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Stochastic inversion of fire test data for the T-dependant thermal diffusivity of SA pine

by

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Project(Civil Engineering)458

Final Draft

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Nomenclature

Constants

g = $9.81\,\mathrm{m/s^2}$

Variables

κ	Thermal conductivity	[W/m·K]
α	Thermal diffusivity	[$\mathrm{m^2/s}$]
c_p	Heat capacity	[J/kg/K]

Chapter 1

Introduction

This chapter will introduce the problem addressed in this project. Previous similar projects as well as the value of this research will also be addressed.

1.1 Background and Motivation

Traditionally the thermal conductivity, otherwise referred to as the κ-value, of timber is based simply off the EN 1995:1-1-2004 or similar standards. This research project will aim to obtain the thermal diffusivity of cross laminated SA-Pine timber by further analysing data obtained by S. van der Westhuyzen for his study of the samples' charring rate.

The thermal conductivity of timber is a unobservable quantity that cannot be measured directly. Instead, it is related to measurements of temperature and time through differential models. When heat diffusion is calculated using Finite Element methods(TODO:choose which FEM), the process is usually simplified to a linear problem (Fish, 2007). Due to the changes in thermal diffusivity of timber with temperature, as can be seen in EN 1995:1-1-2004(pg number TODO), the diffusivity cannot be linearly modelled. Therefore, the problem lends itself to being analysed by inversion techniques. The aforementioned approach will allow us to obtain information about the diffusivity based on the combination of the information assumed prior to measuring, further referred to as the prior, and the measured data. Using statistical inversion leads to a probability distribution that provides us with a collection of diffusivity estimates and their corresponding probabilities.

Currently the fire rating of specific timber samples are based on fire tests conducted in a furnace. The furnace is kept at increasing temperatures corresponding with the Standard or ISO 834 fire curve as specified in ISO 834 ISO (1999). This process becomes very costly if it has to be repeated every time that timber is used for construction, as timber usage for multiple story construction projects have increased over the past decades. This increase is partially due to the sustainability of timber as a construction material: not only is it renewable but it also has a small carbon footprint (Salvadori, 2017).

1.2 Aim and objectives

During the course of the project, the student will aim to meet the following objectives:

1. Modify a Finite Element Model into an accurate and effective function;
2. Compare the model data to the actual acquired data;
3. Solve for the thermal diffusivity using Bayes' theorem of inverse problems; and
4. Evaluate and explore the posterior probability distribution using the following methods:
   (a) Maximum a Posteriori
   (b) Markov-Chain Monte Carlo

1.3 Literature study

In their article *Simple Method to Determine the Diffusivity of Green Wood*, Frayssinhes *et al.* determine the global diffusivity of a Douglas fir green log using inverse identification methods. Their experiment was set up by immersing the log with K-type thermocouples into a boiler filled with water at 60°C. These K-type thermocouples were very specifically placed to improve the accuracy of the diffusivity ratio calculation. The finite element model constructed for their calculations used linear interpolation with four node quadrangle elements. An analytical model was also constructed using the heat propagation equation(TODO?heat diffusion?). The intent of this research was to assist the peeling industry in making the pretreatment process more cost effective. The method proved to be effective at determining the thermal diffusivity of green Douglas fir logs, as the κ-values obtained were comparable to those form literature. The methods used by Frayssinhes *et al.* (2020) are similar to the methods described later in the report. A crucial difference remains as the temperatures at which these experiments were conducted as well as the final usage of the data differ greatly.

A similar method of analysis was used by De Koker and Bekker (2021) in their article *Assessment of ice impact load threshold exceedance in the propulsion shaft of an ice-faring vessel via Bayesian inversion.* Bayesian inversion is used to determine the impact of ice on the propellers from the measurements taken at a specified distance from the propeller. (TODO)

The current κ-values used for the design of timber elements are taken from the EURO code (ref TODO (CEN, 2004)) and are shown in figure 1.3.

