Finite Element Modelling Of Thermal Processes With Phase Transitions

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Interim Master's Thesis

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PREFACE

This interim Masters thesis is written for the degree of Master of Science for the study Applied Mathematics, faculty of Electrical Engineering, Mathematics and Computer Science of Delft University of Technology. The graduation work is done in the unit of Numerical Analysis. The Masters project is being carried out at TNO Science and Industry, department of Process Modeling and Control, business unit Industrial Modeling and Control. At TNO Science and Industry nine months of work will be done on the Finite Element Modelling Of Thermal Processes With Phase Transitions. The Masters project is separated into two parts: the first three months are intended for literature study to introduce the Masters project, the last six months are designed to carry out the planned research. This interim Masters thesis comprises the first part of the project.

Delft, December 2006   Abdelhaq Abouhafç

1 Introduction

Adding and removing heat and mass to and from a product take place in several processes in the industry. For example: steam production, freezing and drying. Improving product quality is the objective of using Physical and chemical models.These models solve a set of heat and mass equations as a function of time and position. The pressure is assumed to be constant, while the temperature and concentration are chosen as state variables. When phase change takes place during these processes the modeling becomes more complicated. In this case using only temperature and concentration is not sufficient for the process description. Additional state variables such as solid, liquid and vapor fractions are needed.

The simulation model should decide which equations are appropriate at a given time during the simulation; one should also take into account that the phase changes usually occur during a part of the entire process. The simulation of thermal process with phase changes is usually quite difficult because we need to solve different sets of equations for different phases of the process. Switching from one set of equations to another can cause instability of the numerical solution. We also need to use a large amount of input parameters, such as specific heat and densities of all phases and latent heat of phase changes. We can take the input parameters constant such that the model becomes easier.

The objective of this project is the combination of the density-enthalpy phase diagram with finite elements methods. The finite element method can be used to solve transport equations (mass, heat and impulse) and the density-enthalpy phase diagram gives the thermodynamics constants. The permeability, viscosity and heat conductance are very important in this case. The developed models can be used to optimize processes and products quality. The structure of this interim thesis is as follows: In Chapter 2, the basic principles and tools of finite element method are discussed, followed by the thermodynamic description in Chapter 3. Chapter 4 discuss the continuation of the Master project.

2 Finite element method

2.1 Introduction

The finite element method is a computational technique for obtaining approximate solutions to partial differential equations that arise in scientific and engineering applications.
Rather than approximating the partial differential equation directly as with e.g. finite difference methods, the finite element method utilizes a variational problem that involves an integral the equation over the problem domain. This domain is divided into a number of subdomains called elements and the solution of the partial differential equation is approximated by a function on each element. These polynomials have to be pieced together so that the approximate solution has an appropriate degree of smoothness over the entire domain. Once this has been done, the variational integral is evaluated as a sum of contributions from each finite element.

The result is an algebraic system for the approximate solution having a finite size rather than the original infinite dimensional partial differential equation. Thus, like finite difference methods, the finite element process has discretized the partial differential equation but, unlike finite difference methods, the approximate solution is known throughout the domain as a piecewise polynomial function and not just at a set of points. A finite element method has a number of advantages relative to other methods including:

- Treatment of problems on complex irregular regions.

- Use of non-uniform meshes to reflect solution gradations(gradual change).

- Treatment of boundary conditions involving fluxes, and

- Construction of high order approximations.

Originally used for steady elliptic problems, the finite element method is now also used to solve transient parabolic and hyperbolic problems.

2.2 1D steady diffusion equation

Let us consider Poisson equation in one dimension

$$
\begin{align}
-k\frac{d^2T}{dx^2} &= f(x), \quad 0 \leq x \leq \pi, \tag{2.2.1}\\
T(0) &= 0, \tag{2.2.2}\\
\frac{dT}{dx}(\pi) &= 0. \tag{2.2.3}
\end{align}
$$

In order to construct the basis functions, we subdivide the interval [0,1] into subelements $e_i = [x_{i-1}, x_i]$, $i = 1, ..., N$ with $x_i = \frac{i}{N}$ as shown in the Figure 2.2.1
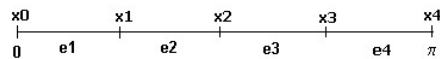
Figure 2.2.1: Subdivision of the interval $[0, \pi]$ in elements

The linear interpolation polynomial of the function $T(x)$ over the element e_i is defined by

$$T_i(x) = \frac{x - x_i}{x_{i-1} - x_i}T(x_{i-1}) + \frac{x - x_{i-1}}{x_i - x_{i-1}}T(x_i) \tag{2.2.4}$$

We define linear Lagrangian polynomials $l_i(x)$ as follows

$$l_{i-1}(x) = \frac{x - x_i}{x_{i-1} - x_i}; \quad l_i(x) = \frac{x - x_{i-1}}{x_i - x_{i-1}} \tag{2.2.5}$$

and write (2.2.4) as

$$T_i(x) = l_{i-1}(x)T(x_{i-1}) + l_i(x)T(x_i) \tag{2.2.6}$$

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Clearly, $l_{i-1}(x)$ and $l_i(x)$ are linear on e_i and are defined by the relations:

$$l_r(x_s) = \delta_{rs}, \quad r, s = i - 1, i. \tag{2.2.7}$$

From (2.2.6), it is clear that $T(x)$ is a linear combination of $T_0, T_1, ..., T_n$ so that we can write:

$$T(x) = \sum_{j=1}^{n} T_j \varphi_j(x), \tag{2.2.8}$$

where for each control point x_j we will choose the piecewise linear function $\varphi_j(x)$:, whose value is 1 at x_j and zero at every other $x_i, j \neq i$, i.e.,

$$\varphi_i(x) = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}} & \text{if } x \in [x_{i-1}, x_i] \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} & \text{if } x \in [x_i, x_{i+1}] \\ 0 & \text{otherwise} \end{cases} \tag{2.2.9}$$

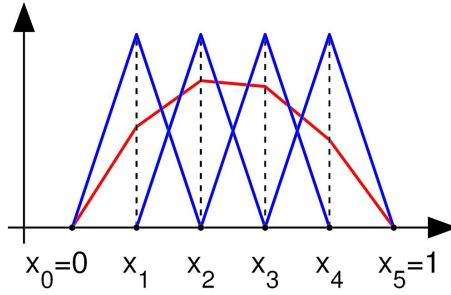The function $\varphi_i(x)$ is illustrated in Figure 2.2

Figure 2.2.2: The basis function in one dimension

Note that $\varphi_i(x)$ is only non-zero in the elements that contain the node x_i, The basis function is defined implicitly by:

- $\varphi_i(x)$ is linear in each element.

- $\varphi_i(x) = \delta_{ij}$

2.2.1   Weak formulation and Galerkin approximation

In order to derive the weak formulation, we multiply the equation (2.2.6) by a test function η, satisfying the homogeneous essential boundary condition $\eta(0) = 0$ and integrate over the domain $\Omega = [0, 1]$, we get:

$$\int_0^\pi \left(k \frac{d^2 T}{dx^2} + f \right) \eta dx = 0. \tag{2.2.10}$$

Integrating by parts, we obtain

$$-\int_0^\pi k \frac{d\eta}{dx} \frac{dT}{dx} d\Omega + \int_0^\pi \eta f d\Omega + \left[\eta (k \frac{dT}{dx}) \right]_0^\pi = 0. \tag{2.2.11}$$

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We get the weak formulation after the application of the boundary conditions as well as the essential boundary condition for the test function

$$\int_0^\pi k \frac{d\eta}{dx} \frac{dT}{dx} d\Omega = \int_0^\pi \eta f d\Omega. \tag{2.2.12}$$

The Galerkin equations corresponding to the weak formulation are given by

$$\sum_{j=1}^n \int_0^\pi k \frac{d\varphi_i}{dx} \frac{d\varphi_j}{dx} d\Omega = \int_0^\pi f \varphi_i d\Omega, \quad i = 1, ..., n. \tag{2.2.13}$$

We obtain the following system of equations

$$ST = F, \tag{2.2.14}$$

where the stiffness matrix is

$$S_{ij} = \int_0^\pi k \frac{d\varphi_j}{dx} \frac{d\varphi_i}{dx} dx, \tag{2.2.15}$$

and the vector F is

$$F_i = \int_0^\pi f \varphi_i dx. \tag{2.2.16}$$

2.2.2 Numerical integration

The right-hand-side vector of (2.2.13) contains an integral over a function $f(x)$. In general, exactly computing this integral is very difficult, so a numerical approximation is required. Well-known integration rules are:

- mid-point rule: $\int_{t_{i-1}}^{t_i} g(x) dx \simeq (t_i - t_{i-1}) g(t_{i-1/2})$,

- Trapezoid rule: $\int_{t_{i-1}}^{t_i} g(x) dx \simeq \frac{t_i - t_{i-1}}{2} \{g(t_{k-1}) + g(t_k)\}$,

- Simpson's rule: $\int_{t_{i-1}}^{t_i} g(x) dx \simeq \frac{t_i - t_{i-1}}{6} \{g(t_{k-1}) + 4g(t_{k-1/2}) + g(t_k)\}$.

