

AN ABSTRACT OF THE THESIS OF
NIKOLAUS PFEIFFER for the degree of MASTER OF SCIENCE in
MECHANICAL ENGINEERING presented on September 26, 1983.

Title: TRANSIENT CONDUCTION WITH COUNTER MASS FLOW IN
WOOD. **Redacted for Privacy**

Abstract approved: _____

Dr. Lorin R. Davis

This paper deals with the thermal decomposition of wood slabs under fire conditions. The partial differential equation is solved numerically by the use of an implicit finite difference method. Wood is treated as two components, Lignin and Hemicellulose on one side, and Cellulose on the other side. The chemical reactions are assumed to have Arrhenius type kinetics. The pyrolysis is represented by three first order reactions from which two are exothermic and one is endothermic. The temperature dependence of the properties is approximated by first and second order equations. The gas mixture is treated as an ideal gas mixture. Two boundary conditions are considered: constant heat flux and convection. Temperature and density profiles are computed for both. From this, the ablating velocity of the wood/char surface is determined. For high

incident heat fluxes the ablating velocity is found to be nearly constant while for lower heat sources the velocity is time dependent. It is also found that under fire condition the reaction only takes place in a thin layer at the surface (1-3 mm). The thickness is dependent on the conductivity and the heat source.

TRANSIENT CONDUCTION WITH COUNTER
MASS FLOW IN WOOD

by

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A THESIS

submitted to

Oregon State University

in partial fulfillment of
the requirements for the
degree of

Master of Science

Completed September 26, 1983

Commencement June 1984

APPROVED:

Redacted for Privacy

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Date Thesis is presented: September 26, 1983

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TABLE OF CONTENTS

| | | |
|-----|--|----|
| 1 | INTRODUCTION..... | 1 |
| 1.2 | LITERATURE RESEARCH..... | 3 |
| 2 | DERIVATION OF THE EQUATIONS..... | 8 |
| 2.1 | INTRODUCTION..... | 8 |
| 2.2 | DERIVATION OF THE GENERAL EQUATION..... | 9 |
| 2.3 | CONTROL VOLUME APPROACH..... | 14 |
| 3 | CHEMICAL COMPONENTS OF WOOD..... | 17 |
| 3.1 | INTRODUCTION..... | 17 |
| 3.2 | CELLULOSE..... | 18 |
| 3.3 | HEMICELLULOSE..... | 19 |
| 3.4 | PECTIN..... | 20 |
| 3.5 | LIGNIN..... | 21 |
| 3.6 | COMPOSITION OF WOOD..... | 23 |
| 4 | PROPERTIES OF WOOD, CHAR, AND THE GASES..... | 24 |
| 4.1 | INTRODUCTION..... | 24 |
| 4.2 | PHYSICAL PROPERTIES OF WOOD..... | 24 |
| 4.3 | PROPERTIES OF THE CHAR..... | 31 |
| 4.4 | PROPERTIES OF THE GASES..... | 34 |
| 5 | THE SOURCE TERM..... | 40 |
| 5.1 | INTRODUCTION..... | 40 |
| 5.2 | MODELING THE CHEMICAL REACTIONS..... | 44 |
| 5.3 | CALCULATION OF THE SOURCE..... | 51 |
| 5.4 | THE CONSTANTS..... | 51 |
| 6 | THE COMPUTER PROGRAM..... | 55 |

TABLE OF CONTENTS (continued)

| | |
|--|-----|
| 6.1 INTRODUCTION..... | 55 |
| 6.2 DERIVATION OF THE FINITE DIFFERENCE EQUATIONS. | 55 |
| 6.3 TREATMENT OF THE BOUNDARY CONDITIONS..... | 61 |
| 6.4 METHOD SOLVING THIS SET OF EQUATIONS..... | 64 |
| 6.5 TREATMENT OF THE ABLATING SURFACE..... | 68 |
| 6.6 REASONS FOR THE IMPLICIT METHOD..... | 68 |
| 7 RESULTS..... | 73 |
| 7.1 CONSTANT HEAT FLUX..... | 73 |
| 7.2 CONVECTIVE BOUNDARY..... | 82 |
| 7.3 CONCLUSIONS..... | 96 |
| BIBLIOGRAPHY..... | 98 |
| APPENDICES..... | 100 |
| APPENDIX A..... | 100 |
| APPENDIX B..... | 107 |

LIST OF FIGURES

| Figure | | Page |
|--------|--|------|
| 1 | Control volume for the wood element..... | 14 |
| 2 | The thermal conductivity of wood versus moisture content for different specific gravities..... | 27 |
| 3 | The specific heat of wood versus temperature for different moisture contents..... | 29 |
| 4 | The expansion coefficients of wood in tangential and radial direction versus specific gravity..... | 33 |
| 5 | The specific heat of CO gas versus temperature..... | 37 |
| 6 | The specific heat of CO versus temperature..... | 38 |
| 7 | The specific heat of 60% CO and 40% CO gas..... | 39 |
| 8 | Local relative heat-source strength in a cylinder with a radius of 1.75 cm..... | 43 |
| 9 | Mass fraction of Hemicellulose and Lignin versus time for different temperatures..... | 48 |
| 10 | Mass fraction of Cellulose versus time for different temperatures..... | 49 |
| 11 | Mass fraction of Char versus time for different temperatures..... | 50 |
| 12 | Temperature and density of wood versus location at time $t=10$ s and constant heat flux $Q=80000$ J/m | 76 |
| 13 | Temperature and density of wood versus location at time $t=60$ s and constant heat flux $Q=80000$ J/m | 77 |
| 14 | Temperature and density of wood versus location at time $t=120$ s and constant heat flux $Q=80000$ J/m | 78 |

LIST OF FIGURES (continued)

| Figure | | Page |
|--------|--|------|
| 15 | Temperature and density of wood versus location at time $t=180$ s and constant heat flux $Q=80000$ J/m | 79 |
| 16 | Temperature and density of wood versus location for time $t= 10,60,120,180$ s and constant heat flux $Q=80000$ J/m | 80 |
| 17 | Temperature and density of wood versus location for time $t=10$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 83 |
| 18 | Temperature and density of wood versus location for time $t=60$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 84 |
| 19 | Temperature and density of wood versus location for time $t=120$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 85 |
| 20 | Temperature and density of wood versus location for time $t=180$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 86 |
| 21 | Temperature and density of wood versus location for time $t=240$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 87 |
| 22 | Temperature and density of wood versus location for time $t=300$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 88 |
| 23 | Temperature and density of wood versus location for time $t=360$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 89 |
| 24 | Temperature and density of wood versus location for time $t=420$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 90 |
| 25 | Temperature and density of wood versus location for time $t=480$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 91 |

LIST OF FIGURES (continued)

| Figure | | Page |
|--------|---|------|
| 26 | Temperature and density of wood versus location for time $t=540$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 92 |
| 27 | Temperature and density of wood versus location for time $t=600$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 93 |
| 28 | Temperature and density of wood versus location for time $t=10, 120, 180, 240, 300$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 94 |
| 29 | Temperature and density of wood versus location for time $t=10, 180, 300, 480, 600$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K) | 95 |

NOMENCLATURE

| | |
|-----|--|
| A | additional specific heat due to the wood-water bond energy |
| a | continuously differentiable vector |
| agr | thermal expansion coefficient in grain direction |
| ar | thermal expansion coefficient in radial direction |
| at | thermal expansion coefficient in tangential direction |
| B | mass or volume dependent scalar property |
| b | $b=B/m$ or $b=B/V$ |
| c | specific heat |
| Co | specific heat of dry wood |
| E | energy |
| e | energy per mass |
| h | enthalpy |
| k | conductivity |
| M | moisture content |
| m | mass |
| M' | mass loss |
| MA | mass fraction |
| mB | burnt mass |
| N | number of moles |
| n | outward normal vector |
| P | pressure |

NOMENCLATURE

| | |
|------|---|
| Pd | work rate done by the system on the surrounding pressure stresses |
| Ps | work rate done by the shaft of the system on the surroundings |
| Pt | work rate done by the system on the surrounding viscous stresses |
| Q | heat flux |
| Qi | heat of pyrolysis of reaction i |
| R | gas constant |
| RHS | right hand side |
| S''' | local heat source or sink per unit volume |
| SPG | specific gravity |
| Su | surface |
| T | temperature |
| t | time |
| TN | right hand boundary temperature |
| TO | left hand boundary temperature |
| V | volume |
| v | frequency |
| Ve | velocity |
| W | work |
| X | location |
| z | defined in equation 6.35 |

NOMENCLATURE

Greek Symbols

| | |
|----------|-------------------------|
| α | defined in equation 5.6 |
| ρ | density |
| θ | time in the integration |

Subscripts

| | |
|---|------------------------|
| B | burnt |
| f | final |
| g | gas |
| i | reaction i |
| j | component j |
| m | solid material |
| n | number of nodal points |
| o | original |

TRANSIENT CONDUCTION WITH COUNTER MASS FLOW IN WOOD

1 INTRODUCTION

Wood is one of the most important resources in the world and is one of the world's most widely used industrial raw materials. It can be easily worked and has an advantage over many other raw materials in that it is renewable. Even though it is the oldest fuel used by mankind, its chemistry is still not totally known. Due to its complicated biochemical complexities, its analysis is very difficult. Its properties vary even within the same plant. Therefore, the results of wood analysis change with each experiment. The two main components of wood, Cellulose and Lignin are second to proteins, the most widely spread organic substance (Ref. 1). In contrast to proteins, there are only a few varieties of Cellulose and Lignin. Wood is not a homogenous chemical structure. It is physically, chemically and anatomically heterogenous.

A lot of houses are made of wood, especially here in Oregon. Therefore, it is important to know and to predict the behavior of wood in a fire. At temperatures below the decomposition temperature with the assumption of constant properties, the conduction equation together with

the relevant boundary conditions can be solved for wood, but as soon as higher temperatures exist and decomposition is involved, an analytic solution can not be determined. Either numerical methods or certain assumptions like linear temperature distribution within the wood and abrupt kinetics are necessary to obtain a solution.

To prevent spreading of fire in a building, so called firestops are used. Firestops are (Ref. 2) designed to interfere with the passage of flames up or across a building. According to (Ref. 3) there are two ways the fire resistance time can be defined:

- a. The time taken by the pyrolysis layer to reach the backface.
- b. The time taken to obtain at the backface a specified critical temperature.

The first definition indicates a resistance due to the ability of wood to bear certain stress-loads, the second one is based on fire penetration.

In order to determine the fire resistance time it is therefore necessary to know the temperature distribution and the decomposition rate of the wood layer.

1.2 LITERATURE RESEARCH

Several articles on charring of wood in inert or oxidative atmospheres have been published. Generally the results reached differ with the experimental techniques used. The constants for the activation energy vary for example from 62 KJ/mol (Ref. 4) to 250 KJ/mol (Ref. 5) and the heat of reaction varies from low endothermic (Ref. 1) to exothermic (Ref. 6). None of the authors included in his theoretical part, ablation of the char-layer or a gasflow or variable properties of the wood.

There are mainly three different models used for the chemical reaction. The simplest model (Ref. 3) assumes abrupt kinetics with a constant endothermic heat of reaction (no gasflow and no reactions with oxygen are considered). This, together with other simplifications, leads to an analytic solution. A more complicated model (Ref. 6) is used by C.H. Bamford, J. Crank, and D.H. Malan. They made the following assumptions:

- a. The combustible properties of the decomposition products remain the same throughout the decomposition.
- b. The rate at which gases escape from the surface is determined by the rate of decomposition, and

not by the rate of diffusion to the surface.

- c. The thermal decomposition can be represented by a single exothermic reaction of the first order.

They tried to make the theoretical results of this model agree with experimental data by adjusting the constants in the equation for the chemical reaction.