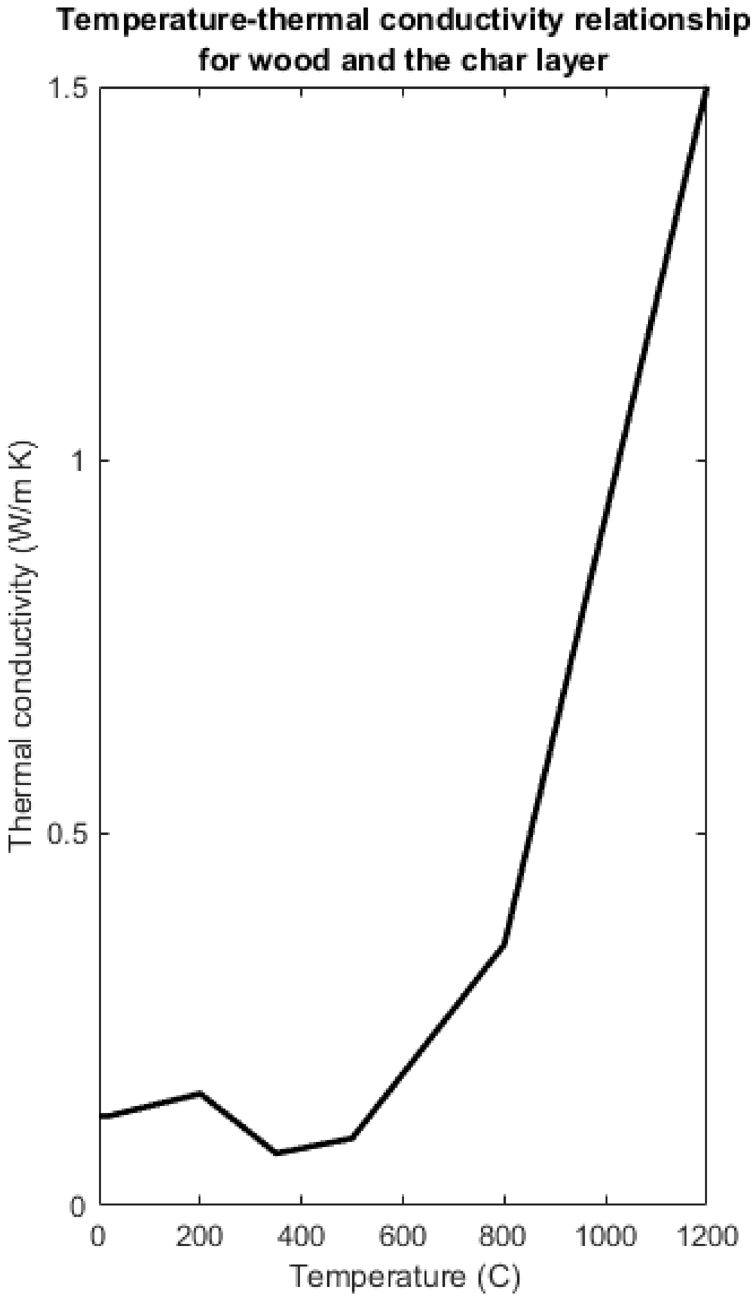


Figure 1.3.1: Standard temperature-thermal conductivity relationship for timber from (CEN, 2004)

Chapter 2

Technical Foundation

2.1 Finite Element Model

Finite element methods (or finite element analysis) is used when the behaviour of an element cannot be accurately depicted by a simple mathematical equation.

2.1.1 History/Origin

The finite element method (FEM) used today is the sum of decades of research. In an article by Gupta and Meek they discuss the five main contributors to the finite element method. According to Gupta and Meek (1996) the idea behind the finite element method was initially explored in the 1943 article by Courant. Courant acknowledges the complex nature of mathematical problems in his first paragraph by stating: "Mathematics is an indivisible organism uniting theoretical contemplation and active application." He goes on to discuss the variational method

2.1.2 method of FEM

A larger element is broken into smaller elements. Assumptions made on the smaller scale have a lesser effect on the final answer than the same assumptions made on a large scale would have had.