All these rules can be written in the general form

$$\int_{t_{i-1}}^{t_i} g(x) dx \simeq \sum_{k=1}^r w_k g(t_k), \tag{2.2.17}$$

with r is the number of the integration points, w_k is the weight, and t_k is the integration point. Another class of integration rules of the form (2.2.17) are the Gaussian rules. An q-point Gaussian quadrature rule is a quadrature rule constructed to yield an exact result for polynomials of degree $2q-1$, by a suitable choice of the q points t_k and q weights w_k. The domain of integration for such a rule is conventionally taken as $[-1, 1]$, so the rule is stated as

$$\int_{-1}^1 g(x) dx = \sum_{k=1}^r w_k f(t_k),$$

where t_k is the integration point, and w_k is the weight of that point in the sum. Some low-order rules for solving the integration problem are listed below

Number of points, n	Points, x_k	Weights, w_k
1	$x_1 = 0$	$w_1 = 2$
2	$x_1 = -\sqrt{\frac{1}{3}}, \; x_2 = \sqrt{\frac{1}{3}}$	$w_1 = w_2 = 1$
3	$x_1 = -\sqrt{\frac{3}{5}}, \; x_2 = 0, x_3 = \sqrt{\frac{3}{5}}$	$w_1 = w_3 = \frac{5}{9}, \; w_2 = \frac{8}{9}$

Change of interval for Gaussian quadrature

An integral over [a, b] must be changed into an integral over [-1, 1] before applying the Gaussian quadrature rule. This change of interval can be done in the following way

$$\int_a^b g(t)dt = \frac{b-a}{2}\int_{-1}^{1} g(\frac{b-a}{2}x + \frac{a+b}{2})dx. \qquad (2.2.18)$$

After applying the Gaussian quadrature rule, the following approximation is obtained

$$\frac{b-a}{2}\sum_{k=1}^{r} w_k g(\frac{b-a}{2}t_k + \frac{a+b}{2}). \qquad (2.2.19)$$

2.2.3 Element matrices and element vectors

In order to construct the large matrix and large vector, it is necessary to evaluate the integrals in (2.2.13) Since $\varphi_i(x)$ is defined element-wise, we write

$$\int_0^\pi \frac{d\varphi_j}{dx}\frac{d\varphi_i}{dx}dx = \sum_{k=1}^{n}\int_{e_k}\frac{d\varphi_j}{dx}\frac{d\varphi_i}{dx}dx.$$

Using the linear basis function, we obtain the element stiffness matrix

$$S^e = \frac{k}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

the element vector is given by

$$F^e = \frac{h}{2}\begin{bmatrix} f(x_1) \\ f(x_2) \end{bmatrix}.$$

where h is the length of the element.

2.2.4 Assembly of the large matrix and vector

All information of the FEM is stored in element matrices, element vectors, and the problem topology. In order to create the large matrix and vector, we apply the assembly process. We consider the subdivision of the region $[0,1]$ into 4 elements as illustrated in Figure 2.2.1, element e_i is defined by: $e_i = [x_{i-1}, x_i]$ and the nodes are numbered from 0 to 4. The large matrix has size (4×4) and the large vector (4×1). The problem topology of this case is very simple, each element contains two unknows.

$$e_1 : \{0, 1\},$$
$$e_2 : \{1, 2\},$$
$$e_3 : \{2, 3\},$$
$$e_4 : \{3, 4\}.$$

In the first step the large matrix and vector are cleared

$$S^0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad (2.2.20)$$

$$f_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \qquad (2.2.21)$$

The element matrix for an arbitrary element e_k has shape

$$S^{e_k} = \frac{1}{t_k - t_{k-1}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \qquad (2.2.22)$$

We apply the Newton-Cotes rule, to obtain the element vector

$$f^{e_k} = \frac{k(t_k - t_{k-1})}{2} \begin{bmatrix} f(t_{k-1}) \\ f(t_k) \end{bmatrix}. \qquad (2.2.23)$$

We assume an equidistant grid with step size

$$t_k - t_{k-1} = h. \qquad (2.2.24)$$

First, we assemble element matrix 1 and element vector 1, Since T_0 is given, only the term involving φ_1 is needed. Hence

$$S^{e_1} = \frac{k}{h}[1], \qquad f^{e_1} = \frac{h}{2}[f(x_1)]. \qquad (2.2.25)$$

Adding matrix and right-hand side to (2.2.20)and (2.2.21) gives

$$S^1 = \frac{k}{h} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad (2.2.26)$$

and

$$f_1 = \frac{h}{2} \begin{bmatrix} f(x_1) \\ 0 \\ 0 \\ 0 \end{bmatrix}. \qquad (2.2.27)$$

Next, we add S^{e_2} and S^{f_2} to S^1 and f^1

$$S^1 = \frac{k}{h} \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad (2.2.28)$$

and

$$f_1 = \frac{h}{2} \begin{bmatrix} 2f(x_1) \\ f(x_2) \\ 0 \\ 0 \end{bmatrix}. \qquad (2.2.29)$$

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Repeating this process for e_3 and e_4 leads to

$$S = S^4 = \frac{k}{h} \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \qquad (2.2.30)$$

and

$$f = f_4 = \frac{h}{2} \begin{bmatrix} 2f(x_1) \\ 2f(x_2) \\ 2f(x_3) \\ f(x_4) \end{bmatrix}. \qquad (2.2.31)$$

2.2.5 Boundary conditions and assembly

Most packages subdivide the finite element process in three steps

- Preprocessing : The mesh generation

- Solving the actual FEM

- Post processing: showing the results

The solve part consists globally of the following steps:

- Read input and mesh

- Compute the structure of the large matrix from the topology

- Clear large matrix and vector

for all elements, including boundary elements, **do**
       Compute element matrix and vector
       Add element matrix to large matrix
       Add element vector to large vector
end for
Apply the essential boundary conditions
Solve system of equations
write results of post processing

Numerical result

Consider the Poisson equation defined in 2.2.1, if we take $f(x) = sin(x)$, the exact solution becomes $T(x) = \frac{1}{k}sin(x) + \frac{x}{k}$. In Figure 2.2.3, we compare between the exact and the numerical solution.

2.3 1D Time Dependent Convection Diffusion Equation

2.3.1 Standard Galerkin Approach: (SGA)

Consider the following 1D time dependent convection diffusion equation

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + u\frac{\partial T}{\partial x} = f(x), \quad 0 \le x \le 1, \quad t \ge 0. \qquad (2.3.1)$$
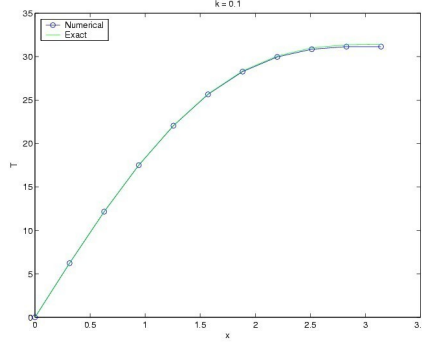
Figure 2.2.3: Exact and numerical solution of poisson equation using finite elements method, k = 0.1

with initial condition

$$T(x,0) = T_0, \tag{2.3.2}$$

and boundary conditions

$$T(0,t) = T_0, \quad \frac{\partial T}{\partial x}(1,t) = 0. \tag{2.3.3}$$

where:

k diffusion number,
u convetion number,
f source term.

To derive the weak formulation, we multiply the equation (2.3.1) by a test function η satisfying the homogenous essential boundary condition $\eta(0,t) = 0$ and integrate over the domain $[0,1]$, we obtain

$$\int_0^1 \left(\frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + u \frac{\partial T}{\partial x} \right) \eta dx = \int_0^1 f\eta dx. \tag{2.3.4}$$

After integrating by parts, we get

$$\int_0^1 \left(\frac{\partial T}{\partial t} \eta + k \frac{\partial T}{\partial x} \frac{\partial \eta}{\partial x} + u \frac{\partial T}{\partial x} \eta \right) dx = \int_0^1 f\eta dx. \tag{2.3.5}$$

The Galerkin equations corresponding to the weak formulation is given by

$$\sum_{j=1}^n \int_0^1 \varphi_j \varphi_i d\Omega \frac{\partial T_j}{\partial t} - \sum_{j=1}^n T_j \int_0^1 \left(k \frac{\partial \varphi_j}{\partial x} \frac{\partial \varphi_i}{\partial x} + u \frac{\partial \varphi_j}{\partial x} \varphi_i \right) dx = \int_0^1 f\varphi_i dx.$$

This gives a system of ordinary differential equations of the form

$$M \frac{dT}{dt} = ST + F, \tag{2.3.6}$$

where the mass-matrix is

$$M_{ij} = \int_0^1 \varphi_j \varphi_i d\Omega, \tag{2.3.7}$$

and the stiffness-matrix is

$$S_{ij} = -\int_0^1 \left(k \frac{\partial \varphi_j}{\partial x} \frac{\partial \varphi_i}{\partial x} + u \frac{\partial \varphi_j}{\partial x} \varphi_i \right) dx, \tag{2.3.8}$$

and

$$F_i = \int_0^1 f \varphi_i dx. \tag{2.3.9}$$

Using linear basis functions, the element stiffness-matrix is given by:

$$S^e = -\frac{k}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} - \frac{u}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}, \tag{2.3.10}$$

The element mass-matrix is given by

$$M^e = \frac{h}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{2.3.11}$$

and the element vector is given by

$$F^e = \frac{hf}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{2.3.12}$$

where h is the length of the element.