The most complicated model was developed by C. Vovelle, H. Mellottee, and R. Delbourgo (Ref. 5). They modeled the burning of wood as three different reactions. They tried to adjust the constants of the reaction equations so that the results agreed with experimental data and that the constants for one of the two components of wood (Cellulose) stayed the same as for a reaction of this component alone. This model is used in this program and later described in detail. Stanley Martin (Ref. 7) examined the diffusion controlled ignition of cellulosic materials. He heated the material with a radiant energy source. Using different radiation levels and different times of exposure, he measured the temperature distribution and the weight loss rate. He also analyzed the volatile pyrolysis products and the remaining liquid and solid material. He suggests that the decomposition of cellulose consists of at least two fundamentally different reactions. One produces most of the volatile fuels, and

the other one produces mainly water and carbon oxides. Other authors (Ref. 4, 8, 9) expressed the heat evolution in cellulosic solids as a function of temperature and distance from the surface. Lee, et al., (Ref. 9) found the effective heat of pyrolysis to be highly dependent on the incident heat flux. The heat of pyrolysis is defined as

$$Q = \frac{\sum_i (Q_i \cdot m_{Bi})}{\sum_i m_{Bi}} \quad (1.1)$$

where Q is the heat of pyrolysis, m_{Bi} is the burned mass, and the subscript i stands for reaction i . For low heating rates, a negative overall mass weighted effective heat of reaction (i.e. endothermic reaction) was determined. For high heating rates a positive heat of reaction (i.e. exothermic reaction) was found. Blackshear, et al. (Ref. 8) show graphs of the evolution of heat as a function of temperature and distance from the surface. They suggest an endothermic decomposition at 300-400 C and an exothermic decomposition above 500 C. C. K. Lee, et al., (Ref. 9) also examined the pressure distribution of the gases within the wood. To measure the pressure of the gases, pressure probes connected to an electronic pressure transducer were inbedded in the material. It was found that the maximum pressure buildup was about 0.3 atm. above

ambient pressure. The pressure was also dependent on location, magnitude, and duration of the heat source. It was also found that the pressure and the occurrence of macroscopic cracks (about 1mm wide) were dependent on the grain direction compared to the heated surface. For perpendicular heating, no cracks were observed. They suggest (without giving any details on the reactions) a five reaction model for the thermal degradation of wood:

Reaction 1: Wood + Heat \longrightarrow Char + Tar + Gas

Reaction 2: Tar \longrightarrow Char + Gas + Heat

Reaction 3: Char + Air \longrightarrow Combustion Products

Reaction 4: Tar + Air \longrightarrow Combustion Products

Reaction 5: Gas + Air \longrightarrow Combustion Products

In Reference 10, a similar physical problem is solved with a totally different application. A finite difference method is used to determine the thermal response of boost and entry heat shields devices. Due to friction, the surface is heated. As high temperatures are reached, a chemical reaction takes place, producing gases and the surface ablates. The author used an explicit method to derive the finite difference equations. The following assumptions were made:

- a. A complete chemical equilibrium at the exposed surface.

- b. A coordinate shift that causes the nodal points to ride with the receding surface .

The receding surface was handled by combining two nodes as soon as one of them reached a specified minimum thickness (this was necessary for stability of the finite difference method (explicit)). The chemical reaction taking place was modeled by an exponential rate equation. A linear combination of virgin material properties and completely charred material was used. Also, temperature equilibrium of the gases and the surrounding materials was assumed. The properties of the gases and the materials were taken from tables using an interpolation program to determine the properties at each temperature. In order to avoid temperature jumps when the surface node was combined with the second node, the nodes that were combined are at the unheated side, i.e. where the temperature difference between the nodal points was small.

2 DERIVATION OF THE EQUATIONS

2.1 INTRODUCTION

Two ways are considered in this paper to obtain the differential form of a physical problem. The first method uses the integral form of the general laws and converts the surface integrals with the use of Green's theorem to volume integrals. A general law is characterized by the fact that its application is independent of the nature of the medium under consideration. Then, particular laws are applied to the physical problem. A particular law is characterized by the fact that its application depends on the nature of the medium under consideration. A second method uses a control volume approach. First a general equation is obtained by the use of the integral forms of two general laws, the 1st law of thermodynamics and the law of mass conservation (continuity), and Fourier's law of conduction. A control volume approach is used to get the final equations which apply to the physical problem.

2.2 DERIVATION OF THE GENERAL EQUATION

The universal integral form of a general law is
(Ref. 11):

$$\left(\frac{dB}{dt}\right)_{\text{system}} = \int \frac{\partial(b \cdot \rho)}{\partial t} dV + \int_{su} b \cdot \rho V_e n dS_u \quad (2.1)$$

where B is a mass or a volume dependent scalar property whose specific value b is given by

$$b = B / m \quad \text{or} \quad b = B / V \quad (2.2)$$

respectively; m represents the mass, V the volume, ρ the density, t the time, Su the surface, V_e the velocity, and n the outward normal vector.

2.2.1 CONSERVATION OF MASS (CONTINUITY)

For the continuity equation $B=m$ and $b=1$. Therefore

$$\left(\frac{dm}{dt}\right)_{\text{system}} = \int_V \frac{\partial \rho}{\partial t} dV + \int_{su} \rho V_e n dS_u \quad (2.3)$$

Since the left hand side of equation 2.3 is equal to zero

$$0 = \int_V \frac{\partial \rho}{\partial t} dV + \int_{su} \rho V_e n dS_u \quad (2.4)$$

Using Green's theorem

$$\int_{S_u} a_n dS_u = \int_V \nabla \cdot a dV \quad (2.6)$$

with a being a continuously differentiable vector and S_u being a piecewise smooth surface, it is found that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V_e) = 0 \quad (2.7)$$

For solids and incompressible fluids, $\rho = \text{constant}$, equation 2.7 reduces to,

$$\nabla \cdot V_e = 0 \quad (2.8)$$

2.2.2 FIRST LAW OF THERMODYNAMICS

Using Green's theorem, equation 2.7, and

$$\nabla \cdot (\alpha \cdot \beta) = \alpha \nabla \cdot \beta + \beta \nabla \cdot \alpha \quad (2.9)$$

equation 2.1 can be transformed into

$$\left(\frac{dB}{dt} \right)_{\text{system}} = \int_V \rho \left(\frac{db}{dt} \right) dV \quad (2.10)$$

The conserved property B in this case is energy E.

Therefore:

$$\left(\frac{dE}{dt}\right)_{\text{system}} = \int_V \rho \left(\frac{de}{dt}\right) dV \quad (2.11)$$

Noting that the rate form of the first law of thermodynamics states

$$(dE/dt)_{\text{system}} = (dQ/dt)_{\text{system}} - (dW/dt)_{\text{system}} \quad (2.12)$$

it is found that

$$\int_V \rho \cdot \left(\frac{de}{dt}\right) dV = - \int_{Su} \mathbf{q} \cdot \mathbf{n} dSu - P_d - P_t - P_s - \int_V S''' dV \quad (2.13)$$

Where P_t , P_s , and P_d are the work rates done by the system on the surrounding viscous stresses, the shaft of the system on the surroundings and the system on the surroundings pressure respectively. S''' represents the rate of a local energy sink or source per unit volume. For frictionless incompressible fluids and for solids $P_t = 0$. If no shaftwork is done by the system on the environment and

$$P_d = \int_{Su} pVn dSu \quad (2.14)$$

equation 2.13 reduces to

$$\rho \left(\frac{de}{dt} \right) + \nabla \cdot (\rho V + Q) = S''' \quad (2.15)$$

using

$$\nabla \cdot (\rho V) = V \cdot \nabla \rho \quad (2.16)$$

equation 2.15 can be transformed into

$$\rho \left(\frac{de}{dt} \right) + V \cdot \nabla \rho + \nabla \cdot Q = S''' \quad (2.17)$$

or if $\rho = \text{constant}$

$$\rho \left(\frac{de}{dt} \right) + \nabla \cdot Q = S''' \quad (2.18)$$

Fourier's law of conduction (1 Dimensional) is given as,

$$Q_x = -k \frac{\partial T}{\partial x} \quad (2.19)$$

where k stands for the conductivity and x for the location.

2.2.3 THE FINAL EQUATIONS

Using equation 2.19 and equation 2.18, one can show that for

$$e = h = cT \quad (2.20)$$

where h , c , T are the enthalpy, the specific heat, and the temperature respectively, equation 2.21 is valid.

$$\rho c \left(\frac{dT}{dt} \right) + \frac{\partial Q}{\partial x} = S''' \quad (2.21)$$

From this it follows

$$\rho c \left(\frac{\partial T}{\partial t} \right) + V_x \rho c \left(\frac{\partial T}{\partial x} \right) + \frac{\partial (-\kappa \frac{\partial T}{\partial x})}{\partial x} = S''' \quad (2.22)$$

or

$$\frac{\partial \kappa \left(\frac{\partial T}{\partial x} \right)}{\partial x} - V_x \rho c \left(\frac{\partial T}{\partial x} \right) + S''' = \rho c \left(\frac{\partial T}{\partial t} \right) \quad (2.23)$$

2.3 CONTROL VOLUME APPROACH

Figure 1 shows the control volume used,

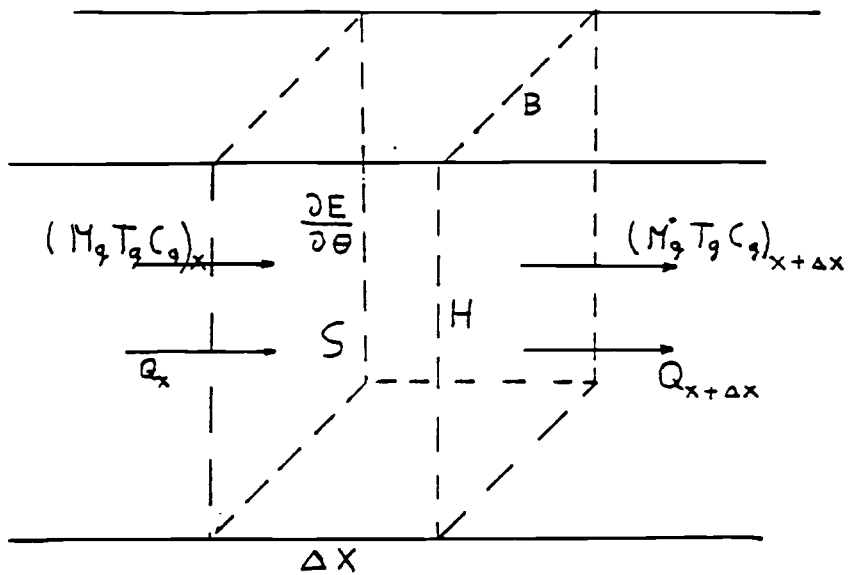


Figure 1. Control volume for the wood element

From the control volume, it follows that,

$$\begin{aligned}
 & B \cdot H \cdot Q_x - Q_{x+\Delta x} B H + (M_g T_g C_g)_x \\
 & - (M_g T_g C_g)_{x+\Delta x} + S = \frac{\partial E}{\partial Q}
 \end{aligned} \tag{2.24}$$

$$E = m_M C_M T + M_g C_g T \tag{2.25}$$

where the subscripts M and g stand for solid material and

gas respectively.

$$\dot{m} = \rho H B V_e \quad (2.26)$$

$$\dot{m} = \rho H B dx \quad (2.27)$$

$$S''' = \frac{S}{H B dx} \quad (2.28)$$

Equations 2.24 to 2.28 lead to

$$\begin{aligned} & (Q_x - Q_{x+\Delta x}) H B + \rho H B V_e C_g (T_x - T_{x+\Delta x}) + S \\ & = H B dx (\rho_M C_M + \rho_g C_g) \left(\frac{\partial T}{\partial \theta} \right) \end{aligned} \quad (2.29)$$

$$\begin{aligned} & \frac{(Q_x - Q_{x+\Delta x})}{\Delta x} - \rho V_e C_g \frac{(T_x - T_{x+\Delta x})}{\Delta x} + S''' \\ & = (\rho_M C_M + \rho_g C_g) \left(\frac{\partial T}{\partial \theta} \right) \end{aligned}$$

with $\lim \Delta x \rightarrow 0$

$$\begin{aligned} & \frac{\partial \left(\kappa \frac{\partial T}{\partial x} \right)}{\partial x} - C_g \rho V_e \left(\frac{\partial T}{\partial x} \right) + S''' \\ & = (\rho_g C_g + \rho_M C_M) \left(\frac{\partial T}{\partial \theta} \right) \end{aligned} \quad (2.30)$$

where S is the sum of

- a. The heat source or energy sink per unit volume.
- b. The thermal energy of the produced gases per unit volume.

3 CHEMICAL COMPONENTS OF WOOD

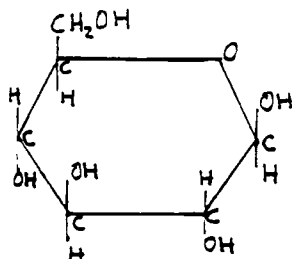
3.1 INTRODUCTION

Wood as a product of biological development is a complex substance both anatomically and chemically. It is non-uniform even within a single tree and varies somewhat between individuals of same species and often greatly between species. Wood is made out of small cells and has a fibrous structure. All wood substances include lignin and a polysaccharide system Holocellulose. Holocellulose consists of Wood Cellulose, Hemicellulose, and subordinate amounts of Pectic materials (Ref. 12). However, these components are not neat, easily identifiable chemical components. Lignin is apparently a series of closely related tridimensional polymers of varying degrees of polymerization, a part of which is linked chemically to a portion of the Holocellulose. Cellulose is closely associated with some of the Hemicellulose (Ref. 12). In this paper a brief description of the most important components of wood is given.

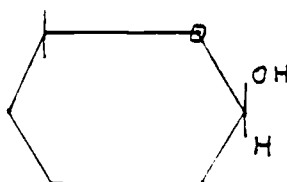
3.2 CELLULOSE

The empirical formula of cellulose is $(C_6H_{10}O_5)_n$.