2.1.3 heat eq

In its simplest form, the one-dimensional heat diffusion equation is a partial differential equation 2.1.1 dependant on the temperature and thickness of the element. The heat diffusion equation is based on Fourier's Law...(TODO)

$$q = -k\frac{dT}{dx} \tag{2.1.1}$$

2.2 Bayes' theorem of inverse problems

The method of statistical inversion is dependant on a fundamental understanding of the Bayes' theorem of inverse problems. The student obtained this understanding through studying Chapter 3 of statistical and Computational Inverse problems by Kaipio and Somersalo (2005), further referred to merely as Kaipio. There are four principles of Statistical inversion that is essential to the thorough understanding of these models. Firstly, it is the principle that any variable in the model needs to be modelled as a random variable. This randomness is based on the extent of information that is available. To ensure that the extent of knowledge is accurately portrayed in the model, the extent of knowledge will be coded into the probability distributions assigned to the different variables. Finally, it needs to be understood that the solution of a statistical inversion is a posterior probability distribution. A generalized equation of Bayes' theorem can be seen in 2.2.1 taken from Kaipio.

$$\pi_{\text{post}}(x) = \pi(x|y_{\text{observed}}) = \frac{\pi_{\text{pr}}(x)\pi(y_{\text{observed}}|x)}{\pi(y_{\text{observed}})} \tag{2.2.1}$$

2.3 Markov Chain Monte Carlo

Markov Chain Monte Carlo (MCMC) is a method of integration. This will be used to determine the mean of the κ-values at specific temperatures. Markov Chain Monte Carlo is a method that was created by combining the concept of Monte Carlo sampling and a Markov Chain. To fully understand MCMC, the methods that it was created from need to be further investigated.

2.3.1 Markov Chains

2.3.2 Monte Carlo Integration

Monte Carlo integration is used to evaluate a probability distributuion. The evaluation is done by drawing a collection of random numbers from the distribution. These numbers are then used as the sample and a sample mean is taken. The arithmetic sample mean can be used to approximate the population mean in accordance with the law of large numbers (Gilks *et al.*, 1996). All of the random samples are not generally accepted. Here the acceptance criteria comes into play. There are multiple options for how a posterior is deemed acceptable, these are elaborated on in the book *Monte Carlo Statistical Methods* by

2.3.3 Metropolis-Hastings Algorithm

The Metropolis-Hastings algorithm is a simulation method based on the MCMC principles.

Chapter 3

Implementation

This chapter will elaborate on the test data used as well as the process that was followed to achieve the results in Chapter 4.

3.1 Existing data

The data used was acquired by van der Westhuyzen *et al.* (2020) for an article assessing the charring rate of both SA-Pine and Eucalyptus. For the purpose of this project, only the data obtained from the SA-Pine test was considered and analysed.

3.1.1 Summary of test

The test was conducted on a sample of 100mm by 0.9m x 0.9m panel of cross-laminated SA-pine. This sample was then divided into nine cubes of 100 mm x 100 mm x 100 mm. Each cube was fitted with seven Type K-thermocouples placed at consecutive 16.5 mm drilled holes, as can be seen in Figure 3.1.1. The test panel was tested in a furnace and was exposed to the standard ISO 834 Fire curve 3.1.2 on one side and room temperature on the other. The panel was exposed to the fire curve for 50 minutes, at which stage near complete de-lamination was observed and the test ended.

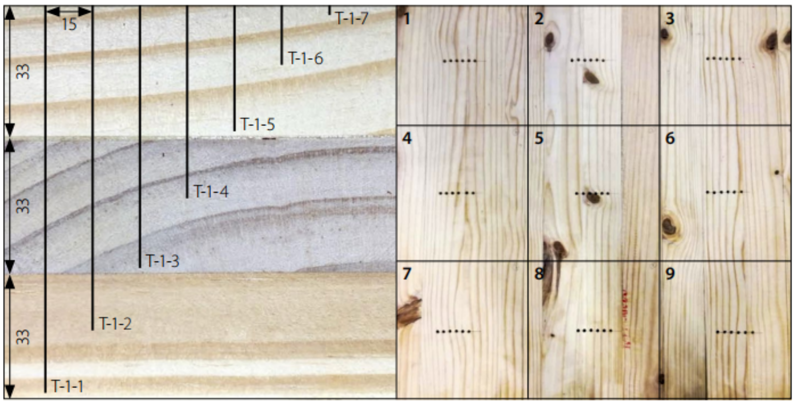


Figure 3.1.1: Thermocouple layout in test conducted by van der Westhuyzen *et al.* (2020) cross-section (left) and overall layout (right)