2.3.2 Comparison between numerical and exact solution

Let us consider the following time dependent 1D convection diffusion equation

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left(\frac{k \partial T}{\partial x} \right) + u \frac{\partial T}{\partial x} = f, \quad 0 \le x \le l, \tag{2.3.13}$$

with initial condition

$$T(x, 0) = T_0, \tag{2.3.14}$$

and boundary conditions

$$T(0, t) = T_0, T(l, t) = T_l. \tag{2.3.15}$$

where:
k diffusion term,
u convection term,
f source term,
l domain length.

The exact solution of this equation is

$$T(x,t) = sin\left(\frac{\pi x}{l}\right) \exp\left[\frac{u}{2k} x - t \left(\frac{u^2}{4k} + \frac{k\pi^2}{l^2} \right) \right] + C_1 exp\left(\frac{ux}{k}\right) + \left(\frac{x}{u}\right) f + C_2,$$

where C_1 and C_2 are defined by

$$C_1 = \frac{T_0 - T_1 + f(\frac{l}{u})}{1 - exp(Pe)}, \tag{2.3.16}$$

$$C_2 = \frac{-T_0 exp(Pe) + T_1 - f(\frac{l}{u})}{1 - exp(Pe)}, \qquad (2.3.17)$$

and Pe is the Peclet number.

$$Pe = \left(\frac{l}{k}\right) u. \qquad (2.3.18)$$

Numerical result

We use Standard Galerkin method and we discretize implicitly in time.

- Boundary conditions: $T(0,t) = 20, \quad T(l,t) = 40.$

- Initial condition: $T(x,0) = 20$
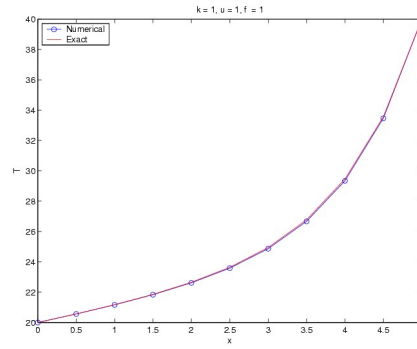
The result is shown in Figure 2.3.1

Figure 2.3.1: Exact and numerical solution of 1D time dependent convection diffusion equation using SGA method and implicit scheme after 500 time steps, dt = 0.1

2.3.3   Comparison between implicit and explicit scheme

We can discretize in time using forward Euler scheme (explicitly) or the backward Euler scheme (implicitly).

Implicit scheme

The implicit scheme for equation (2.3.6) is given by

$$M\frac{T^{\tau+1} - T^{\tau}}{\Delta t} = ST^{\tau+1} + F, \qquad (2.3.19)$$

which means that

$$\left(\frac{M}{\Delta t} - S\right) T^{\tau+1} = F + \frac{M}{\Delta t}T^{\tau}. \qquad (2.3.20)$$

Explicit scheme

The explicit scheme for the equation (2.3.6) is given by

$$M\frac{T^{\tau+1} - T^{\tau}}{\Delta t} = ST^{\tau} + F, \qquad (2.3.21)$$

which means that

$$\frac{M}{\Delta t}T^{\tau+1} = F + \left(S + \frac{M}{\Delta t}\right)T^{\tau}. \qquad (2.3.22)$$

A time step with an implicit scheme requires much more computing work than an explicit scheme. An implicit scheme is unconditionally stable, while an explicit scheme is only stable if two conditions are satisfied, that will be shown in the following section.

2.3.4 Stability analysis

First example

Consider the 1D convection equation:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = 0, \quad 0 \le x \le l, \qquad (2.3.23)$$

with initial condition:

$$T(x,0) = T_0, \qquad (2.3.24)$$

and boundary condition:

$$T(0,t) = T_0. \qquad (2.3.25)$$

where u is a convetion term.
We discretize in space with the upwind scheme (assuming $u > 0$) and in time with explicit scheme, we get:

$$T_j^{\tau+1} = T_j^{\tau} - c\left(T_j^{\tau} - T_{j-1}^{\tau}\right), \quad c = \frac{u\Delta t}{\Delta x}. \qquad (2.3.26)$$

where:

Δt time step,
Δx mesh size.

The dimensionless number c is called the *Courant number* or *CFL number*. If we use an explicit scheme, the following stability condition on the time step must be satisfied:

$$\frac{Speed(PDE)}{Speed(mesh)} = \frac{u}{\left(\frac{\Delta x}{\Delta t}\right)} \le 1 \qquad (2.3.27)$$

If the condition (2.3.27) is not satisfied, then we get instability as illustrated in Figure 4.3.4.
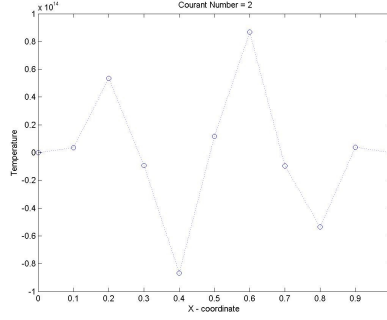
Figure 2.3.2: Numerical solution of 1D time dependent Convection equation using explicit scheme, Courant number = 2

Second example

Consider 1D heat equation

$$\frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(\frac{k \partial T}{\partial x}\right) = 0, \quad 0 \le x \le l. \tag{2.3.28}$$

with initial condition

$$T(x,0) = T_0, \tag{2.3.29}$$

and boundary conditions

$$T(0,t) = T_0, \quad \frac{\partial T}{\partial x}(1,t) = 0. \tag{2.3.30}$$

where k is a diffusion term.

We discretize in space with a central scheme and in time with explicit scheme, we get:

$$T_j^{\tau+1} = dT_{j-1}^{\tau} + (1 - 2d)T_j^{\tau} + dT_{j+1}^{\tau}, \quad d = \frac{k\Delta t}{\Delta x^2}. \tag{2.3.31}$$

where:

Δt time step
Δx mesh size

The dimensionless number d is called the *Diffusion number*. If we use an explicit scheme, the following stability condition on the time step must be satisfied:

$$\frac{k\Delta t}{\Delta x^2} \le 1 \tag{2.3.32}$$

If the condition (2.3.32) is not satisfied, then we get instability as illustrated in Figure 2.3.3.
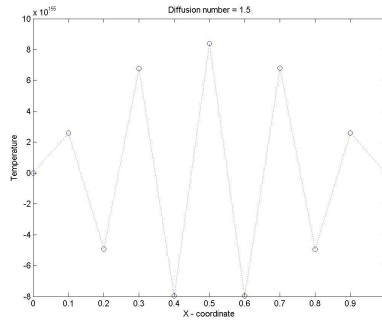
Figure 2.3.3: Numerical solution of 1D time dependent heat equation using explicit scheme, Diffusion number = 2

2.3.5 Streamline Upwind Petrov Galerkin method

To show the difference between SGA and SUPG we consider the previous problem of time dependent convection diffusion equation with source term, we discretize implicitly in time, $T(0,t) = 20, \quad T(l,t) = 40$. The result is shown in Figure 2.3.4
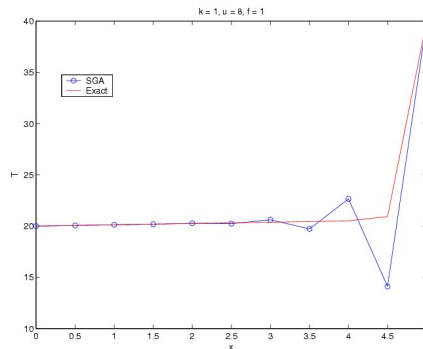

Figure 2.3.4: Numerical solution of 1D time dependent Convection diffusion equation using SGA method and implicit scheme after 500 time steps, dt = 0.1

The wiggles we get are due to convection. To avoid it, let us apply the upwind technique, we split $\eta(x)$ into two parts $w(x)$ and $p(x)$, $(\eta(x) = w(x)+p(x))$ where $w(x)$ is the classical test function, it ensures the consistency of the scheme and $p(x)$ is used to take care of the upwind behavior. In order to make integration by parts possible, the function $w(x)$ must be so smooth that integration by parts is allowed. $p(x)$ is defined elementwise, which means that it may be discontinuous over the elements boundaries. In practice, one chooses $p(x) = \frac{h\xi}{2}\frac{d\varphi_i}{dx}$ with ξ some parameter depending on the ratio of k and u. In this example ξ is chosen equal to $sign(u)$ which corresponds to the classical upwind scheme. Popular choices for ξ can be found in [7].