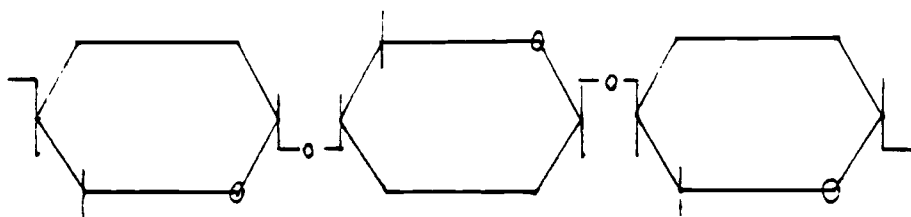
Its monomer has the following structure



or (in a short form)



The polymer is of the following structure



The weight per molecule of Cellulose is very high and is determined by the degree of polymerization. A Macromolecule of a Cellulose contains up to 15,000 glucose residues and it is about 0.01 mm long. Its diameter is about $5.1 \cdot 10^{-10}$ m and can not be seen in a microscope. In wood the degree of polymerization is, according to Ref. 1,

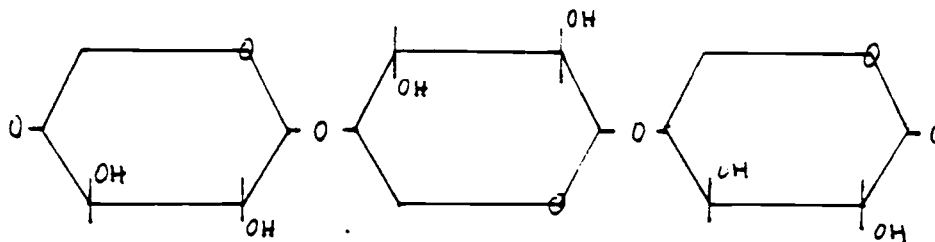
about 1000-1600.

3.3 HEMICELLULOSE

Hemicellulose consists mainly of two components, Pentosans and Hexosans. It is far less resistant to action of dilute acids than other cell wall components, and it might also be combined in other components of high molecular weight.

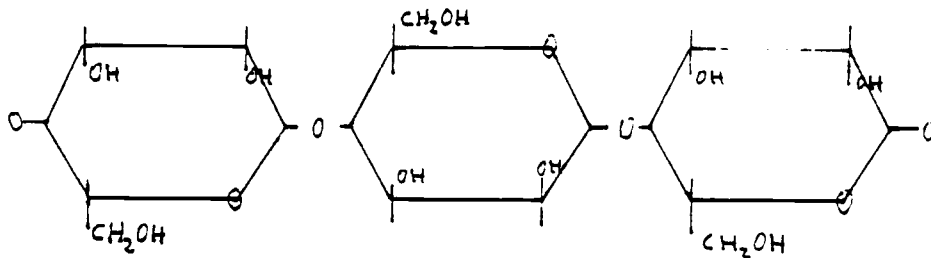
3.3.1 PENTOSANS

The most important Pentosan in Hemicellulose is Xylan. Its degree of polymerization is between 70 and 200. Its chemical structure is



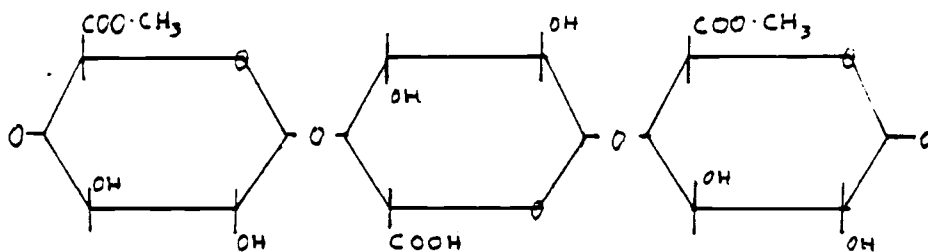
3.3.2 HEXANS

Mannan is the most common Hexan of Hemicellulose.
 Its degree of polymerization is about 160 and its
 chemical structure is as follows



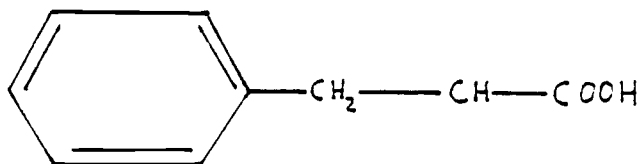
3.4 PECTIN

Pectin mainly exists in young plants. In older woods
 the percentage of pectin is only around 0.5%. The weight
 per Mol is around 100,000. The chemical structure is

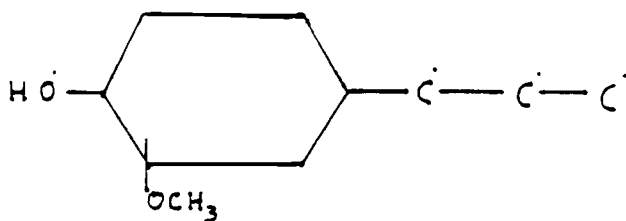


3.5 LIGNIN

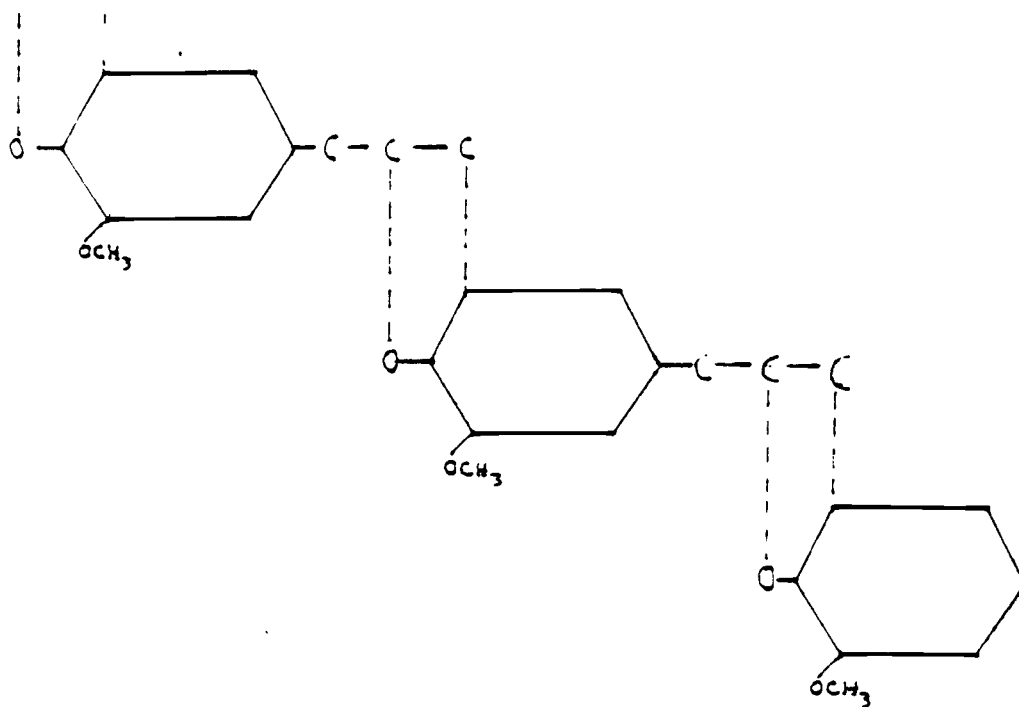
Lignin is defined as that incrusting material of the plant which is built mainly, if not entirely, of phenylpropane building stones (Ref. 12). The chemical structure of phenylpropane is



In contrast to the polysaccharides, Lignin is resistant towards strong mineral acids, and is aromatic in nature. Lignin is a group of high-molecular, amorphous compounds that are chemically very closely related. A typical monomer of Lignin is dihydroeuganol



By condensing this typical monomer to a polymer, the following structure is reached.



3.6 COMPOSITION OF WOOD

A table showing the composition of Fir (*Picea excelsa*) is shown below (Ref. 1). Due to different experiments the data for the constituents vary. Therefore, three values are presented for each component:

- a. the maximum value MAX (%)
- b. the minimum value MIN (%)
- c. the mean value MEAN (%)

| Component | MAX | MIN | MEAN |
|---------------|-------|-------|-------|
| Holocellulose | 75.7 | 67.9 | 71.87 |
| Cellulose | 59.13 | 41.0 | 49.13 |
| Hemicellulose | | | |
| total | 26.25 | 16.39 | 20.87 |
| Pentosans | 12.86 | 8.0 | 9.28 |
| Hexosans | 13.38 | 8.38 | 11.59 |
| Lignin | 28.5 | 16 | 23.9 |

4 PROPERTIES OF WOOD, CHAR, AND THE GASES

4.1 INTRODUCTION

Generally all physical properties are temperature dependent. As wood is not a uniform material, its properties are also, up to a certain amount, dependent on the species and the individual plant. In this paper average values are used, and in the case of temperature dependence, linear approximations are made. For the gases, an ideal gas approach is used to determine the properties of the gas mixture. For each individual gas first and second order approximations for the temperature dependence are made. Generally for all mixtures the principle of superposition (i.e. linear relationships are assumed) is used.

4.2 PHYSICAL PROPERTIES OF WOOD

First it is necessary to define specific gravity and grain: Specific gravity is the ratio of the weight of a given volume of wood to that of an equal volume of water at a standard temperature (Ref. 2).

Since the weight of wood in a given volume changes with the shrinkage and swelling caused by changes in moisture content, specific gravity is an indefinite quantity unless the conditions under which it is obtained are specified.

Grain is often used in reference to annual rings but also employed to indicate the direction of the fibers. It is also used by painters as open grained and closed grained, meaning the relative size of the pores.

In this text grain is used to indicate the direction of the fibers.

4.2.1 THERMAL CONDUCTIVITY

The factors that affect conductivity in wood are:

- a. direction of grain
- b. specific gravity
- c. moisture contents
- d. kind, quantity, and distribution of extractives
- e. checks, knots, cross grains

Thermal conductivity is approximately the same in radial and tangential direction, but it is generally 2.25 to 2.75 times larger along the grain than in transverse

directions. It increases with specific gravity (i.e. the lighter weight woods are the better insulators) and moisture contents.

The values for thermal conductivity of oven-dry wood range from 0.41 W / m K for Balsa (specific gravity of 0.16) to 1.3 W / m K for Sugar Marbel (specific gravity of 0.66).

If the specific gravity S (based on volume at current moisture content and weight when oven-dry) and the moisture content M of the wood are known, the conductivity can be determined by (Ref. 2):

$$k = [S(1.39 + 2.8 M) + 0.165] \cdot 0.14413 \quad (4.1)$$

where k is the thermal conductivity in W / m K. A chart of conductivity verses moisture content for several different specific gravities is shown in Figure 2.

4.2.2 SPECIFIC HEAT

Specific heat of dry wood is mainly temperature dependant. It is approximately related to temperature T in Kelvin by

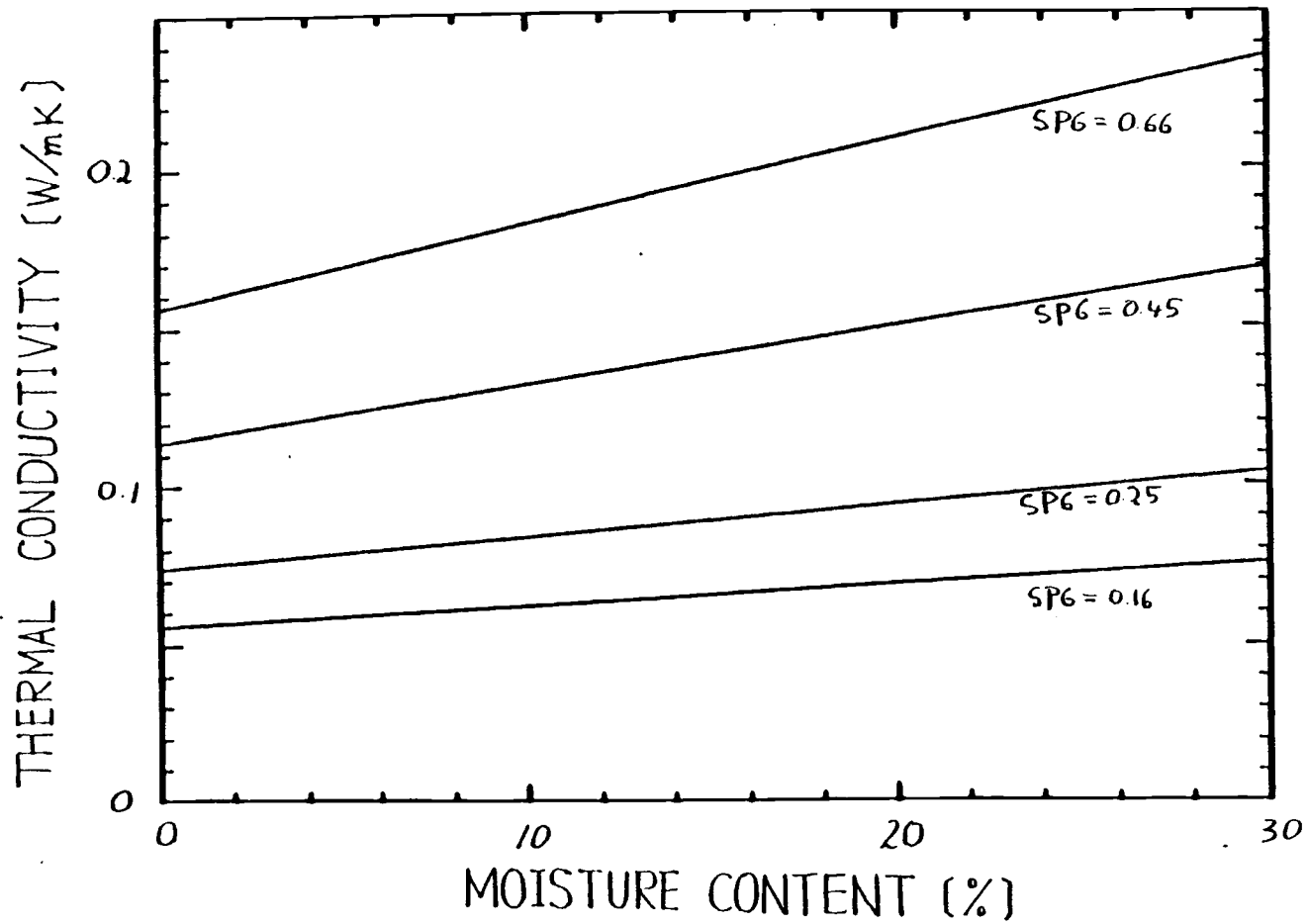


Figure 2. The thermal conductivity of wood versus moisture content for different specific gravities.

$$C_o = [0.25 + 0.006 (1.8T - 459.67)] \cdot 4.184 \quad (4.2)$$

where C_o has the units J / g K. When wood contains water, the specific heat is increased because the specific heat of water is larger than that of dry wood and because of an additional specific heat due to a water-wood bond energy. The specific heat of moist wood is given by

$$C = \left[\frac{(M + C_o)}{(1 + M)} + A \right] \cdot 4.184 \quad (4.3)$$

where M is the fractional moisture content of the wood, C_o is the specific heat of dry wood, and A is the additional specific heat due to the wood-water bond energy. For M being around 10%, A ranges from about 0.02 at 302.6 K to about 0.04 at 333.2K. For M around 30%, A ranges from about 0.04 at 302.6 K to about 0.09 at 333.2K.