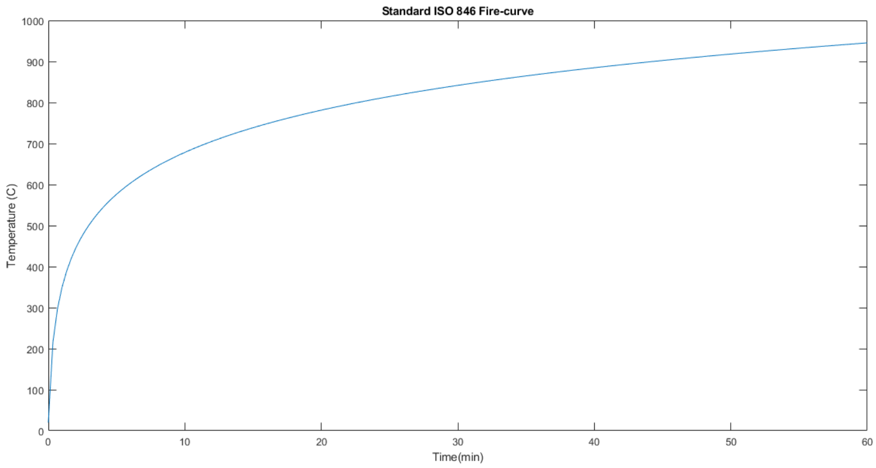


Figure 3.1.2: Standard ISO fire curve TODO

3.1.2 Potential inaccuracies

As with most tests, everything is not always perfect. The potential inaccuracies are discussed below.

In the data, it was observed that two of the thermocouples broke during testing, this resulted in temperature with a magnitude of 10^{13}. That temperature is not possible as the highest ever recorded temperature reached was $4x10^{12}$ and that only occurred in a atomic explosion. This malfunction required that two of the depth measurements were no longer the average between nine samples but instead the average between eight. Another inaccuracy that could potentially influence the accuracy of the final result is the accuracy of the depth of the holes in which the thermocouples were placed.

There is also debate about the significance of the contribution of the timber burning to the temperature inside the furnace. For the purposes of this project, it will be assumed that the timber burning does not contribute to the temperature inside the furnace.

3.2 Finite Element Modelling

A one-dimensional finite element model that simulates what we expect to obtain from the fire tests based on the simplified *kappa*-values provided in EN 1995:1-2-2004 is modified into a function. This function should provide the temperature of the modelled element based on a specified location and thermal conductivity. The derivation and adaptation of the model are expanded on below.

3.2.1 Derivation

Assumptions were made to simplify the model, they were as follows

1. The air on the side of fire follows the temperature of the fire curve.
2. The air on the cold side remains at 20°C.

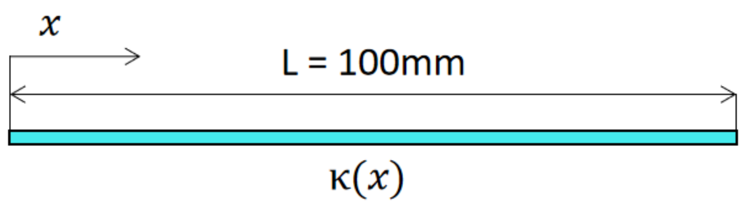


Figure 3.2.1: Visualisation of element that is modelled in one-dimension

The derivation started as a one-dimensional stationary heat conduction problem with the below equations as a starting point.

$$q_{,x} - f = 0 \text{ ...(1)}; q = -\kappa u_{,x} \text{ ...(2)} \tag{3.2.1}$$

Integrating Equation 3.2.1 (1) over the length of the element(shown in Figure 3.2.1) and introducing a weighting function $w(x)$ we obtain 3.2.2. Since the derivative of $w(0)$ is known and $q_{,x}$ is unknown. The first term in 3.2.2 is integrated by parts. After the integration by parts and substituting q with 3.2.1 (2) Equation 3.2.3 is created.