Following the same steps as in the previous method, we obtain a system of

16

ordinary differential equations of the form (2.3.6), where the mass-matrix is given by

$$M_{ij} = \int_0^1 \varphi_j \varphi_i d\Omega + \int_0^1 \varphi_j p dx, \qquad (2.3.33)$$

the stiffness-matrix is:

$$S_{ij} = -\int_0^1 \left(k \frac{\partial \varphi_j}{\partial x} \frac{\partial \varphi_i}{\partial x} + u \frac{\partial \varphi_j}{\partial x} \varphi_i \right) dx - \int_0^1 u \frac{\partial \varphi_j}{\partial x} p dx, \qquad (2.3.34)$$

and

$$F_i = \int_0^1 f \varphi_i dx + \int_0^1 f p dx. \qquad (2.3.35)$$

Element matrices and element vectors

Using the linear basis functions defined in , the element stiffness-matrix is given by:

$$S^e = -\frac{k}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} - \frac{u}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} - \frac{u}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \qquad (2.3.36)$$

The element mass-matrix is given by:

$$M^e = \frac{h}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{h}{4} \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}, \qquad (2.3.37)$$

and the element vector is given by:

$$F^e = \frac{hf}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \frac{hf}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

where h is the length of the element. Let us consider again the numerical test in Figure 2.3.4. Applying SUPG technique, we can avoid the wiggles causes by high convection, as illustrated in Figure 2.3.5.
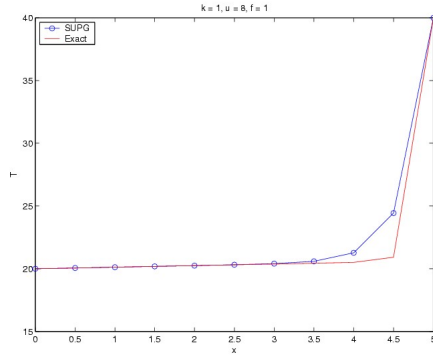
Figure 2.3.5: Numerical solution of 1D time dependent Convection diffusion equation using SUPG method with full upwind, and implicit scheme after 500 time steps, dt = 0.1

In the following numerical test, we will take the source term $f(x)$ as function of x, for example: $f(x) = x^2, f(x) = sin(x)$ and $f(x) = exp(x)$, the result is shown in Figure 2.3.6
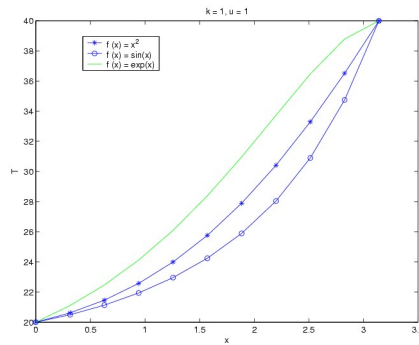

Figure 2.3.6: Numerical solution of 1D time dependent Convection diffusion equation using and implicit scheme and SUPG method with full upwind after 500 time steps, dt = 0.1

2.4   Linear elements in two dimensions

As in one dimension finite element bases are constructed implicitly in an element-by-element manner in terms of shape functions. Once again a shape function on an element "e" is the restriction of a basis function $\varphi_j(x, y)$ to element "e". The extension of the linear line element in $\mathbf{R}$ is the triangle in $\mathbf{R^2}$.
Figure 2.4.1 shows a subdivision of a region into triangles. Three parameters are needed to construct a linear polynomial on each triangle. We choose the function values in three vertices of the triangle in order to make the approxima-
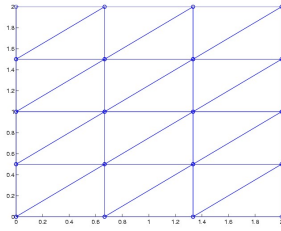
Figure 2.4.1: Subdivision in triangles

tion continuous across the element boundary. We proceed as in $\mathbf{R}$ to construct the basis function in $\mathbf{R^2}$ which is implicitly defined by:

- $\varphi_i(x)$ is linear per triangle.

- $\varphi_i(x^j) = \delta_{ij}$

But the explicit expression of the basis function is required to compute the solution of the PDE. Consider the triangle in Figure 2.4.2
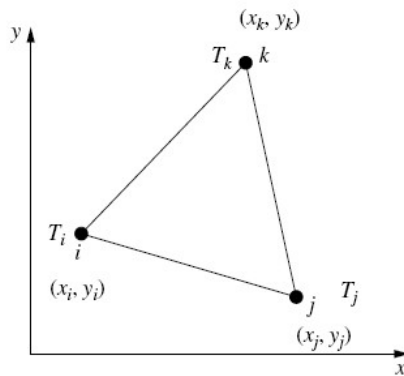

Figure 2.4.2: Linear triangle with nodal points

A Linear polynomial is defined by

$$\varphi_i(x^j) = a_0^i + a_1^i x_j + a_2^i y_j \qquad (2.4.1)$$

with

$$x^j = \begin{pmatrix} x_j \\ y_j \end{pmatrix} \qquad (2.4.2)$$

Substitution of (2.4.1) and (2.4.2) leads to the following system of linear equations

$$\begin{pmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{pmatrix} \begin{pmatrix} a_0^1 & a_0^2 & a_0^3 \\ a_1^1 & a_1^2 & a_1^3 \\ a_2^1 & a_2^2 & a_2^3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Solving this system by Cramer's rule, give the following results:

$$a_1^1 = \tfrac{1}{\Delta}(y_2 - y_3), \quad a_1^2 = \tfrac{1}{\Delta}(y_3 - y_1), \quad a_1^3 = \tfrac{1}{\Delta}(y_1 - y_2)$$

$$a_2^1 = \tfrac{1}{\Delta}(y_3 - y_2), \quad a_2^2 = \tfrac{1}{\Delta}(y_1 - y_3), \quad a_2^3 = \tfrac{1}{\Delta}(y_2 - y_1)$$

$$a_0^i = 1 - a_1^i x_i - a_2^i y_i$$

with:

$$\Delta = \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} = (x_2 - x_1)(y_3 - y_2) - (y_2 - y_1)(x_3 - x_2)$$

Δ is equal to two times the area of the triangle in Figure 2.4.2

2.5 Isoparametric transformation

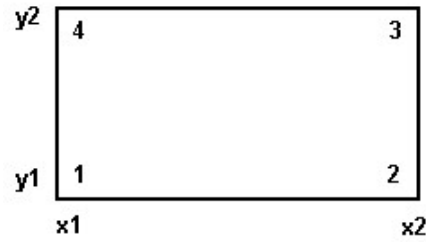Consider a rectangle and local node numbers 1 to 4 as depicted in Figure 2.5.1

Figure 2.5.1: Nodes of rectangle

The basis functions of this element have the shape

$$\varphi_i(x, y) = a_0^i + a_1^i x + a_2^i y + a_3^i xy \qquad (2.5.1)$$

Since these basis functions are not continuous for a general quadrilateral, and since we do not know what the general shape of the basis functions must be, we

have to use a standard technique known under the name *isoparametric trans-formations*. To apply this technique we transform the general quadrilateral element in the (x, y) plane with a coordinate transformation $(x, y) \rightarrow (\xi, \eta)$ to a standard element (the unit square) in the (ξ, η) plane. Such a transformation is called isoparametric if it satisfies the following properties

- The nodes $x^1, x^2, ...x^k$ are transformed to the fixed points $\xi_1, \xi_2, ...\xi_k$.

- Straight sides in *the original* element remain straight in *the reference* element.

- If the basis functions in the transformed element are given by $\varphi_1(x), ..., \varphi_k(x)$, then the inverse transformation $(\xi, \eta) \rightarrow (x, y)$ is given by

$$x = \sum_{j=1}^{k} x_j \varphi_j(\xi, \eta), \tag{2.5.2}$$

and the interpolation by:

$$T(x) = \sum_{j=1}^{k} T_j \varphi_j(\xi, \eta). \tag{2.5.3}$$

In other words we use the same elements for transformation and interpolation. Note that the basis functions are only known explicitly in *the reference* element. To compute their values in *the original* element we must do a back transformation. The transformation of the quadrilateral element to a unit square is illustrated in Figure 2.5.2
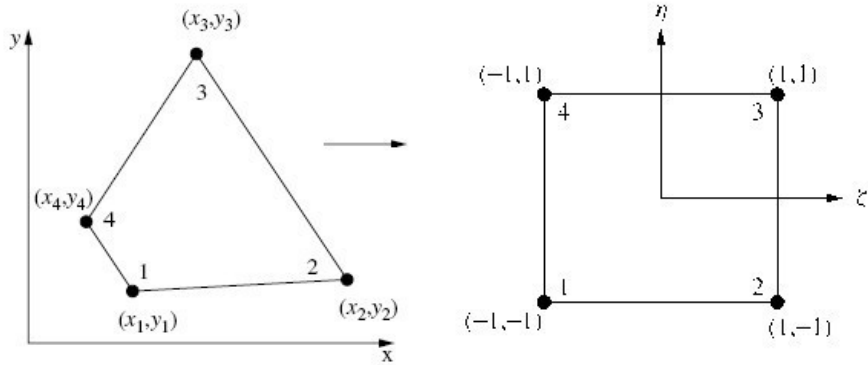