A graph using linear interpolation and extrapolation of this data showing the specific heat verses temperature for oven-dry wood and wood with 10% and 30% moisture content is shown in Figure 3.

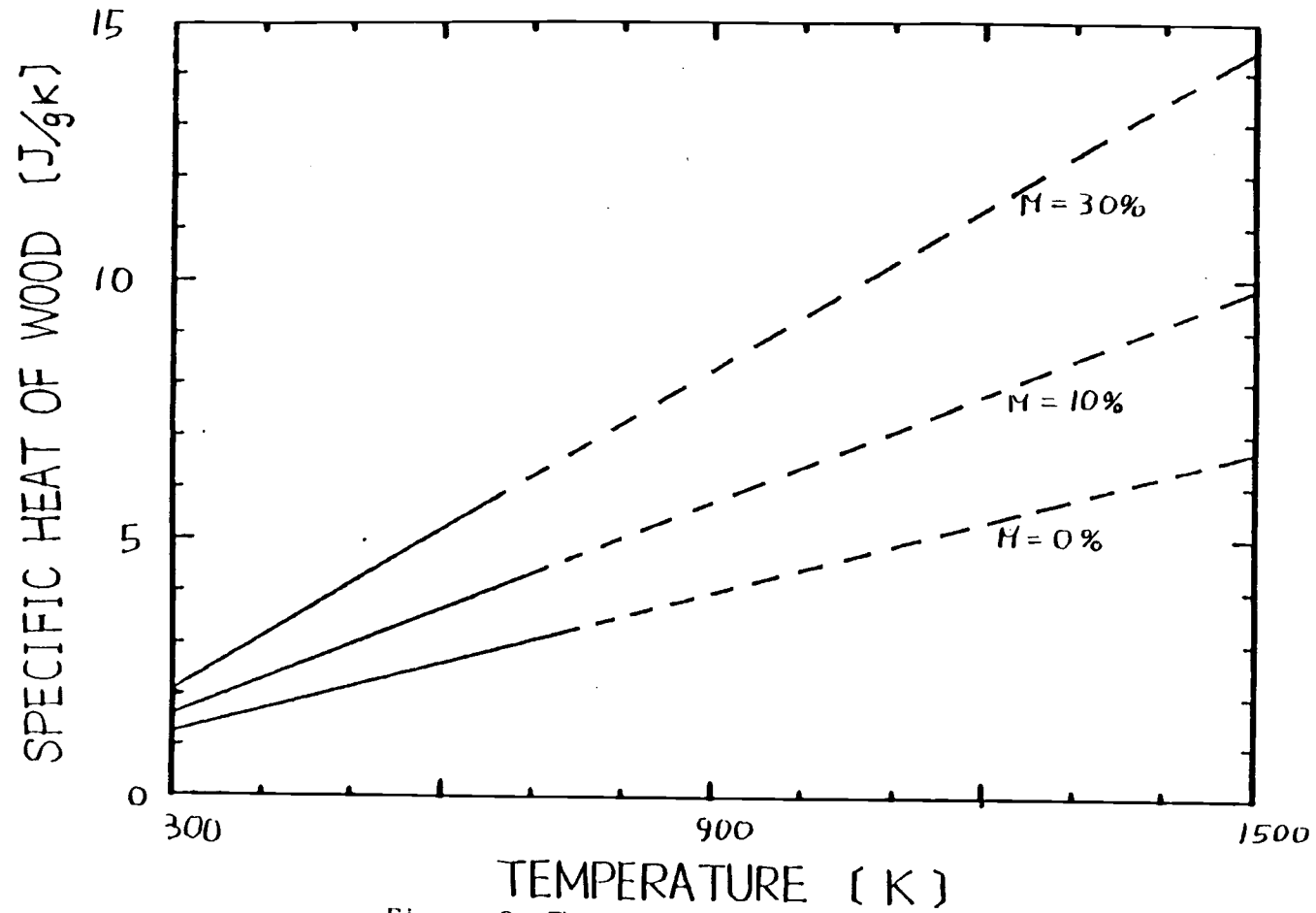


Figure 3. The specific heat of wood versus temperature for different moisture contents.

4.2.3 SPECIFIC GRAVITY

The thermal expansion coefficients of oven-dry wood are positive in all directions. The thermal expansion coefficients are, however, dependent on the direction.

PARALLEL TO THE GRAIN

The thermal expansion coefficients vary only slightly with specific gravity and species. They range from $3.1 \cdot 10^{-6}$ to $4.5 \cdot 10^{-6}$ per degree Kelvin.

RADIAL AND TANGENTIAL

The radial and tangential thermal expansion coefficients are proportional to wood density. They are 5 to 10 times greater than the parallel to the grain coefficient. For a specific gravity range of 0.1 to 0.8, they can be approximated by (Ref. 2):

$$\alpha_r = 1.8 (33 \cdot \text{SPG} + 9.9) \cdot 10^{-6} / \text{deg K} \quad (4.4)$$

$$\alpha_t = 1.8 (33 \cdot \text{SPG} + 18.4) \cdot 10^{-6} / \text{deg K} \quad (4.5)$$

From this, the specific gravity can be calculated by:

$$SPG = \frac{SPGR}{(1 + \alpha_r \Delta T)(1 + \alpha_t \Delta T)(1 + \alpha_{gr} \Delta T)} \quad (4.6)$$

where spg is the specific gravity, spgr is the specific gravity at reference temperature, α_r , α_t , α_{gr} are the thermal expansion coefficients in radial, tangential, and grain direction, and ΔT is the temperature difference to the reference temperature.

Only the thermal expansion coefficients for dry wood are generally of interest since shrinkage due to loss of moisture is much larger than the thermal expansion. Values for α_r , α_t , and α_{gr} are shown on Figure 4.

4.3 PROPERTIES OF THE CHAR

Very little has been published about the properties of char. In this paper constant properties are assumed. The density of char is assumed to be about 40% of the density of wood (Ref. 3). The thermal conductivity is dependent on direction. The difference for the directions

is about 30%. In this paper an average value is assumed.

The specific heat of char is assumed to be 2 J / g K (Ref. 3).

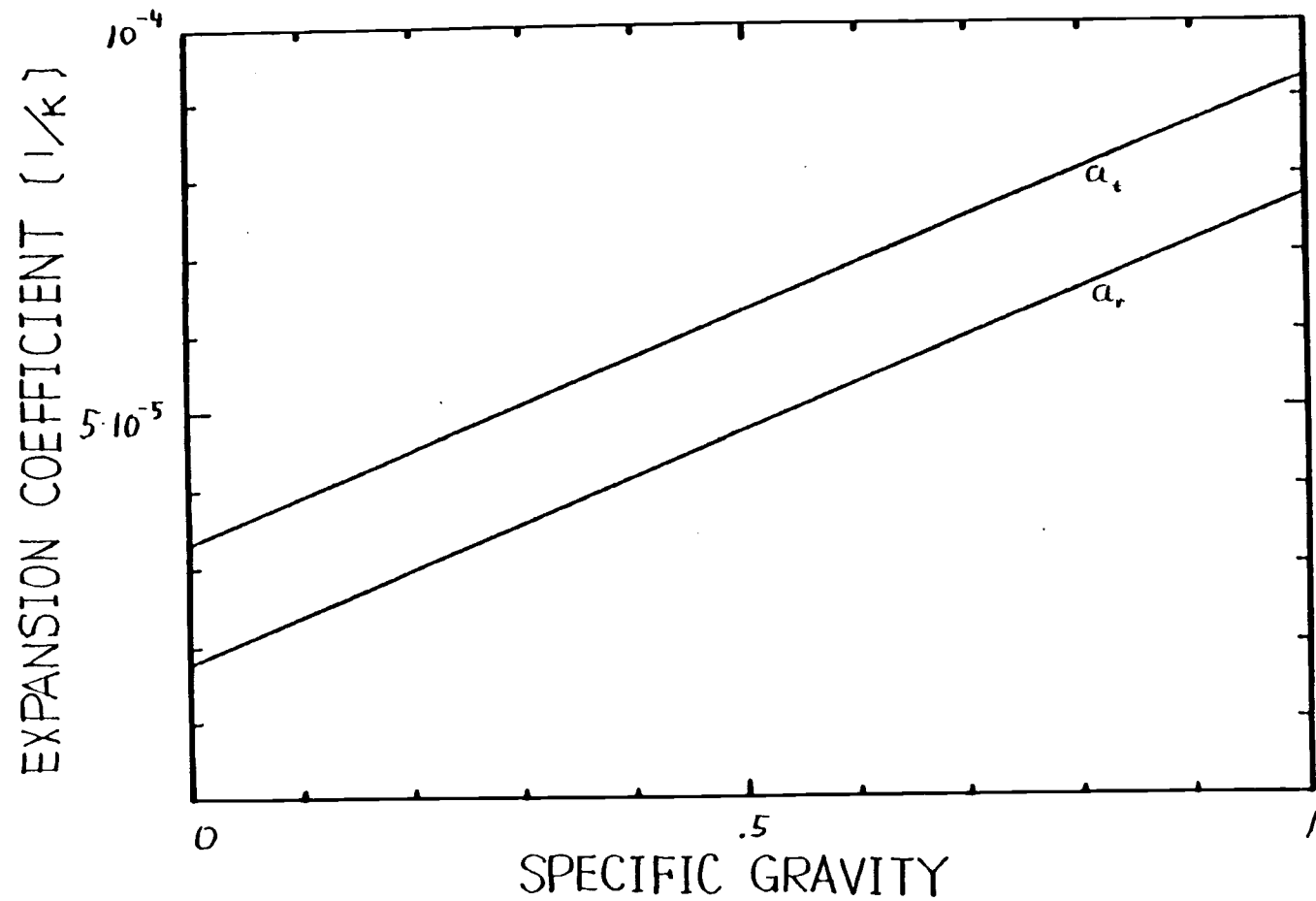


Figure 4. The expansion coefficients of wood in tangential and radial direction versus specific gravity

4.4 PROPERTIES OF THE GASES

According to Stanley Martin (Ref. 7) approximately 97 to 98 % of the gas products are carbon dioxide and carbon monoxide. The rest is H_2 , CH_4 , C_2H_4 , and C_2H_6 . In this paper the effects of H_2 , CH_4 , C_2H_4 , and C_2H_6 are neglected. The gas products are treated as a mixture of CO and CO_2 . The following properties are of interest for this paper:

- a. density
- b. specific heat

The gases are treated as ideal gases. Therefore,

$$P_j = \frac{N_j \cdot R \cdot T_m}{V_m} \quad (4.7)$$

where the subscript m stands for mixture, P_j and N_j are the pressure and the number of mols of component j respectively. T is the temperature and R is the gas constant. From the laws for ideal gases it can be shown, that

$$P_j = \frac{P_m N_j}{N_m} \quad (4.8)$$

It is assumed that the gases are at atmospheric pressure.

With these assumptions the density of component j , ρ_j

$$\rho_j = \frac{P_j M_j}{(R \cdot T)} \quad (4.9)$$

can be determined M_j is the mass of component j per mol of component j . Putting equation 4.8 to 4.10 together we obtain:

$$\rho_j = \frac{N_j M_j}{RT N_m} \quad (4.10)$$

$$\frac{N_j}{N_m} = \frac{MA_j \cdot M_m}{M_j} \quad (4.11)$$

where MA_j is the mass fraction of component j .