$$\int_{x=0}^{L} wq_{,x}dx - \int_{x=0}^{L} wfdx = 0 \tag{3.2.2}$$

$$\int_{x=0}^{L} wku_{,x}dx + \int_{x=0}^{L} wfdx - wq|_0^L = 0 \tag{3.2.3}$$

3.2.2 Existing Model

For this project an existing finite element model of heat diffusion by Prof. N de Koker was modified for usage in the Bayes' theorem 2.2.1. This model is used to determine the likelihood function. The current model uses the standard Euro code κ-values as well as the specific heat specified in the (CEN, 2004).

The model discretises the wooden element into 32 different elements. For finite element analysis, there are always more elements used to generate the model than usually evaluated. This is done to improve the accuracy of said model. The model is a one dimensional finite element model that takes time differentiation into account.

3.2.3 Adapted Model

The model was changed into a function that takes κ-values and provides a new temperature distribution over the elements for the different κ-values. This function is used in the posterior calculation to determine the likelihood function.

3.3 Inversion method

The basis of the stochastic analysis is the adapted Bayesian equation 3.3.1 below. TODO: further interpret

$$\pi^*(x|T) = \exp\left(-\frac{(\mu - x)^2}{2\sigma_\mu^2}\right) \cdot \exp\left(-\frac{(T - M(x))^2}{2\sigma_{\text{temp}}^2}\right) \tag{3.3.1}$$

3.3.1 Prior probability

$$\pi(x) = \exp\left(-\frac{(\mu - x)^2}{2\sigma_\mu^2}\right) \tag{3.3.2}$$

The prior probability function (Equation 3.3.2) is based on the κ-values assumed prior to any simulation or analysis. The σ_μ in this equation was assumed to be equal to 0.13 W/m·K, In this case, the prior values are indicated as μ and refer to the vector of κ-values(3.3.3) at specific temperatures ?TODO how to indicate?

$$\mu = \begin{bmatrix} 0.12 \\ 0.12 \\ 0.12 \\ 0.12 \\ 0.15 \\ 0.07 \\ 0.09 \\ 0.35 \\ 1.5 \end{bmatrix} \tag{3.3.3}$$

The x (in Equation 3.3.2) refers to a vector of randomised κ-values that correspond with the same temperatures as the values in the μ vector. The first iteration of randomised κ-values are generated by creating a random perturbation of the μ vector. By multiplying the μ vector with $(0.5 + \vec{\text{rand}}) \cdot 1.5)$ the first values of x are guaranteed to be within an acceptable range of the prior values. The process of obtaining the x vector after the first iteration is discussed later in section 3.3.3.

Initially the program was written to generate completely random new values for the first iteration of x. This later proved to not only be unnecessary, but also made the process less accurate as there was a larger burn-in period* before the values were anywhere near the actual solution. To increase the accuracy and reduce the number of times the program needed to run to produce a sufficient number of accurate samples, the program was changed to the current method. The prior function in this case was relatively easy to generate and incorporate into the program as a well defined list of prior values exists.

* explain and validate burn-in for machine learning (TODO)

3.3.2 Likelihood probability function

$$\pi(T) = \exp\left(-\frac{(T - M(x))^2}{2\sigma_{\text{temp}}^2}\right) \tag{3.3.4}$$

The likelihood probability was more complex to implement, as this required utilisation of the function created from the finite element model as discussed in section 3.2. This function will output the probability of the modelled values $M(x)$ given the measured temperature values (T). As can be seen in Equation 3.3.4, the $M(x)$ vector is written as a function. The function indicated here takes the new randomised x vector and then runs the model to provide a new temperature distribution over time at various nodes. The output of the finite element model was reduced such that only the nodes at the same depths as the thermocouples are provided to the likelihood function. For the likelihood function, the σ_{temp} value was assumed to be 15°C.

3.3.3 MCMC itegration

The two main parts of the MCMC integration (as mentioned in section 2) are: how a value is deemed acceptable (Monte Carlo), and how the next random sample is selected after a previous sample is accepted (Markov Chain).