Figure 2.5.2: Transformation of quadrilateral to unit square

In this case the isoparamtric transformation is a bilinear transformation. The nodes of the quadrilateral are transformed to the vertices of the unit square as follows

$$x_1 \longrightarrow (0,0), \quad x_2 \longrightarrow (1,0), \quad x_3 \longrightarrow (1,1), \quad x_4 \longrightarrow (0,1). \tag{2.5.4}$$

The basis functions in the (ξ, η) plane are bilinear and defined by

$$
\begin{array}{rcll}
\varphi_1(\xi, \eta) &=& (1-\xi)(1-\eta), & (2.5.5) \\
\varphi_2(\xi, \eta) &=& \xi(1-\eta), & (2.5.6) \\
\varphi_3(\xi, \eta) &=& \xi\eta, & (2.5.7) \\
\varphi_4(\xi, \eta) &=& (1-\xi). & (2.5.8)
\end{array}
$$

To show how this transformation can be utilized to compute an element matrix or vector, we consider the following integral $s_{ij} = \int_e \nabla\varphi_i(x)\nabla\varphi_j(x)d\Omega$. Since the basis functions are only known in the reference element we have to transform this integral to an integral in the (ξ, η) plane. Hence:

$$
s_{ij} = \int_{e_{xy}} \nabla\varphi_i(x).\nabla\varphi_j(x)dxdy = \int_{e_{\xi\eta}} \nabla\varphi_i.\nabla\varphi_j|J|d\xi d\eta \qquad (2.5.9)
$$

with $|J|$ the absolute value of $det(J)$. In order to compute the value of $\nabla\varphi_i$, we should express the derivatives to x and y into derivatives of ξ and η, since φ_i is only known in the (ξ, η) plane:

$$
\frac{\partial\varphi_k}{\partial x} = \frac{\partial\varphi_k}{\partial\xi}\frac{\partial\xi}{\partial x} + \frac{\partial\varphi_k}{\partial\eta}\frac{\partial\eta}{\partial x}, \qquad (2.5.10)
$$

$$
\frac{\partial\varphi_k}{\partial y} = \frac{\partial\varphi_k}{\partial\xi}\frac{\partial\xi}{\partial y} + \frac{\partial\varphi_k}{\partial\eta}\frac{\partial\eta}{\partial y}. \qquad (2.5.11)
$$

This relation can be written in the following matrix form:

$$
\left[\begin{array}{cc} \frac{\partial\varphi_k}{\partial x} & \frac{\partial\varphi_k}{\partial y} \end{array} \right] = \left[\begin{array}{cc} \frac{\partial\varphi_k}{\partial\xi} & \frac{\partial\varphi_k}{\partial\eta} \end{array} \right] \left[\begin{array}{cc} \frac{\partial\xi}{\partial x} & \frac{\partial\xi}{\partial y} \\ \frac{\partial\eta}{\partial x} & \frac{\partial\eta}{\partial y} \end{array} \right] \qquad (2.5.12)
$$

For more details see [3].

2.6   2D convection diffusion equation

2.6.1   Standard Galerkin method

We consider the convection diffusion equation:

$$\frac{\partial T}{\partial t} - \vec{\nabla}.\left(k\vec{\nabla}T\right) + \left(\vec{u}.\vec{\nabla}T\right) = f \qquad (2.6.1)$$

On the boundary Γ_1 we assume the Dirichlet boundary condition:

$$T|_{\Gamma_1} = g_1 \qquad (2.6.2)$$

On the boundary Γ_2 we assume the Neumann boundary condition:

$$k\frac{\partial T}{\partial n}|_{\Gamma_2} = g_2 \qquad (2.6.3)$$

In order to derive the weak formulation, we multiply the equation (2.6.1) by a test function η satisfying the homogeneous essential boundary condition $\eta|_{\Gamma_1} = 0$ and integrate over the domain Ω, we obtain:

$$\int_\Omega \left[\frac{\partial T}{\partial t} - \vec{\nabla}.\left(k\vec{\nabla}T\right) + \left(\vec{u}.\vec{\nabla}T\right) - f\right]\eta d\Omega = 0. \qquad (2.6.4)$$

Integrating by parts (i.e., using Green's formula), we obtain:

$$\int_\Omega \frac{\partial T}{\partial t}\eta d\Omega + \int_\Omega k\left(\vec{\nabla}T.\vec{\nabla}\eta\right)d\Omega + \int_\Omega \left(\vec{u}.\vec{\nabla}T\right)\eta d\Omega - \int_{\Gamma_2} k\left(\vec{\nabla}T.\vec{n}\right)\eta d\Gamma_2 = \int_\Omega f\eta d\Omega.$$

Since $\vec{\nabla}T.\vec{n} = \frac{\partial T}{\partial n}$, and after substituting the boundary condition as well as the essential boundary condition for the test function, we get the weak formulation:

$$\int_\Omega \frac{\partial T}{\partial t}\eta d\Omega + \int_\Omega k\left(\vec{\nabla}T.\vec{\nabla}\eta\right)d\Omega + \int_\Omega \left(\vec{u}.\vec{\nabla}T\right)\eta d\Omega = \int_\Omega f\eta d\Omega + \int_{\Gamma_2} k\frac{\partial T}{\partial n}\eta d\Gamma_2.$$

The solution T can be approximated by : $T^n = \sum_{j=1}^n T_j\varphi_j(x)$. If the test function η takes the values $\varphi_i, \quad i = 1,...,n$, we obtain the following system of equations:

$$\sum_{j=1}^n \int_\Omega \varphi_j\varphi_i d\Omega \frac{dT_j}{dt} = -\sum_{j=1}^n \left[\int_\Omega k\left(\vec{\nabla}\varphi_j.\vec{\nabla}\varphi_i\right)d\Omega + \int_\Omega \left(\vec{u}.\vec{\nabla}\varphi_j\right)\varphi_i d\Omega\right]T_j + \int_\Omega f\varphi_i d\Omega \quad + \int_{\Gamma_2} g_2\varphi_i d\Gamma_2, \quad i = 1,...,n.$$

Using the following notations:
The mass matrix:

$$M_{ij} = \int_\Omega \varphi_j\varphi_i d\Omega, \qquad (2.6.5)$$

The stiffness matrix:

$$S_{ij} = -\int_\Omega k\left(\vec{\nabla}\varphi_j.\vec{\nabla}\varphi_i\right)d\Omega - \int_\Omega \left(\vec{u}.\vec{\nabla}\varphi_j\right)\varphi_i d\Omega, \qquad (2.6.6)$$

And:

$$F_i = \int_\Omega f\varphi_i d\Omega + \int_{\Gamma_2} g_2\varphi_i d\Gamma_2. \qquad (2.6.7)$$

We have to solve the linear, large and sparse ODE system(2.3.6).

2.6.2 Comparison between numerical and exact solution

To test our numerical solution in two dimensions, we can compare the exact solution in one dimension, in x-direction with the numerical solution in two dimensions in x-direction such that the velocity in y-direction is equal to 0, i.e, $u2 = 0$, This test is illustrated in the following example

On $\Gamma_1(y = 0)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_2} = 0$

On $\Gamma_2(x = 2)$, we prescribe Dirichlet boundary condition: $T|_{\Gamma_4} = 40$

On $\Gamma_3(y = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 0$

On $\Gamma_4(x = 0)$, we prescribe Dirichlet boundary condition: $T|_{\Gamma_4} = 20$

Number of elements in x-direction is 10.

Number of elements in y-direction is 10.
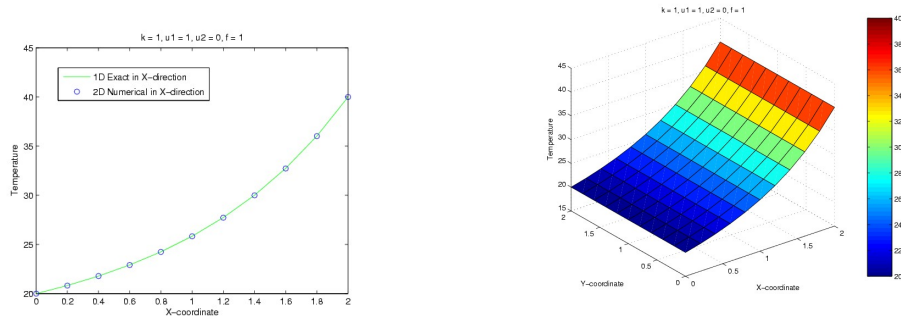
The result is shown in Figure 2.6.1:

Figure 2.6.1: Comparison between numerical solution of 2D time dependent convection diffusion equation in X-direction and 1D time dependent exact solution in X-direction using SGA method after 500 time steps, dt = 0.1

we can also compare the exact solution in one dimension, in y-direction with the numerical solution in two dimensions in y-direction such that the velocity in x-direction is equal to 0, i.e, $u1 = 0$, This test is illustrated in following example

On $\Gamma_1(y = 0)$, we prescribe Dirichlet boundary condition: $T|_{\Gamma_1} = 20$

On $\Gamma_2(x = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_2} = 0$

On $\Gamma_3(y = 2)$, we prescribe Dirichlet boundary condition: $T|_{\Gamma_3} = 40$

On $\Gamma_4(x = 0)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_4} = 0$

Number of elements in x-direction is 10.