For the specific heat, a second order temperature dependency is assumed:

$$SH = a + bT + cT^2 \quad (4.12)$$

From Ref. 13 the constants are as follows:

$$CO: a = 26.881; b = 6.971 \cdot 10^{-3}; c = -0.821 \cdot 10^{-6} \quad (4.13)$$

$$\begin{aligned} \text{CO}_2 : \quad a &= 26.018 \quad ; \quad b = 43.528 \cdot 10^{-3} \\ c &= -14.843 \cdot 10^{-6} \end{aligned} \quad (4.14)$$

The units for the specific heat c are J / mol K and T is in Kelvin. C_m is then calculated by:

$$C_m = \sum_j (C_j M A_j) \quad (4.15)$$

A chart for CO₂, CO, and a mixture of 60% CO₂ and 40% CO is shown in Figure 5,6,and 7.

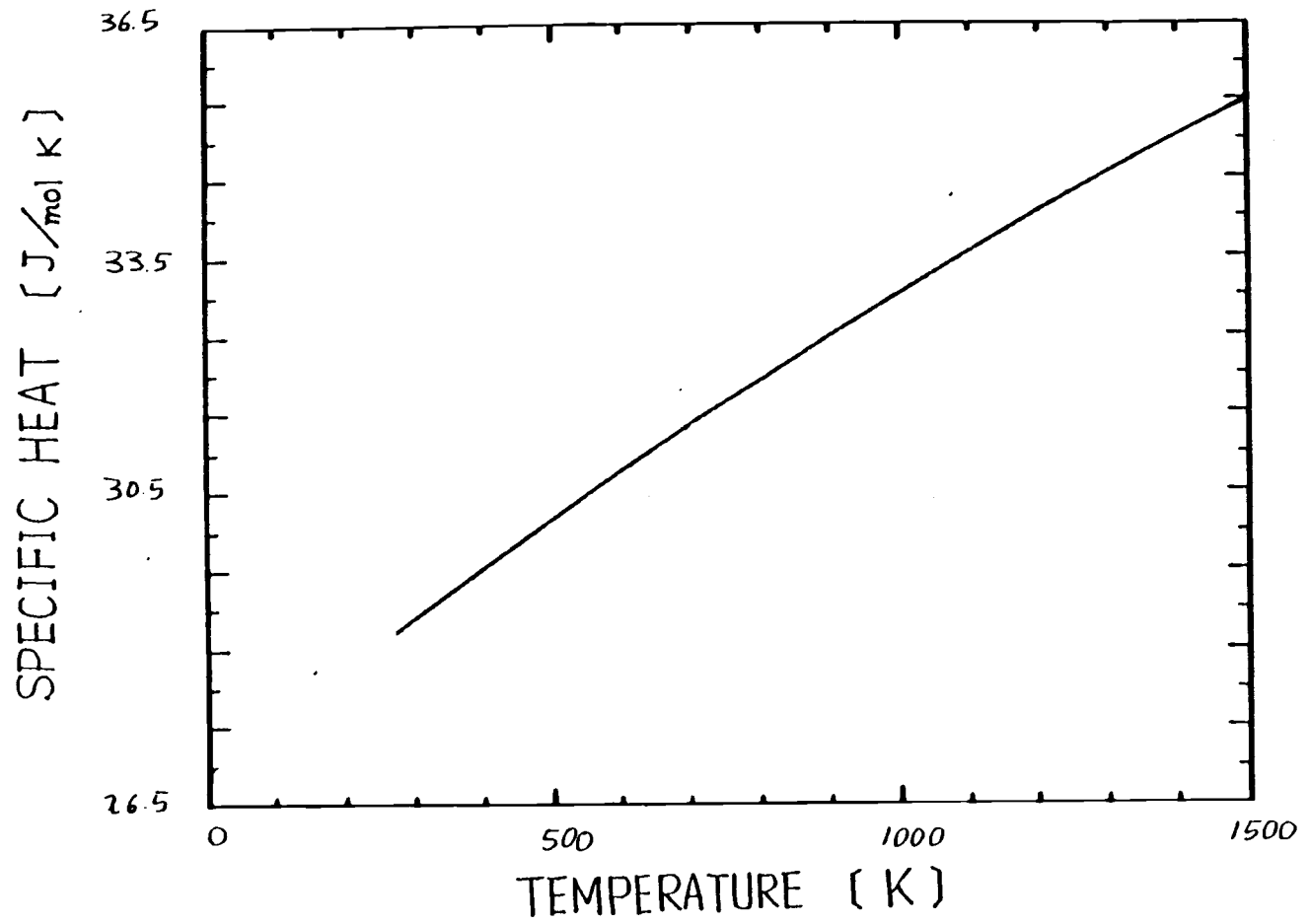


Figure 5. The specific heat of CO gas versus temperature

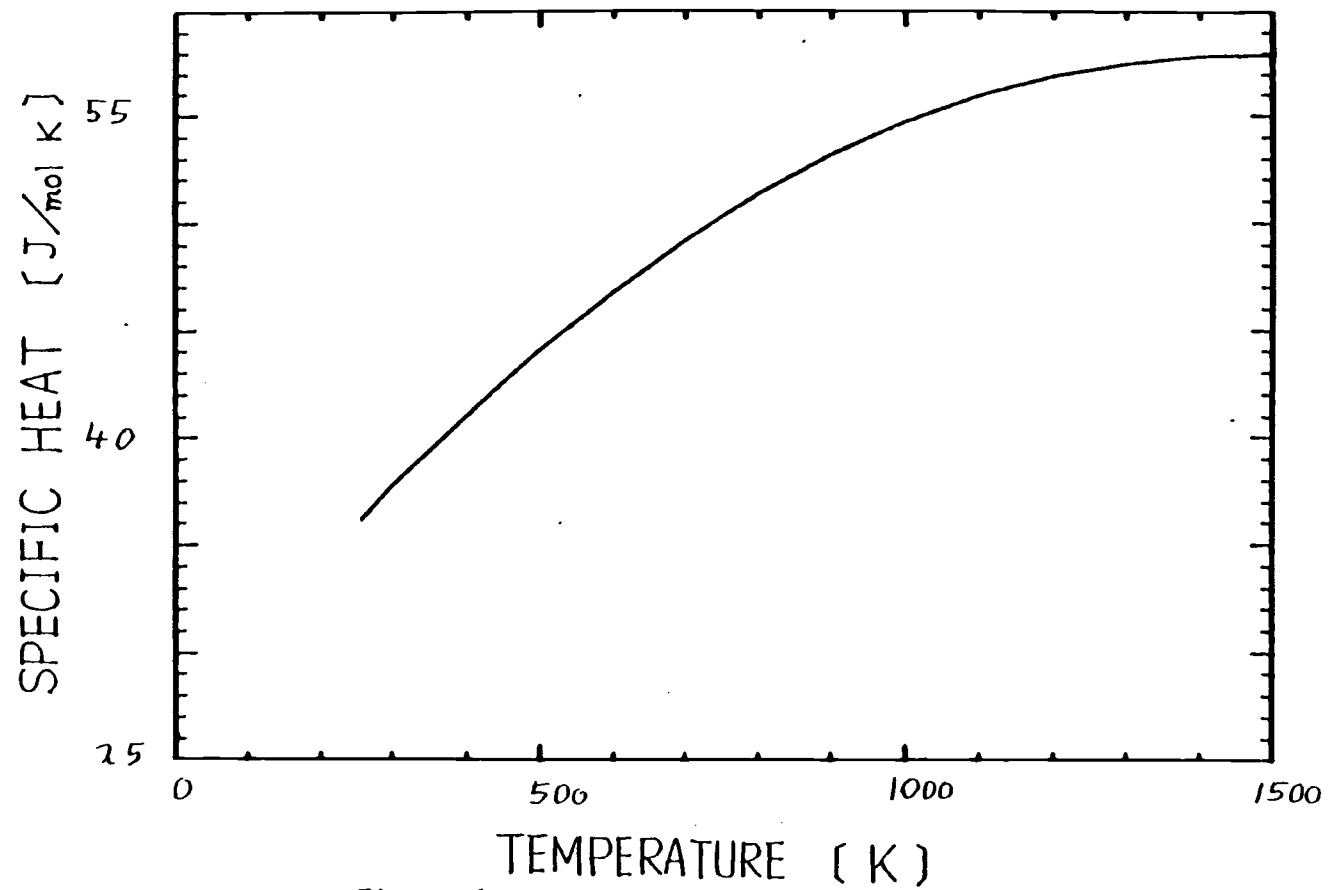


Figure 6. The specific heat of CO₂ gas versus temperature

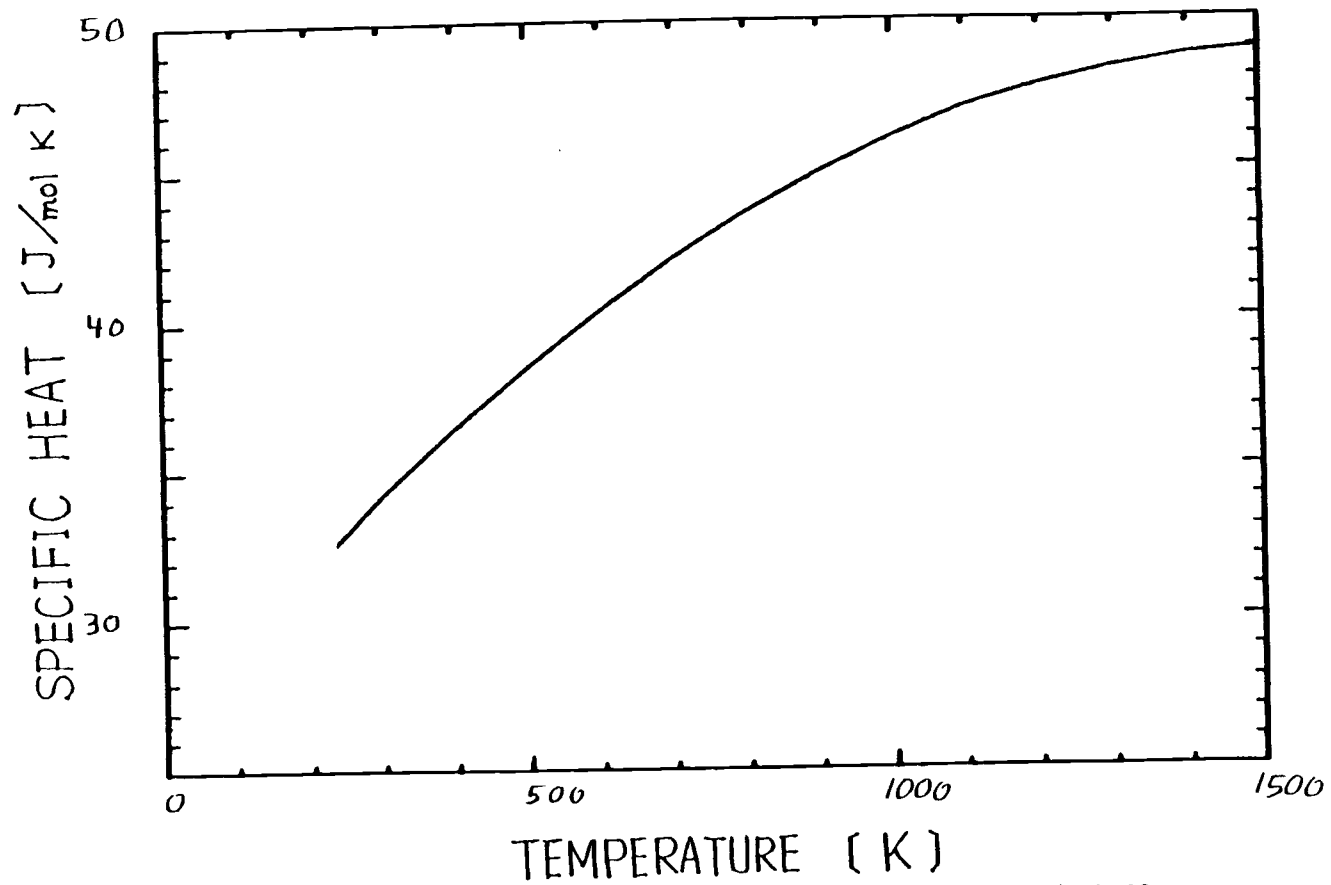


Figure 7. The specific heat of a 60% CO₂ and 40% CO gas mixture.

5 THE SOURCE TERM

5.1 INTRODUCTION

Burning of wood in air is the sum of various complex reactions. Due to differences in composition and complexity of the reactions, averaging and some simplifications are necessary to model degradation of wood. In this paper, the following assumptions are made (Ref. 5): a. Wood consists only of three components; Lignin, Hemicellulose, and Cellulose. b. The reactions can be modeled by two parallel 1st order reactions, and one successive 1st order reaction. c. Lignin and Hemicellulose can be treated as one uniform component.

Linear approximations are used to calculate the mass fraction of each component and it is assumed that superposition can be used to determine the mass loss of each component. Constant (i.e. temperature independent) heat of reaction for each chemical reaction are used.