To assist in choosing the next random sample, a step size that indicates how wide the range should be in which the next step will be found was chosen. For this project a step size of 0.05 W/m·K was chosen. This concept can be visualized as follows: our accepted point(x1) is in the center of a cube. The next possible random point is randomly generate but still within the cube. After this next number is selected, the cube moves such that the new point(x2) is now the centre ,and so it continues. See Figure 3.3.1 for clarification. The above example simplifies the concept, but this understanding can now be expanded. If every coordinate direction in the simple example is seen as a single entry into the x vector, then the example has only three κ-values. There are however 10 values, so the imaginary cube in this situation is now ten-dimensional (don't worry, no attempt at drawing that will be made). Another level of complication can be added if it is taken into account that every point in the cube is no longer equally likely. A distribution within the cube can be chosen; in this case a log-normal distribution was chosen. The shape of the cube then warps into a stranger shape with points closer to the center being more likely choices and the edges being less likely.

The acceptance criteria of the new x-vector is based on the proximity of the value to

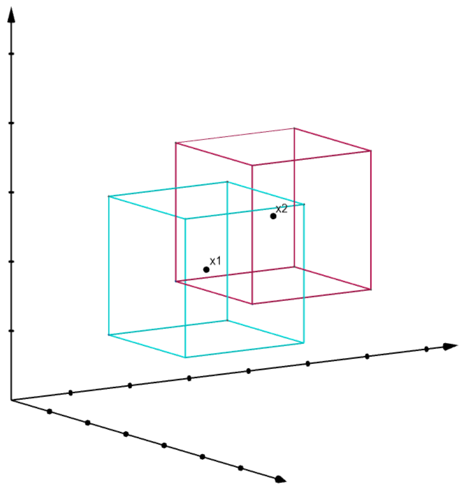
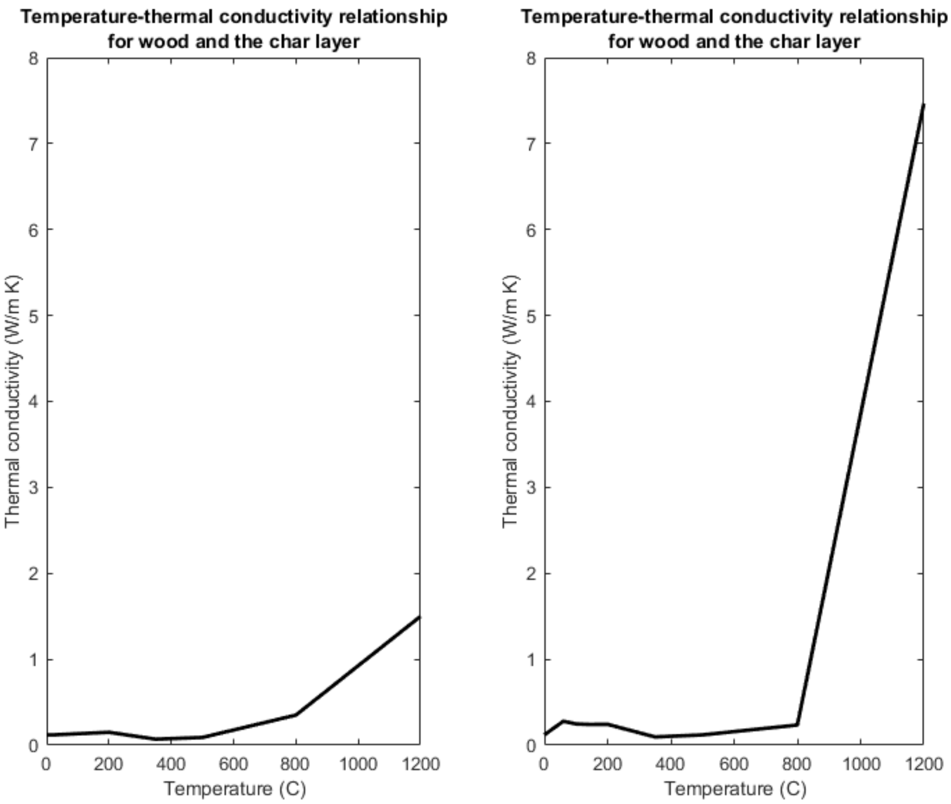


