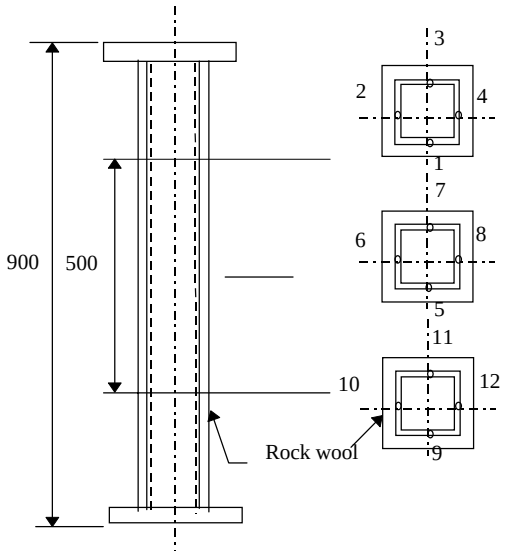

Figure 15. Column specimen details and location of thermocouples.

Thermal conductivity as a function of temperature is determined from these tests. Heat losses are also estimated. Thus, the problem is to estimate the thermal conductivity and heat loss terms appearing in the energy conservation equation. The heat losses, in the direction perpendicular to the cross section, are the terms Q_1 (through steel) and Q_2 (Wool). These terms are due to the treatment of the original 3-D heat conduction problem as a 1-D problem.

Therefore, the inverse problem consists of estimating the thermal conductivity of the thermal insulation (rock wool) as a function of the temperature using data (measured temperatures) from 'full scale' fire tests on an insulated steel structure, i.e. $\mathbf{a} = (\lambda(T)\ \ Q_1\ \ Q_2)$.

Consider the insulated steel structure, Figure 16. The direct problem is now trcated as a one dimensional problem using three elements. One element is used for the steel part and two linear elements for the insulation part. For the steel part it is assumed that the temperature is uniform (one basis function $N_1 = 1$).

In the first case (a 50x50x5 column) only the temperature of the steel section was measured while in the second case (a 40x40x4 column) the temperature of the fire protection at the centre was also measured (Fig. 16b). In both cases, the direct problem was formulated using two linear elements in the fire protection as in (56).The system (56) of ODEs was integrated using the explicit Euler scheme.

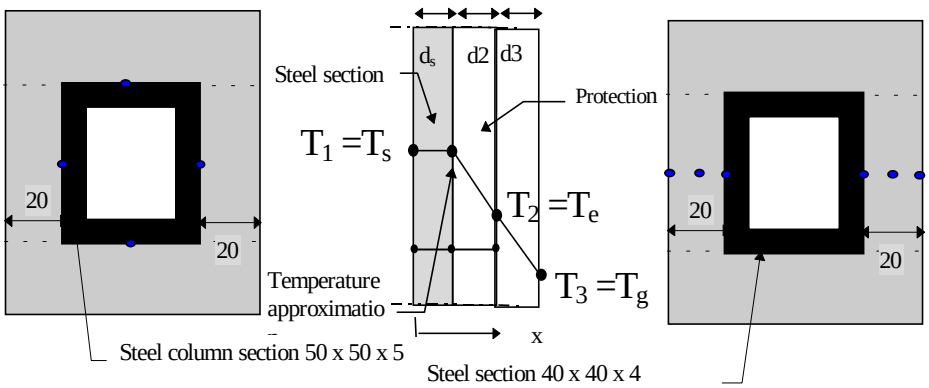

Figure 16. The cross-section of the test columns and one dimensional idealization of insulated steel structure in fire, linear elements at the fire protection.

Integration of the heat conductivity matrix $\mathbf{K^e}$ and of the force vector $\mathbf{f^e}$ are performed using one Gauss integration point at the centre of the elements. The element capacity matrix $\mathbf{C^e}$ was integrated using two-point Newton-Cotes integration (at the nodal points of the element, $\xi = -1$ and $\xi = +1$ in Eq. (56)) in order to get a diagonal matrix ($\mathbf{C}_{ij} = 0$, when i differs from j, i.e. C_{12}, C_{13}, C_{23} *and* C_{21} in Eq. (60) are all zero). In this way we avoid unstable numerical differentiation of T_g in Eq. (60), since the gas temperature is very noisy as seen in Figure 17b (the upper curve).