Number of elements in y-direction is 10.
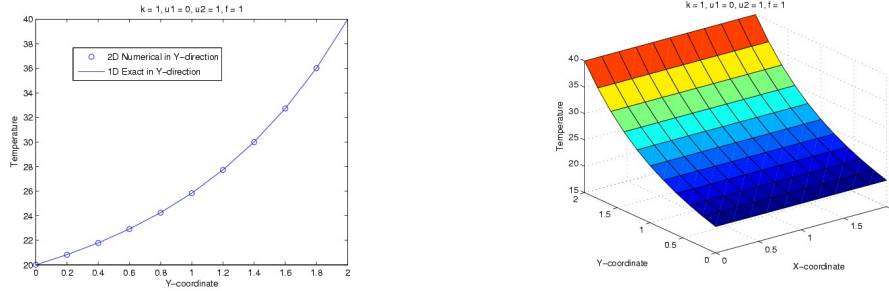
The result is shown in Figure 2.6.2

Figure 2.6.2: Comparison between numerical solution of 2D time dependent convection diffusion equation in Y-direction and 1D time dependent exact solution in Y-direction using SGA method after 500 time steps, dt = 0.1

2.6.3 Streamline Upwind Petrov Galerkin method

Let us consider this example to see the effect of SUPG method.

On $\Gamma_1(y = 0)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_1} = 0$

On $\Gamma_2(x = 1)$, we prescribe the essential boundary condition: $T|_{\Gamma_2} = 40$

On $\Gamma_3(y = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 0$

On $\Gamma_4(x = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_4} = 20$

Number of elements in x-direction is 10.

Number of elements in y-direction is 10.

The result is shown in Figure 2.6.3:

Figure 2.6.3: Numerical solution of 2D time dependent convection diffusion equation using SGA method and implicit scheme after 500 time steps, $dt = 0.1$

The wiggles we get are due to convection (the solution jump around the exact solution, if the convection dominates), we should apply upwind only in the direction of flow, so a natural choice for upwind in more dimensions is to apply the one-dimensional upwind in the velocity direction, this can be achieved by replacing the term $p(x) = \frac{h\xi}{2}\frac{d\varphi_i}{dx}$ by $p(x) = \frac{h\xi}{2}\frac{\vec{u}.\vec{\nabla}\varphi_i}{\|\vec{u}\|}$. This means that the x-derivative of the basis function in the one dimensional problem is replaced by the directional derivative of the basis function in the direction of the velocity. Since streamlines are always in the direction of the velocity this method is commonly

called the Streamline Upwind Petrov Galerkin method (SUPG). Using the same procedure as in SGA method, we get the matrix notation (2.3.6) where The mass matrix is:

$$M_{ij} = \int_\Omega \varphi_j \varphi_i d\Omega + \int_\Omega \varphi_j p d\Omega, \qquad (2.6.8)$$

The stiffness matrix is:

$$S_{ij} = -\int_\Omega k \left(\vec{\nabla}\varphi_j . \vec{\nabla}\varphi_i \right) d\Omega - \int_\Omega \left(\vec{u} . \vec{\nabla}\varphi_j \right) \varphi_i d\Omega - \int_\Omega \left(\vec{u} . \vec{\nabla}\varphi_j \right) p d\Omega, \quad (2.6.9)$$

And:

$$F_i = \int_\Omega f \varphi_i d\Omega + \int_\Omega f p d\Omega + \int_{\Gamma_2} k \frac{\partial T}{\partial n} \varphi_i d\Gamma_2. \qquad (2.6.10)$$

The wiggles can be avoided after using supg method, as illustrated in Figure 2.6.4, we prescribe the same boundary conditions as in the previous test.
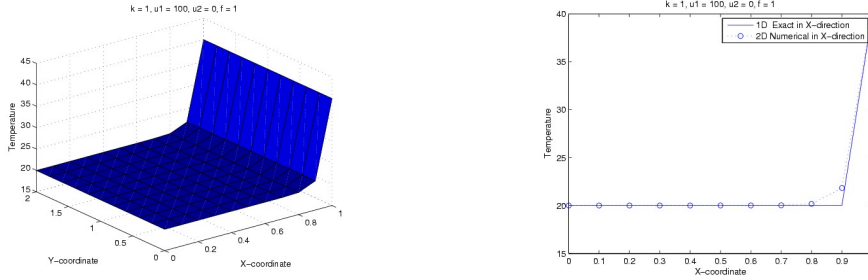
Figure 2.6.4: Numerical solution of 2D time dependent convection diffusion equation using SUPG method and implicit scheme after 500 time steps, dt = 0.1

2.6.4 Role of boundary conditions

The occurence of boundary layers is strongly influenced by the type of boundary conditions. The following tests illustrate the effect of boundary conditions
The first example studies a heat metal block with a square form, the inferior and the left sides of the block are heated to 20 °C, the other block boundaries are isolated. This leads to the following set of boundary conditions
On $\Gamma_1(y = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_1} = 20$
On $\Gamma_2(x = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_2} = 0$
On $\Gamma_3(y = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 0$
On $\Gamma_4(x = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_4} = 20$
Number of elements in x-direction is 10.
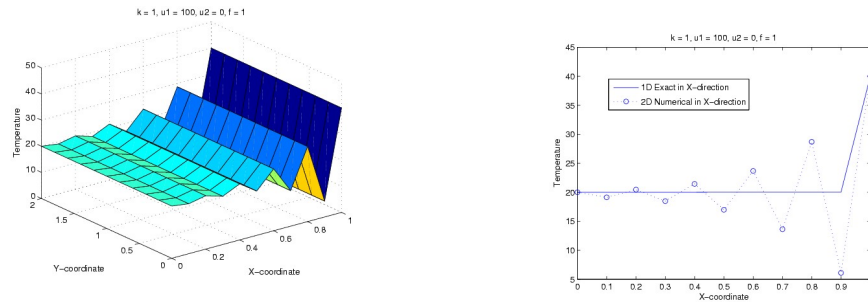Number of elements in y-direction is 10.
The result is shown in Figure 2.6.5

Figure 2.6.5: Numerical solution of 2D time dependent convection diffusion equation using SGA method after 500 time steps, dt = 0.1

In the following test, we assume that heat is flowing from the surrounding air to the block at constant rate.

On $\Gamma_1(y = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_1} = 20$

On $\Gamma_2(x = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_2} = 50$

On $\Gamma_3(y = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 50$

On $\Gamma_4(x = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_4} = 20$

Number of elements in x-direction is 10.

Number of elements in y-direction is 10.

The result is shown in Figure 2.6.6
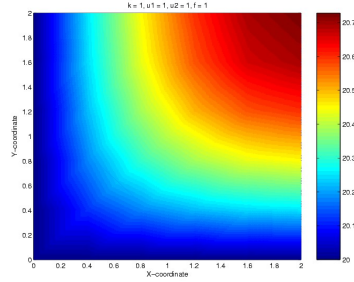

Figure 2.6.6: Numerical solution of 2D time dependent convection diffusion equation using SGA method after 500 time steps, dt = 0.1

In the following test, we assume that the left and the right sides are heated to 20 °C, while at the other sides, heat is flowing from the surrounding air to the block at constant rate

On $\Gamma_1(y = 0)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 10$

On $\Gamma_2(x = 2)$, we prescribe the essential boundary condition: $T|_{\Gamma_2} = 20$

On $\Gamma_3(y = 2)$, the flux is given by: $k\frac{\partial T}{\partial n}|_{\Gamma_3} = 10$

On $\Gamma_4(x = 0)$, we prescribe the essential boundary condition: $T|_{\Gamma_4} = 20$

Number of elements in x-direction is 10.

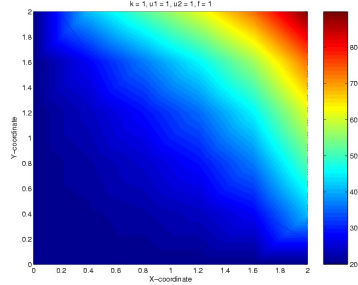Number of elements in y-direction is 10.
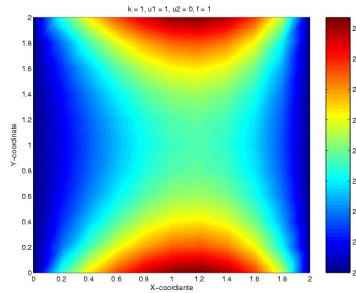
The result is given in Figure 2.6.7

Figure 2.6.7: Numerical solution of 2D time dependent convection diffusion equation using SGA method after 500 time steps, dt = 0.1

3   Thermodynamic description

3.1   Heat or mass balance alone

The techniques given by voller et al.(1990) to solve phase change problems are related only to the enthalpy balance, which means that the use of these techniques to model processes with mobile components is not possible because of the absence of the mass balance. Moreover, a fixed phase change temperature is required to apply those techniques, but this temperature profile is not known in advance because of the coupled mass and heat balances. The coupling between the mass and heat balance is very important. For instance, the evaporation of water from a product not only affects the mass balance, but will also lower the temperature due to the heat of evaporation. Another technique which is only related to the mass balance is the effective diffusivity model and is often used to model moisture transport during drying. This technique neglects the coupling between the mass and the heat balance and therefore the effect of the heat of evaporation on the temperature, as well.