Figure 3.3.1: Three-dimensional example of Markov Chain application(Generated on `https://www.geogebra.org/3d`)


Temperature-thermal conductivity relationship for wood and the char layer
Thermal conductivity (W/m K)
Temperature (C)
0
1
2
3
4
5
6
7
8
0
200
400
600
800
1000
1200
Temperature-thermal conductivity relationship for wood and the char layer
Thermal conductivity (W/m K)
Temperature (C)

Chapter 4

Results

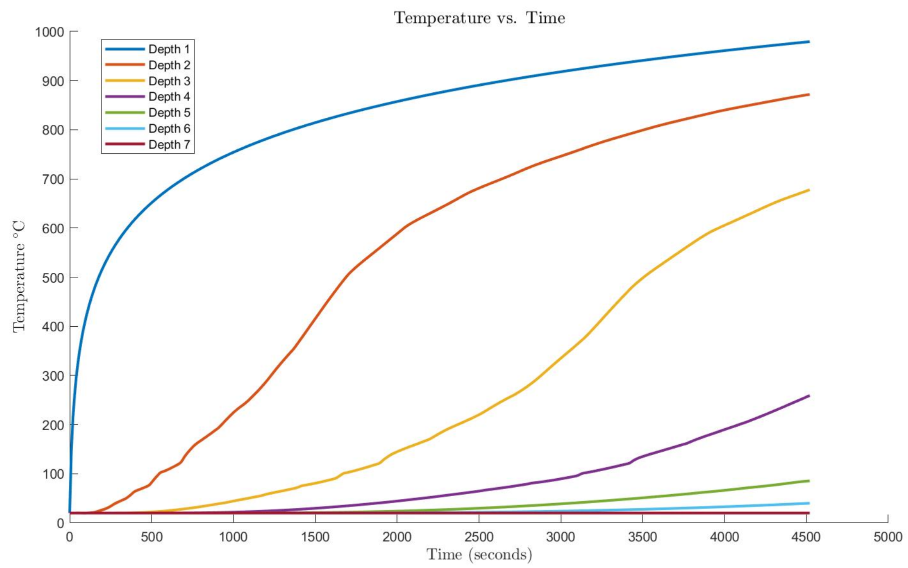
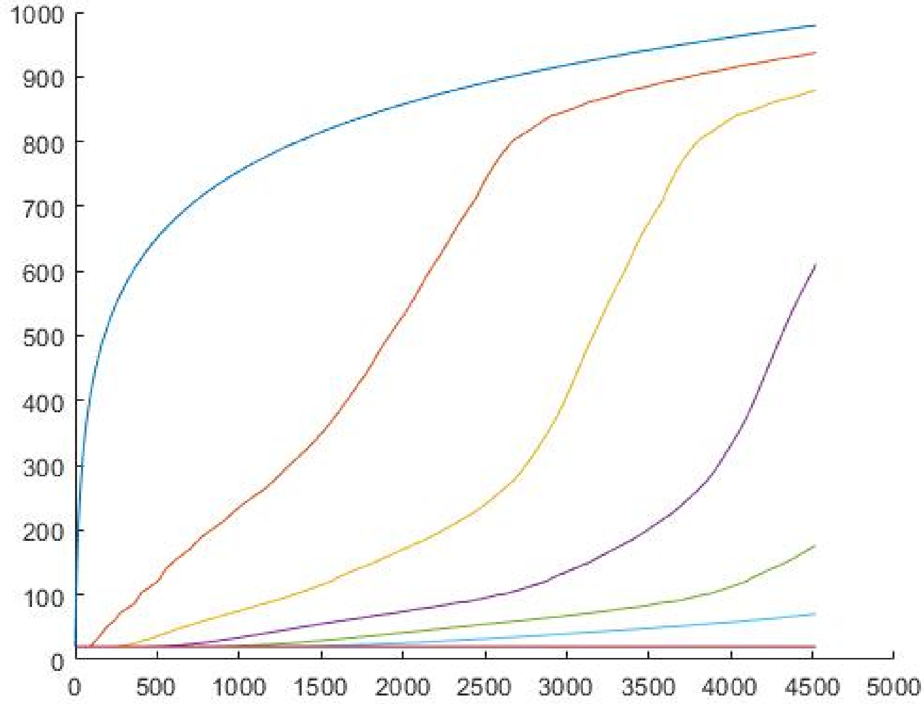