5.1.1 THE CHEMICAL REACTIONS

The decomposition of wood can be subdivided into three different chemical reactions. The first reaction takes place at temperatures of about 250 C. It is an endothermic pyrolysis of Lignin and Hemicellulose. With higher temperatures (T around 350 C) wood undergoes active pyrolysis. Decomposition of Lignin and Hemicellulose continues and the onset of pyrolysis of Cellulose occurs (Reaction 2). This process, in contrast to the first one, is an exothermic reaction. The third reaction takes place at temperatures above 350 C. The surface char layer reacts in an exothermic reaction with air.

5.1.2 HEAT OF REACTION

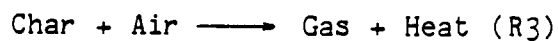
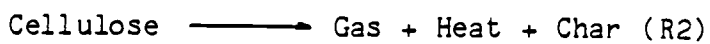
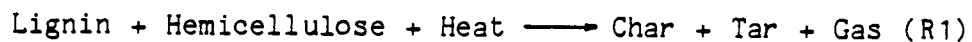
The overall mass weighted effective heat of pyrolysis is defined by (Ref. 9)

$$Q_o = \frac{\sum_j Q_j M_j}{\sum_j M_j} \quad (5.1)$$

where Q_j is the heat of pyrolysis of control mass j , M_j is the mass loss of component j and Q_o is the overall effective heat of pyrolysis. Q_o is dependent on the magnitude of the heat source the wood is exposed to. For

low heating rates it is negative, i.e. the overall reaction is endothermic and for higher heating rates it is positive i.e. the overall reaction is exothermic. The heat evolution in a cylinder with a radius of 1.75 cm as a function of location and temperature is shown in Figure 8. (Ref. 8).

The chemical reactions taking place can be simplified to the following:



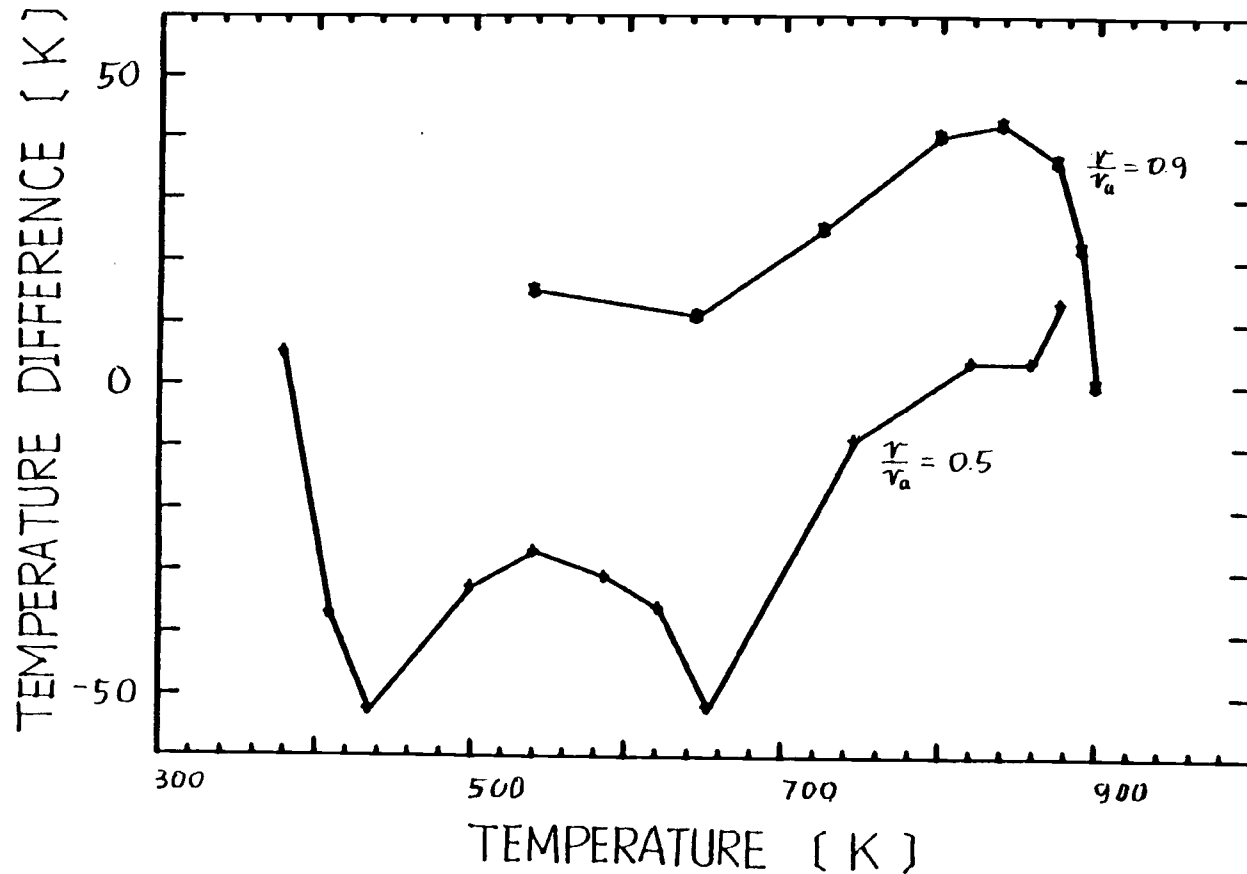


Figure 8. Local relative heat-source strength in a cylinder with a radius of 1.75 cm.

5.2 MODELING THE CHEMICAL REACTIONS

5.2.1 RATE OF REACTION

The rate of reaction is defined (Ref. 14) as the decrease in concentration per unit time of one of the reactants.

$$\text{rate} = -d[A]/dt \quad (5.2)$$

where A represents the concentration of reactant A measured at time t . If " a " represents the initial concentration of A and " x " represents the concentration of the product at time t , then the rate can be also expressed by:

$$\text{rate} = dx/dt \quad (5.3)$$

$$\text{rate} = - d(a-x)/dt \quad (5.4)$$

5.2.2 RATE CONSTANT

The rate constant is the rate of change in concentration of reactant or product with time for a reaction in which all the reactants are at unit concentration (Ref. 14). The rate of reaction can then be expressed by (Rate law):

$$\frac{dx}{dt} = k F(a, b, c, \dots) \quad (5.5)$$

where x is the concentration of the product, k is the rate constant and $F(a, b, c, \dots)$ represents a function of the concentrations of reactants a, b, c, \dots .

5.2.3 ORDER OF REACTION

The order of reaction is defined as the sum of the powers of the concentration terms that occur in the differential form of the rate law (Ref. 14). The order is usually a small whole number, but in special cases it may have a fractional value or be zero. Typical rate laws are:

$$\frac{dx}{dt} = k (a - x)^0$$

$$\frac{dx}{dt} = k (a - x)$$

$$\frac{dx}{dt} = k (a - x)^2$$

To model the decomposition of wood three, 1st order

reactions are assumed. The term α is defined as

$$\alpha = \frac{M_{0j} - M_i}{M_{0j} - M_{fi}} \quad (5.6)$$

where M_{0j} is the initial mass of component i for reaction j , M_i is the mass of constituent i at time t and M_{fi} is the final mass of component i for reaction j .

With M_j being the order of the j th reaction the rate expression for α_j is:

$$\frac{d\alpha_j}{dt} = k_{0,j} \cdot \exp\left(-\frac{E_j}{RT}\right) (1 - \alpha_j) \quad (5.7)$$

Assuming 1st order reactions

$$\frac{d\alpha_j}{dt} = k_{0,j} \cdot \exp\left(-\frac{E_j}{RT}\right) (1 - \alpha_j) \quad (5.8)$$

As T is an unknown function of time, this equation can not be integrated directly. Therefore a Taylor's series

$$f(z) = f(a) + f'(a)(z-a) + \frac{f''(a)(z-a)^2}{2!} + \dots \quad (5.9)$$

is used. α at $t + dt$ can then be expressed as

$$\alpha_{t+dt} = \alpha_t + \sum_k dt^k \frac{d^k \alpha}{k! dt^k} \quad (5.10)$$

where k is the order of approximation. In this program a 1st order approximation is made i.e.

$$\alpha_{t+\Delta t} = \alpha_t + \Delta t \left(\frac{d\alpha}{dt} \right) \quad (5.11)$$

5.2.4 THE COMPOSITION OF WOOD

Very little is known or has been published on thermal degradation of Hemicellulose and Lignin. In this evaluation therefore, the wood is considered to be made out of two components (Ref. 5):

- a. Hemicellulose and Lignin treated as a uniform Material with a starting mass-fraction of 50%.
- b. Cellulose

Figures 9, 10, 11 show the mass-fraction of each component for each of the three reactions verses time for several different temperatures.

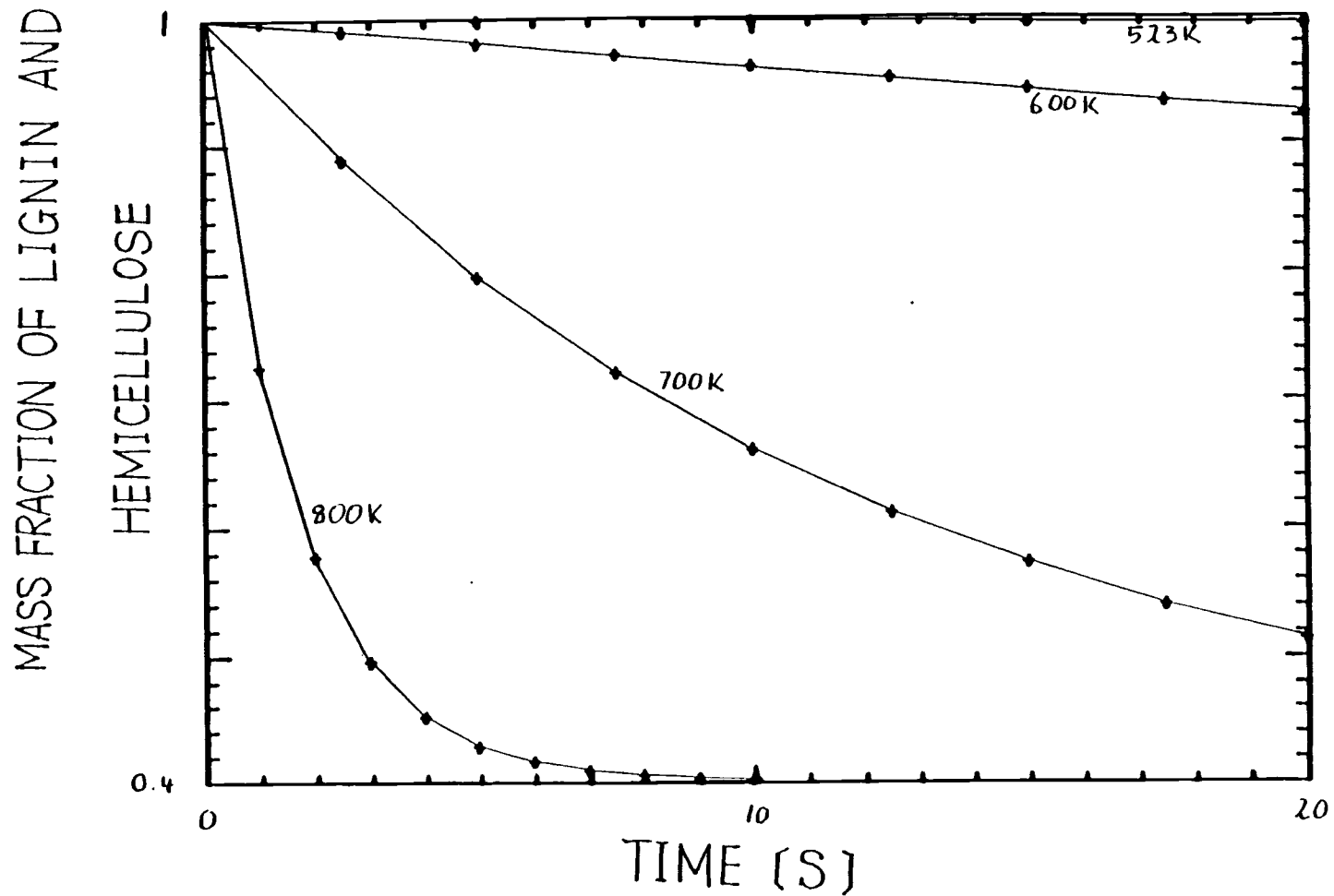


Figure 9. Mass fraction of Hemicellulose and Lignin versus time for different temperatures.