3.2   Density-enthalpy phase diagram

In order to increase the accuracy, numerical stability, calculation speed and to minimize the number of assumptions of models, describing processes that involve phase transitions, a *density-enthalpy* phase diagram has been developed.

It is possible to calculate directly the temperature, pressure and phase fractions given the density and enthalpy of the system if we use *density-enthalpy* phase diagram. Indeed, the state variables, density and enthalpy are sufficient to determine the current state of a homogeneous system completely if the thermodynamic equilibrium is assumed. In other words, if temperature, pressure and mass distribution over the phases can be obtained as functions of density and enthalpy, then the thermal processes can be simulated by solving only one set of equations for the entire process, without switching between sets of equations. Moreover, we can obtain all thermal properties using the partial derivatives of these functions, so that , we can minimize the set of input parameters. Density and enthalpy can be obtained by solving mass and heat balances. However, we need temperature, pressure and phase fractions to calculate flux and boundary

conditions. A thermodynamic analysis is required to obtain temperature, pressure and mass distribution at any given density and enthalpy. The method of the density-enthalpy phase diagram is based on dividing the density-enthalpy plane into different zones. The phase diagram of pure water shown in Figure 3.2.1 is used as an example to describe the principle of the density-enthalpy phase diagram. For more details see[1]
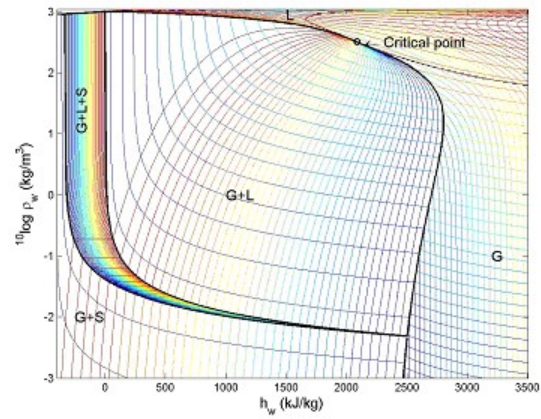

Figure 3.2.1: Density-enthaply phase diagram for pure water, G : gas, L : liquid, S : solid

4 Further research

4.1 Introduction

In the next part of the master thesis research, a 0D boiler system described in [1] will be solved using MATLAB, secondly a 1D problem described in [2] will be set up and solved using MATLAB, and finally a 2D and 3D problem will set up and solved using a FE package SEPRAN. The different problems are described as follows:

4.2 0D Boiler system

Figure 4.2.1 illustrates a boiler system: Liquid Propaan (C_3H_8) at constant inlet pressure P_i and temperature T_i flows into the system since we have taken pressure inside the boiler P relatively low compared to the pressure in the inlet ($P_i >> P$). The system is constructed in such a way that only gas can leave the boiler at the top. The gas has the same pressure and temperature as the system. Since pressure outside the system Pe is relatively low compared to the pressure P inside the system ($P_e << P$), the formed gas will flow out.
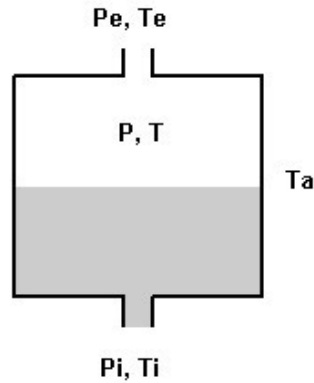

Figure 4.2.1: Boiler

This system can be described using the following differential equations (mass and heat balance)

$$V\frac{d\rho}{dt} = \Phi_i - \Phi_e, \tag{4.2.1}$$

$$V\frac{d(\rho h)}{dt} = \Phi_i.h_i - \Phi_e.h_e + Q + V\frac{dP}{dt}. \tag{4.2.2}$$

where

V Volume $[m^3]$,
ρ Density $[Kg/m^3]$,
Φ_i Inflow mass $[Kg/s]$,
Φ_e Outflow mass $[Kg/s]$,
Q Heat flow $[W]$,
h Specific enthalpy $[J/Kg]$,
P Pressure $[Pa]$.

Since $P = P(\rho, h)$, the total differential of P equals:

$$\frac{dP}{dt} = \left(\frac{\partial P}{\partial \rho}\right)_h \frac{d\rho}{dt} + \left(\frac{\partial P}{\partial h}\right)_\rho \frac{dh}{dt}. \tag{4.2.3}$$

If we model the inlet and outlet flows using Bernoulli's Law and if we assume that the amount of the heat transfered into the system is a function of the wall temperature, then inflow mass Φ_i, outflow mass Φ_e and heat flow Q can be expressed as follows, for more details see [1].

$$\Phi_i = A_i\sqrt{2\rho_i(P_i - P)}, \tag{4.2.4}$$
$$\Phi_e = A_e\sqrt{2\rho_e(P - P_e)}, \tag{4.2.5}$$
$$Q = AU(T_a - T). \tag{4.2.6}$$

where

A_i Inlet area $[m^2]$,
A_e Exit area $[m^2]$,
T_a Ambient temperature $[K]$,
U Heat transfer coefficient $[W/m^2/K]$.

The level of the system can be calculated according to the following equation

$$Le = \rho\left(\frac{X^L e}{\rho^L e}\right) \tag{4.2.7}$$

where

X^L Mass fraction of the liquid,
ρ^L Density of the liquid,
ρ Density of the liquid and gas.

We can solve this system using the following initial conditions

$$\rho(0) = \rho\left(P_0, T_0, X^G(0)\right), \tag{4.2.8}$$
$$h(0) = h\left(P_0, T_0, X^G(0)\right). \tag{4.2.9}$$

4.3   1D Darcy flow in porous media

Let us consider one dimensional flow of fluid which experience phase change through inert porous media as illustrated in Figure 4.3.1. The fluid can appear as a pure liquid or as gas or as a liquid in thermodynamic equilibrium with a gas.

The velocity can be written as:

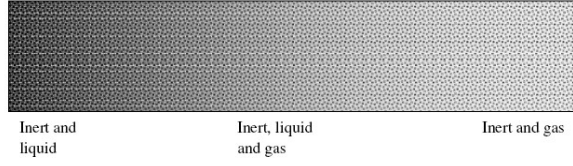$$\nu = -\frac{K}{\mu}\frac{\partial P}{\partial x}. \tag{4.3.1}$$

Figure 4.3.1: Porous media in one dimension

where:

ν velocity $[m/s]$,
μ dynamic viscosity $[Pa.s]$,
P pressure $[Pa]$,
K permeability $[Darcy]$

The permeability is a measure of the flow resistance, a high permeability means a better mass transport. The mass balance can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \nu}{\partial x} = 0. \tag{4.3.2}$$

where:

ν velocity $[m^3/m^3]$,
ρ density $[Kg/m^3]$.

The heat balance can be given by:

$$\frac{\partial (\rho h)}{\partial t} - \frac{\partial P}{\partial t} + \frac{\partial (\rho h \nu)}{\partial x} = \frac{\partial}{\partial x} \lambda \frac{\partial T}{\partial x} + q. \tag{4.3.3}$$

where:
λ heat conductance coefficient $[W/K]$,
ρ density $[Kg/m^3]$,
μ dynamic viscosity $[Pa.s]$,
h enthlpy $[J/Kg]$,
T temperature $[K]$,
P pressure $[Pa]$,
q heat flow $[W]$.
After neglecting potential and kinetic energies, and eliminating a velocity, the general set of PDE for non-isothermal flow in porous media is given by:

$$\frac{\partial \rho}{\partial t} - \frac{K}{\mu} \frac{\partial P}{\partial x} \frac{\partial \rho}{\partial x} = \rho \frac{\partial}{\partial x} \frac{K}{\mu} \frac{\partial P}{\partial x}, \tag{4.3.4}$$

$$\rho \frac{\partial h}{\partial t} - \frac{\partial P}{\partial t} - \rho \frac{K}{\mu} \frac{\partial P}{\partial x} \frac{\partial h}{\partial x} = \frac{\partial}{\partial x} \lambda \frac{\partial T}{\partial x} + q. \tag{4.3.5}$$

Initial and boundary conditions:

$$P|_{t_0} = P_a, \tag{4.3.6}$$

$$T|_{t_0} = T_a, \tag{4.3.7}$$

$$\frac{K}{\mu}\frac{\partial P}{\partial x} = k_m\left(P_a - P\right), \tag{4.3.8}$$

$$\lambda\frac{\partial T}{\partial x} = k_h\left(T_a - T\right). \tag{4.3.9}$$

where:

t_0 starting time $[S]$,
λ heat conductance coefficient $[W/K]$,
μ dynamic viscosity $[Pa.s]$,
ρ density $[Kg/m^3]$,
K permeability $[Darcy]$,
k_h heat transfer coefficient $[W/m^2/K]$,
k_m mass transfer coefficient $[Kg/m^2/K]$,
q heat fllow $[W]$.