Figure 4.0.1: Output of finite element model using κ-values as indicated in EN 1995:1-2-2004


1000
900
800
700
600
500
400
300
200
100
0
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000

Chapter 5

Discussion

Chapter 6

Summary and Conclusion

Further development of this concept could lead to simplified methods of calculating the fire rating of specifically SA-Pine as well as other timber samples.

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van der Westhuyzen, S., Walls, R. and de Koker, N. (2020). Fire tests of south african cross-laminated timber wall panels: Fire ratings, charring rates, and delamination. *Journal of the South African Institution of Civil Engineering*, vol. 62, no. 1, pp. 33–41. ISSN 23098775.

Relevant code segments

Below are the relevant code segments taken from the Matlab code that was used to generate the final samples used for analysis.

Prior function

Determines the probability of x assuming a (NORMAL) probability over the prior values.

```
function q_val = prior_pdf(x_values,sigmaMU)

 global mu_values
 q_val = -0.5*((x_values - mu_values)*(x_values -
    mu_values)')/(sigmaMU^2);

end
```

Likelihood Function

```
function likelihood_pi = likelihood_func(kinput,sigmaT)

% Global variables: physical constants
global_const;
% Global variables: material properties
global_prop
% Global variables: time integration values
global_time;
% Global variables: mesh geometry
global_mesh;
% Global variables of measured temperatures
global_measuredtemp;

udepths = model_kinput(kinput);
```

```
depths_measured = [depth1;depth2;depth3;depth4;depth5;depth6;depth7];
%Where depths measure is the actual measured temperature data from
    the experiment and udepths is the temperature at the same points
    generated by the model using the new k-values.

tempmat = depths_measured - udepths;
likelihood_pi = tempmat(:)'*tempmat(:)/(-2*sigmaT^2);

end
```

Function to take next step

This function takes the current x-vector and generates a new probable x-vector.

```
function xvalue2 = takexsteps(xvalue1)
  global temps mu_values stepsize sigmastepMU sigmastepT

  locsigma = stepsize*mu_values;
  locxvalue = xvalue1 ;;

  lnMu = log(locxvalue.^2 ./ sqrt(locsigma.^2+locxvalue.^2));
  lnSigma = sqrt(log(locsigma.^2./xvalue1.^2 + 1));

  xvalue2 = max(0, lognrnd(lnMu, lnSigma));
  xvalue2(1) = xvalue1(1);

  xvalue2(xvalue2<locsigma/20) =
      (mu_values(xvalue2<locsigma/20)+xvalue2(xvalue2<locsigma/20))/2;

end
```

Program

Date	What should be done before then
4 Jun	Topic allocated. Contact study leader
23 Jun - 31 Jul	Exams and Recess
10 Aug - 23 Aug	Work on Introduction and Literature study for project proposal
24 Aug	Submit project proposal
25 Aug - 2 Sep	Familiarize with FEM model and MCMC process
2 - 10 Sep	Begin coding a basic MCMC process
10 - 17 Sep	Testweek, minimal time can be alloted to skripsie
18 - 30 Sep	Work on MCMC code during recess
1-8 Oct	Finalise Matlab program for MCMC analysis
8-10 Oct	Run simulation
10 - 17 Oct	Add results, discussion of result and conclusion to report
18 Oct	Submit final draft report
20 - 28 Oct	Finalise report and correct as suggested by study leader
28 - 30 Oct	Print and bind report
1 Nov	Submit report

GA outcomes

GA1:Problem Solving

The problem is described in Chapter 1 t

GA2:Application of scientific and engineering knowledge

GA4:Investigations,experiments and data analysis

GA5: Engineering methods , skill and tools, including IT