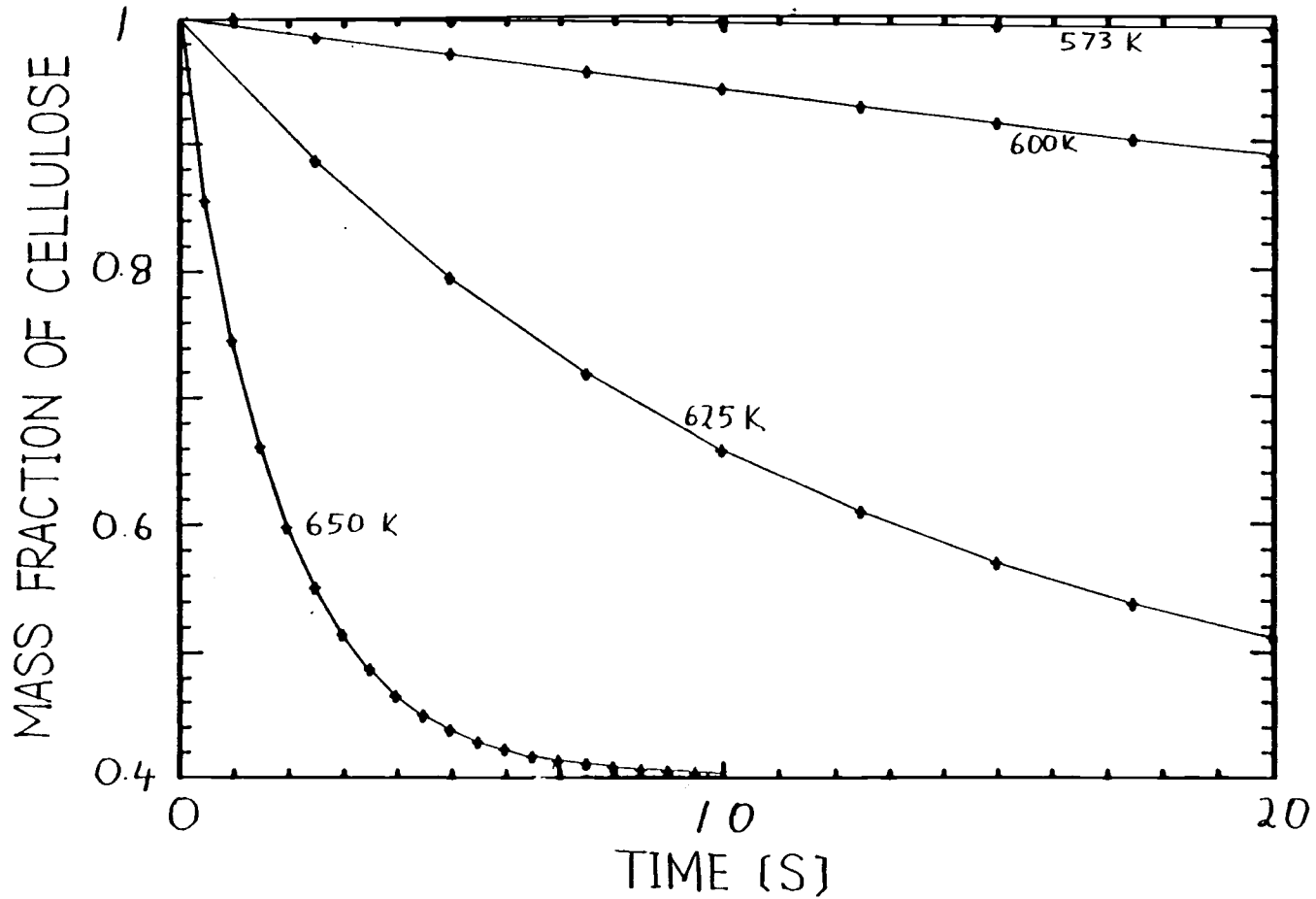


Figure 10. Mass fraction of Cellulose versus time for different temperatures.

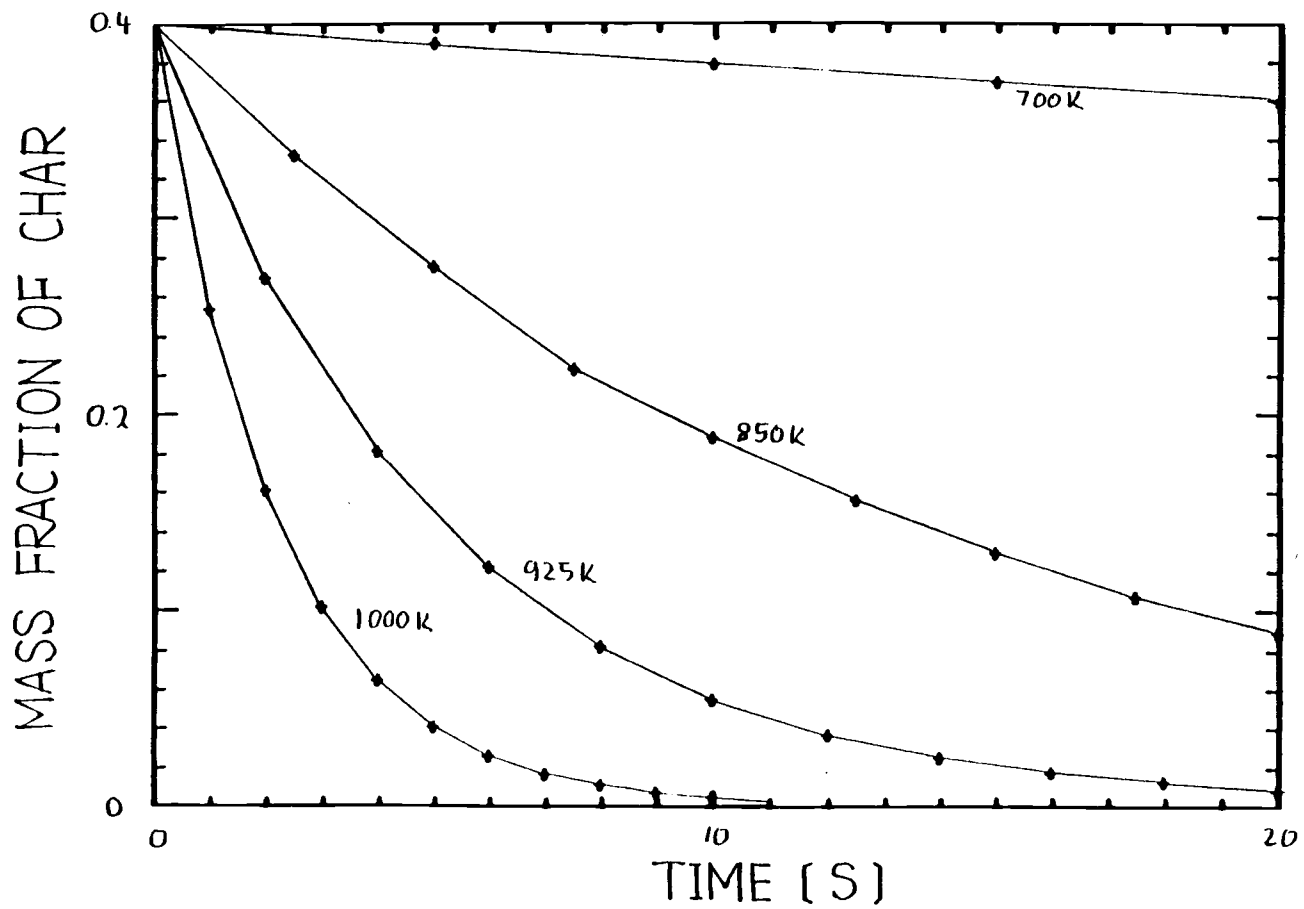


Figure 11. Mass fraction of Char versus time for different temperatures.

5.3 CALCULATION OF THE SOURCE

With these assumptions, the source term S can be calculated by the following equations

$$S_j = M_{Bj} Q_j \quad (5.12)$$

where M_{Bj} is the mass-loss and Q_j is the effective heat of pyrolysis for component j . M_{Bj} can be determined from

$$M_{Bj} = M_{0j} - M_j \quad (5.13)$$

The overall effective source can then be calculated by superposition

$$S = \sum_j S_j \quad (5.14)$$

5.4 THE CONSTANTS

5.4.1 ACTIVATION ENERGY AND RATE CONSTANTS

The activation energy for reaction 1 (Lignin + Hemicellulose) is, for all species, approximately 84 KJ/mol. The rate constant varies from $1.4 \cdot 10^5$ /s for Fir to 3.7

$\cdot 10^5$ /s for Oak. The final mass-fraction, Y_f , is 0.4. For Cellulose the activation energy (reaction 2) is 250 KJ/mol and the rate constant varies from $6.2 \cdot 10^{19}$ for Fir to $4.5 \cdot 10^{20}$ for Oak. The final mass-fraction varies from 0.38 for Fir to 0.23 for Poplar. The third reaction (Char) has an activation energy of 84 KJ/mol and a rate constant varying from $7 \cdot 10^3$ for Redwood to $1 \cdot 10^4$ for Fir. The final mass-fraction is zero.

5.4.2 THE HEAT OF REACTION

For the heat of decomposition an average of each temperature field was taken (relative high heating rates are assumed).

5.4.3 THE HEAT SOURCE

From the above data the strength of the heat source for each reaction can be calculated by

$$S_j = Q_j \Delta M'_j \quad (5.15)$$

where $\Delta M'_j$ is the burnt mass per unit time of reaction j . Then the overall effect is obtained by summation of all heat sources. All constants used in the program are

summarized in Table 1.

Cellulose:

activation energy : 250 KJ/mol
rate constant : $6 \cdot 10^{19}$ /s
heat of reaction : 1883 J/g
initial mass fraction : 1
end mass fraction : 0.4

Hemicellulose and Lignin:

activation energy : 84 KJ/mol
rate constant : $1.4 \cdot 10^5$ /s
heat of reaction : -168 J/g
initial mass fraction : 1
end mass fraction : 0.4

Char:

activation energy : 84 KJ/mol
rate constant : $1 \cdot 10^4$ /s
heat of reaction : 1465 J/g
initial mass fraction : 0.4
end mass fraction : 0

Table 1. Constants used in the computer program.

6 THE COMPUTER PROGRAM

6.1 INTRODUCTION

The partial differential equation derived in chapter 2 was solved numerically. An implicit method was used to obtain a set of finite difference equations. These equations were then solved by a matrix decomposition method. For the linear problem (constant properties), a stability analysis was investigated. The program was able to handle four different boundary conditions on each side of the slab: insulated, constant temperature, constant heat flux, and convection to an ambient temperature.

6.2 DERIVATION OF THE FINITE DIFFERENCE EQUATIONS

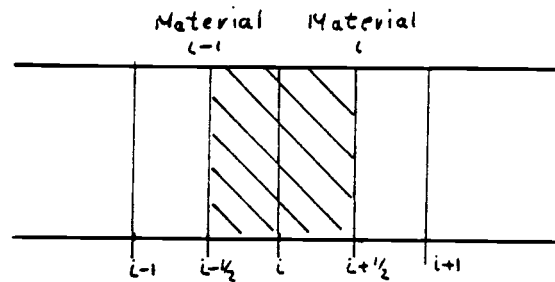
The partial differential equation solved in the program is shown in equation 6.1 and 6.2.

$$\begin{aligned} & \frac{\partial(k(\frac{\partial T}{\partial x}))}{\partial x} - C_g \rho_g V_e (\frac{\partial T}{\partial x}) + S''' \\ & = (\rho_g C_g + \rho_m C_m) \frac{\partial T}{\partial \theta} \end{aligned} \quad (6.1)$$

or

$$\begin{aligned} & \frac{\partial(k(\frac{\partial T}{\partial x}))}{\partial x} - C_g \rho_g V_e (\frac{\partial T}{\partial x}) \\ & = (\rho_g C_g + \rho_m C_m) \frac{\partial T}{\partial \theta} - S''' \end{aligned} \quad (6.2)$$

Using a control volume shown below



and dividing equation 6.2 into four parts

$$A = \frac{\partial(k(\frac{\partial T}{\partial x}))}{\partial x} \quad (6.3)$$

$$B = C_g \rho_g V_e (\frac{\partial T}{\partial x}) \quad (6.4)$$

$$C = (\rho_g C_g + \rho_m C_m) \frac{\partial T}{\partial \theta} \quad (6.5)$$

$$D = S''' \quad (6.6)$$

equation 6.2 is first integrated from $(x_i - \frac{1}{2} \Delta X)$ to $(x_i + \frac{1}{2} \Delta X)$ and then over the time interval. The integration of A is written

$$\begin{aligned}
 \int_{x_i - \frac{1}{2}}^{x_i + \frac{1}{2}} \partial(k(\frac{\partial T}{\partial x})) dx &= k(\frac{\partial T}{\partial x}) \Big|_{x_i - \frac{1}{2}}^{x_i + \frac{1}{2}} \\
 &= k_i (\frac{\partial T}{\partial x}) \Big|_i - k_{i-1} (\frac{\partial T}{\partial x}) \Big|_{i-1}
 \end{aligned} \tag{6.6}$$

Using first order approximations for the derivatives, equation 6.7 is obtained.

$$\int A = k_i (T_{i+1} - T_i) / \Delta x - k_{i-1} (T_i - T_{i-1}) / \Delta x \tag{6.7}$$

Now equation 6.7 is integrated from θ_i to θ_{i+1} by the use of an implicit method.

$$\begin{aligned}
 \int_{\theta_i}^{\theta_{i+1}} (k_i (T_{i+1} - T_i) / \Delta x - k_{i-1} (T_i - T_{i-1}) / \Delta x) d\theta \\
 = k_i (T_{i+1, l+1} - T_{i, l+1}) / \Delta x - k_{i-1} (T_{i, l+1} - T_{i-1, l+1}) / \Delta x
 \end{aligned} \tag{6.8}$$

where the subscripts $i-1, i, i+1$ stand for location and $l+1$ for time.