Since $P = P(\rho, h)$ and $T = T(\rho, h)$, the partial derivatives of P and T can be written as:

$$\frac{\partial P}{\partial x} = \left(\frac{\partial P}{\partial \rho}\right)_h \frac{\partial \rho}{\partial x} + \left(\frac{\partial P}{\partial h}\right)_\rho \frac{\partial h}{\partial x}, \tag{4.3.10}$$

$$\frac{\partial P}{\partial t} = \left(\frac{\partial P}{\partial \rho}\right)_h \frac{\partial \rho}{\partial t} + \left(\frac{\partial P}{\partial h}\right)_\rho \frac{\partial h}{\partial t}, \tag{4.3.11}$$

$$\frac{\partial T}{\partial x} = \left(\frac{\partial T}{\partial \rho}\right)_h \frac{\partial \rho}{\partial x} + \left(\frac{\partial T}{\partial h}\right)_\rho \frac{\partial h}{\partial x}. \tag{4.3.12}$$

The partial derivatives of pressure and temeprature with respect to enthalpy and density will be calculated using a thermodynamic model. By eliminating partial derivatives of pressure and temperature in the transport model, we obtain a system of PDE with only density and enthalpy as states. In the mathematical model (4.3.4) and (4.3.5), we have separated between the transport model and the thermodynamic model. Moreover, the transport model does not depend on the phases of the fluid. This method is called $\rho - h$ method.

4.4   2D Darcy flow in porous media

Let us consider 2D Darcy flow in porous media, heat and mass balances can be written as:

$$\frac{\partial \rho}{\partial t} - \frac{K}{\mu}\vec{\nabla}P.\vec{\nabla}\rho = \rho\frac{K}{\mu}\Delta P, \tag{4.4.1}$$

$$\rho\frac{\partial h}{\partial t} - \rho\frac{K}{\mu}\vec{\nabla}P.\vec{\nabla}h = \vec{\nabla}.\left(\lambda\vec{\nabla}T\right) + q. \tag{4.4.2}$$

To describe this process completely, we should determine the boundary conditions which describe the transfer of mass and heat. The external heat transfer

can be given by:

$$\lambda \vec{\nabla} T.\vec{n} = k_h \left(T_a - T \right).$$

(4.4.3)

The external mass transfer can be represented by:

$$\frac{K}{\mu} \vec{\nabla} P.\vec{n} = k_m \left(P_a - P \right).$$

(4.4.4)

The initial conditions can be given by:

$$
\begin{aligned}
P|_{t_0} &= P_a, \\
T|_{t_0} &= T_a.
\end{aligned}
$$

where:

P	pressure $[Pa]$,
T	temperature $[K]$,
P_a	ambient pressure $[Pa]$,
T_a	ambient temperature $[K]$,
h	enthalpy $[W]$,
t_0	starting time $[S]$,
λ	heat conductance coefficient $[W/K]$,
μ	dynamic viscosity $[Pa.s]$,
ρ	density $[Kg/m^3]$,
K	permeability $[Darcy]$,
k_h	heat transfer coefficient $[W/m^2/K]$,
k_m	mass transfer coefficient $[Kg/m^2/K]$,
q	heat fllow $[W]$,
$\vec{n}$	normal vector.

5 Appendix A

5.1 Thermodynamic words

Porous:
A porous medium or a porous material is a solid (often called frame or matrix) permeated by an interconnected network of pores (voids) filled with a fluid (liquid or gas).

Porosity:
The porosity of a porous material is the proportion of the non-solid volume to the total volume of material, and is defined by the ratio:

$$\phi = \frac{V_p}{V_m}$$

where V_p is the non-solid volume (pores and liquid) and V_p is the total volume of material, including the solid and non-solid parts.

Darcy:
Permeability measures the ability of fluids to flow through porous media. The darcy is defined using Darcy's Law which can be written as:
where:
v is the superficial fluid flow rate through the medium $[m/s]$,
k is the permeability of a medium $[Darcy]$,
μ is the dynamic viscosity of the fluid $[Pa.s]$,
ΔP is the applied pressure difference $[Pa]$,
Δx is the thickness of the medium $[m]$.

Mass balance:
A mass balance (also called a material balance) accounts for material entering and leaving a system (The matter can not disappear or be created).

Heat balance:
First law of thermodynamics (the conservation of energy). The increase in the energy of a closed system is equal to the amount of energy added to the system by heating, minus the amount lost in the form of work done by the system on its surroundings.

Inert:
A medium is inert if it is not reacting chemically with other substances.

Enthalpy:
In thermodynamics, the quantity enthalpy, symbolized by H is the sum of the internal energy of a thermodynamic system plus the energy associated with work done by the system on the atmosphere which is the product of the pressure times the volume.

$$H = U + P \ V,$$

H   is the enthalpy [J],
U   is the internal energy $[J]$,
P   is the pressure of the system $[Pa]$,

V   is the volume $[m^3]$.

Phase transition:

In physics, a phase transition or phase change is the transformation of a thermodynamic system from one phase to another. The distinguishing characteristic of a phase transition is an abrupt sudden change in one or more physical properties, in particular the heat capacity, with a small change in a thermodynamic variable such as the temperature.

Examples of phase transitions include the transitions between the solid, liquid, and gaseous phases, due to the effects of temperature and pressure:

The solid-to-liquid transition is called melting.

The liquid-to-solid transition is called freezing.

The liquid-to-gas transition is called boiling / evaporation.

The gas-to-liquid transition is called condensation.

The solid-to-gas transition is called sublimation.

The gas-to-solid transition is called deposition.

Phase diagram:

In physical chemistry and materials science, a phase diagram is a type of graph used to show the equilibrium conditions between the thermodynamically-distinct phases

Air pressure:

Air pressure is the pressure above any area in the Earth's atmosphere caused by the weight of air. As elevation increases, there are exponentially fewer and fewer air molecules. Therefore, atmospheric pressure decreases with increasing altitude at a decreasing rate. The following relationship is a first-order approximation:

$$\log_{10} P \approx 5 - \tfrac{h}{15500}$$

where P is the pressure in Pascal and h the height in meters. This shows that the pressure at an altitude of 31 km is about $10^{(5-2)} Pa = 1000 Pa$, or 1% of that at sea level. A rough approximation valid for the first few kilometers above the surface is that pressure decreases by 100 hPa per kilometer.

Permeability $[Darcy]$**:**

The permeability is a measure of the ability of a material to transmit fluids.

Isothermal process:

An isothermal process is a thermodynamic process in which the temperature of the system stays constant: $\Delta T = 0$

Thermodynamic equilibrium:

In thermodynamics, a thermodynamic system is said to be in thermodynamic equilibrium, when it is in thermal equilibrium, mechanical equilibrium, and chemical equilibrium. The local state of a system at thermodynamic equilibrium is determined by the values of its intensive parameters, as pressure, temperature, etc. Specifically, thermodynamic equilibrium is characterized by the minimum of a thermodynamic potential, such as the Helmholtz free energy, i.e. systems at constant temperature and volume:

$$A = U - TS,$$

or as the Gibbs free energy, i.e. systems at constant pressure and temperature:

$$G = H - TS,$$

where H is the enthalpy $[J]$,
T is the temperature $[K]$,
S is the entropy $[J/K]$.

The process that leads to a thermodynamic equilibrium is called thermalization

Gibbs free energy:
The Gibbs free energy is a thermodynamic potential and is therefore a state function of a thermodynamic system. It is defined as:

$$G = H - TS,$$

where (in SI units)
G is the Gibbs energy $[J]$,
H is the enthalpy $[J]$,
T is the temperature $[K]$,
S is the entropy $[J/K]$.

Entropy:
Symbolized by S, is defined by the differential quantity $dS = dQ/T$, where dQ is the amount of heat absorbed in a reversible process in which the system goes from one state to another, and T is the absolute temperature. Entropy is one of the factors that determines the free energy of the system.

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6 NOTATIONS

Roman symbols

A	area $[m^2]$
C_p	heat capacity $[J/Kg/K]$
f	source term
G	gaz
h	specific enthalpy $[J/Kg]$
k	diffusion term
K	permeability
l	domain length
L	liquid
Le	level $[m/m]$
n	normal vector
P	pressure $[Pa]$
S	solid
T	temperature $[K]$
t	time $[s]$
u	convection term
U	heat transfer coefficient $[W/m^2/K]$
V	volume $[m^3]$
X	mass fraction $[Kg/Kg]$

Greek symbols

ϵ	porosity $[m^3/m^3]$.
λ	effective heat conductance coefficient $[W/m/K]$
μ	dynamic viscosity $[Pa.s]$
ρ	density $[Kg/m^3]$
Φ	mass flow $[Kg/s]$