The following values of parameters were assumed in the calculation: density of the fire protection ρ_p = 220 kg/m^3, specific heat of the protection c_p =1000 J/kgK, the density of steel ρ_s = 7850 kg/m^3 and specific heat of the steel c_p =540 J/kgK. The mean of the measured temperatures of the steel section and of the insulation (at the midpoint) at the centre of the column were used as collocation points.

Thus, the effective thermal conductivity $\lambda(\mathrm{T})$ was found as the regularized solution of the constrained minimization problem

$$\min\left(\left\| \tilde{T}_{test}^{\ \delta}(t) - \tilde{T}_{calc.}(\vec{a};t) \right\|^2 + \alpha \left\| \mathbf{L}\vec{\lambda} \right\|^2 \right), \qquad with\ \lambda_j \in D(\vec{\lambda}) \tag{61}$$

where the operator $\mathbf{L}$ is the central difference discretization of the second derivatives $\partial^2 \lambda\ (T)/\partial T^2$ of the thermal conductivity. The accuracy measurements of the temperature were estimated to be $\left\| \tilde{T}^{\delta}(t) - \tilde{T}(t) \right\| \le \delta \approx \int_{t_\infty} 10\ ^{o}C\, dt$ when applying the Morozov discrepancy principle.

The solution to the problem is presented in Fig. 17a) and compared with the values provided by the producer of rock wool (the dashed line). For heat loss, these valves, (Q_1,Q_2) = (-2.2, -0.4) W/m are achieved. The calculated temperature history (for one test) is compared to the experimental one in Fig. 17 b. Legends for Figure 17 a are:

- The balls (column: 40x40x4), calculated using two elements and two collocation points (the steel and the mineral wool)

- The triangles (column: 40x40x4), the same as the balls but only one collocation point was used (the steel temperature)

- The squares represent the case where two data tests were used simultaneously (column 40x40x4 with two collocation points: the steel and the wool at the midpoint and column 50x50x5 with one collocation point: the steel). The temperature calculations were made using two elements for both columns.

- The dashed line shows values provided by the producer.

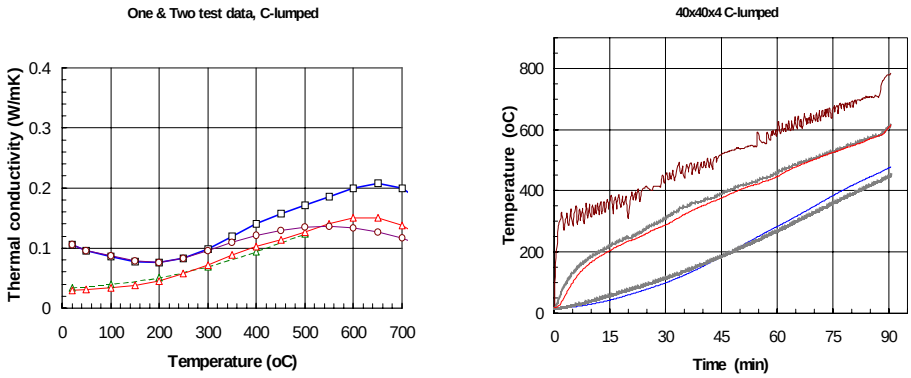

Figure 17. a) Calculated thermal conductivity of mineral wool using a different number of elements and collocation points with test data (columns: 40x40x4 and 50x50x5). b) The calculated temperatures (thick) and the measured ones (thin) for the 40x40x4 column (the temperature of the protection at the midpoint and of the steel). The upper curve represents the gas temperature.

7. SUMMARY

Several applications of the regularised output least square method (ROLS) to the parameter identification of heat transfer in structures were presented. Although the examples shown consist only of a one or two ODEs, the method is directly applicable to a system of ODEs obtained by semi-discretization of the variational formulation of the general heat conduction problem using a finer FEM-mesh.

The presented method (with only one or two ODEs) can be applied to the assessment of fire protection of steel structures. Other applications in fire technology may need a finer mesh.

The new method is a reliable way to identify the non-linear coefficients of a system of ODEs. It can be applied to other problems of fire technology as well. The authors have applied the method to the identification of mechanical properties, such as temperature dependent variables of rate dependent plastic (i.e. the viscoplastic material model of metals). One application might be the identification of parameters of fire models (zone model etc.).

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