Integrating B

$$\begin{aligned}
 \int_{x_i - \frac{1}{2}}^{x_i + \frac{1}{2}} C_g \rho_g V_e (\frac{\partial T}{\partial x}) dx &= C_g \rho_g V_e T \Big|_{x_i - \frac{1}{2}}^{x_i + \frac{1}{2}} \\
 = \rho_{g,i} C_{g,i} V_{e,i} T_{i+\frac{1}{2}} - \rho_{g,i-1} V_{e,i-1} C_{g,i-1} T_{i-\frac{1}{2}}
 \end{aligned} \tag{6.9}$$

Using a linear temperature distribution within x , equation 6.10 is obtained.

$$\int B = \rho_{g,i} C_{g,i} V_{e,i} (T_{i+1} - T_i)/2 \quad (6.10)$$

$$- \rho_{g,i-1} C_{g,i-1} V_{e,i-1} (T_i - T_{i-1})/2$$

Now equation 6.10 is integrated from θ_i to θ_{i+1} .

$$\int_{\theta_i}^{\theta_{i+1}} (\rho_{g,i} C_{g,i} V_{e,i} (T_{i+1} + T_i)/2 - \rho_{g,i-1} C_{g,i-1} V_{e,i-1} (T_i + T_{i-1})/2) d\theta = k_i (T_{i+1, \ell+1} + T_{i, \ell+1})/2 \quad (6.11)$$

$$- \rho_{g,i-1} C_{g,i-1} V_{e,i-1} (T_{i-1, \ell+1} + T_{i, \ell+1})/2$$

where the subscripts are the same as in equation 6.8.

Integrating C

$$\int_{x_{i-1/2}}^{x_{i+1/2}} (\rho_g C_g + \rho_m C_m) \frac{\partial T}{\partial \theta} dx = ((\rho_{g,i} C_{g,i} + \rho_{m,i} C_{m,i}) \Delta x/2 + (\rho_{g,i-1} C_{g,i-1} + \rho_{m,i-1} C_{m,i-1}) \Delta x/2) \frac{\partial T}{\partial \theta} \quad (6.12)$$

Integrating equation 6.12 from θ_i to θ_{i+1} one can get

$$\int_{\theta_i}^{\theta_{i+1}} ((\rho_{g,i} C_{g,i} + \rho_{m,i} C_{m,i}) \Delta x/2 + (\rho_{g,i-1} C_{g,i-1} + \rho_{m,i-1} C_{m,i-1}) \Delta x/2) \frac{\partial T}{\partial \theta} d\theta \quad (6.13)$$

$$= \Delta x/2 (\rho_{g,i} C_{g,i} + \rho_{m,i} C_{m,i} + \rho_{g,i-1} C_{g,i-1} + \rho_{m,i-1} C_{m,i-1}) (T_{i,l+1} - T_{i,l})$$

where the subscripts $i, i-1$ indicate the location and $l, l-1$ indicate the time.

Integration of D over time leads to

$$\int_{\theta_i}^{\theta_{i+1}} (S''_i + S'''_{i-1}) \Delta x/2 d\theta = ((S''_i + S'''_{i-1}) \Delta x/2) \Delta \theta \quad (6.14)$$

where S''' stands for (see chapter 3) the sum of:

- The heat source or energy sink per unit volume S .
- The thermal energy of the produced gases per unit volume, S_g .

Assuming that the gases in each control volume are produced at an average temperature (i.e. a linear temperature distribution within each element):

$$S_g = m_{B,i-1} C_{g,i-1} (T_{i-1,l+1} + T_{i,l+1})/2 \quad (6.15)$$

where $m_{B,i-1}$ is the amount of gas produced in element $i-1$.

6.2.1 THE FINITE DIFFERENCE EQUATION (IMPLICIT FORM)

Putting equations 6.8, 6.11, 6.13, 6.15, and 6.16 together an equation of the following form can be obtained:

$$\begin{aligned} a_i T_{i-1, l+1} + b_i T_{i, l+1} + c_i T_{i+1, l+1} \\ = \text{RHS}_{i, l} \end{aligned} \quad (6.16)$$

where RHS stands for the right hand side and

$$\begin{aligned} a_i = k_{i-1} \Delta \theta_i / \Delta x_i + \rho_{g, i-1} C_{g, i-1} V_{e, i-1} \Delta \theta / 2 \\ + m_{B, i-1} C_{g, i-1} / 2 \end{aligned} \quad (6.17)$$

$$\begin{aligned} b_i = -(k_i - k_{i-1}) \Delta \theta / \Delta x - (\rho_{g, i} V_{e, i} C_{g, i} \\ - \rho_{g, i-1} V_{e, i-1} C_{g, i-1}) \Delta \theta / 2 - \Delta x / 2 (\rho_{g, i} C_{g, i} \\ + \rho_{m, i} C_{m, i} + \rho_{g, i-1} C_{g, i-1} + \rho_{m, i-1} C_{m, i-1}) \\ + m_{B, i-1} C_{g, i-1} / 2 \end{aligned} \quad (6.18)$$

$$c_i = k_i \Delta \theta / \Delta x - \rho_{g, i} C_{g, i} V_{e, i} \Delta \theta / 2 \quad (6.19)$$

$$\begin{aligned} \text{RHS}_{i,l} = & -\Delta x/2 (S_i + S_{i-1}) \Delta \theta - \Delta x/2 (P_{g,i} C_{g,i} \\ & + P_{m,i} C_{m,i} + P_{g,i-1} C_{g,i-1} + P_{m,i-1} C_{m,i-1}) T_{i,l} \end{aligned} \quad (6.20)$$

6.3 TREATMENT OF THE BOUNDARY CONDITIONS

Four different boundary conditions are considered: insulated, constant temperature, constant heat flux, and convection to an ambient temperature. The boundary conditions influence only the first and the last of the finite difference equations, the rest stay unchanged.

6.3.1 INSULATED BOUNDARY

A pseudo or image point is used. The velocity in the pseudo area is supposed to be zero. The other properties used are the same as in the boundary. This leads to the following equations:

Insulated left side:

$$T_{i-1,l+1} = T_{i+1,l+1} \quad (6.21)$$

$$b_i T_{0, l+1} + (a_i + C_i) T_{1, l+1} = \text{RHS} \quad (6.22)$$

Insulated right side:

$$T_{n+1, l+1} = T_{n-1, l+1} \quad (6.23)$$

$$(a_i + C_i) T_{n-1, l+1} + b_i T_{n, l+1} = \text{RHS} \quad (6.24)$$

6.3.2 CONSTANT TEMPERATURE

The number of equations is reduced by one for each boundary with a fixed temperature. Thus, for a given left boundary temperature, T_0 :

$$b_1 T_{1, l+1} + C_1 T_{2, l+1} = \text{RHS} - a_1 T_0 \quad (6.25)$$

or for a given right boundary temperature T_N :

$$\begin{aligned} a_{n-1} T_{n-2, l+1} + b_{n-1} T_{n-1, l+1} \\ = \text{RHS} - C_{n-1} T_N \end{aligned} \quad (6.26)$$

6.3.3 CONSTANT HEAT FLUX

As the material is not uniform a 1st order approximation for the temperature derivative is made:

$$Q = -k(T_i - T_{i-1})/2 \quad (6.27)$$

With this assumption the equations are as follows:

$$T_0 - T_1 = Q/k\Delta x \quad (6.28)$$

for a given heat flux at the left boundary. For a given heat flux at the right boundary:

$$T_{n-1} - T_n = Q/k\Delta x \quad (6.29)$$

with Q being defined as positive if in the +x direction.

6.3.4 CONVECTIVE BOUNDARY CONDITION

Similar to the constant heat flux boundary condition, a 1st order approximation for the temperature derivatives is made. This leads to the following equation for a left

convective boundary

$$T_0 (h + k_0/\Delta x) - k_1/\Delta x T_1 = h * TH \quad (6.30)$$

and for a right convective boundary

$$T_n (h + k_n/\Delta x) - k_{n-1}/\Delta x T_{n-1} = h * TH \quad (6.31)$$

where h is the convective heat transfer coefficient and TH is the ambient temperature.

6.4 METHOD SOLVING THIS SET OF EQUATIONS

Any matrix AA can be decomposed into a lower triangular (LL) and an upper triangular (UU) matrix, i.e.

$$AA = LL * UU \quad (6.32)$$

where $*$ implies matrix multiplication. The equations to be solved can then be rewritten as

$$LL * UU * x = f \quad (6.33)$$

where f , z and x are vectors. Or

6.4.2 SOLUTION FOR X

First equation 6.35 is solved for z. z is defined as

$$Z_1 = f_1 / \alpha_1 \quad (6.39)$$

$$Z_i = (f_i - b_i Z_{i-1}) / \alpha_i \quad i = 2, 3, 4, \dots, n \quad (6.40)$$

Then the final solution for x is given by

$$x_n = Z_n \quad (6.41)$$

$$x_i = Z_i - \gamma_i Z_{i+1} \quad (6.42)$$

6.4.3 OPERATIONAL COUNT FOR THIS METHOD

There are (Ref. 15)

3n - 2 operations necessary to find α and γ

3n - 2 operations necessary to find z

2n - 2 operations necessary to find x.

Therefore, only approximately 8n operations are necessary for each solution. It should also be mentioned that it is

not necessary to store the whole triangular Matrix (nxn). All zero value elements can be omitted. So it is sufficient to store only a 3xn matrix.

6.5 TREATMENT OF THE ABLATING SURFACE

For each time step the density of the char is calculated. As soon as the density goes below a certain value, this interval is treated as being burnt, i.e. the current boundary condition is transferred to the next nodal point.

6.6 REASONS FOR THE IMPLICIT METHOD

A nonlinear equation has at least (necessary condition) to satisfy the stability criterion for a linear equation of the same type. (The linear case can be looked at as a limit for very slowly varying properties.) The corresponding linear equation to equation 2.30 is (The source term can be neglected for the stability analysis):

$$k \left(\frac{\partial^2 T}{\partial x^2} \right) - C \rho V_e \left(\frac{\partial T}{\partial x} \right) = \rho C \left(\frac{\partial T}{\partial t} \right) \quad (6.43)$$

To get the stability criterion a "von Neumann Criterion" (Ref. 16) is used. Assume that the solution of the

homogenous finite difference equation is of the form $H(t) \cdot \exp(jv \cdot x)$, where j denotes $\sqrt{-1}$ and v is a positive constant. Whether the solution remains bounded as t becomes large can be determined by the amplification factor KSI.

$$KSI = H(t + dt) / H(t) \quad (6.44)$$

If KSI is smaller than one, the function $H(t)$ remains bounded. In general, components of all frequencies v may be present, i.e. $H(t)$ must be bounded for all v .

6.6.1.1 STABILITY ANALYSIS

The finite difference equation (implicit) of equation 6.43 is

$$K(T_{i+1, l+1} - 2T_{i, l+1} + T_{i-1, l+1}) / h_x^2 - PCV_e / 2h_x T_{i+1, l+1} - T_{i-1, l+1} = PC / h_x T_{i, l+1} - T_{i, l-1} \quad (6.45)$$

with

$$L_a = \frac{k}{PC} \cdot \frac{h_t}{h_x^2} \quad G_a = \frac{PCV_e}{2} \cdot \frac{h_t}{h_x}$$

equation 6.45 transforms to

$$L_a (T_{i+1, l+1} - 2T_{i, l+1} + T_{i-1, l+1}) - G_a (T_{i+1, l+1} - T_{i-1, l+1}) = T_{i, l+1} - T_{i, l} \quad (6.46)$$

or

$$(L_a - G_a) T_{i+1, l+1} + (L_a + G_a) T_{i, l+1} + (2L_a + 1) T_{i, l} = -T_{i, l} \quad (6.47)$$

Assuming

$$T = H(t) \exp(jv x_i) \quad (6.48)$$

and

$$W = jv x \quad (6.49)$$

leads to

$$2L_a \cos(W) - 2G_a \sin(W)j - (2L_a + 1)j = -H_i / H_{i+1} \quad (6.50)$$

The absolute value of $H(i)/H(i+1)$ is therefore

$$\text{Abs} (4L_a^2 \cos^2(W) - 8L_a^2 \cos(W) - 4L_a \cos(W) + 4L_a^2 + 1 + 4L_a + 4G_a^2 \sin^2(W)) = \text{Abs} (H_i / H_{i+1}) \quad (6.51)$$

For stability, the absolute value has to be bigger than 1.

First G_a is discussed. For $G_a = 0$ the absolute value has a minimum. Therefore, it is sufficient to show stability for $G_a = 0$. For $G_a = 0$ equation 6.52 reduces to

$$\text{Abs} \{ 2La [\cos(w) - 1] - 1 \} = \text{Abs} (H_i / H_{i+1}) \quad (6.52)$$

or

$$\text{Abs} \{ 1 + 2La [1 - \cos(w)] \} = \text{Abs} (H_i / H_{i+1}) \quad (6.53)$$

From this it can be seen that the implicit method for the linear problem is always stable.

6.6.2 MATRIX DECOMPOSITION VERSES ITERATIVE SOLUTION

Three different methods of solving 1-dimensional heat-transfer problems were considered:

- a. Matrix decomposition
- b. Gauss-Seidel iterative method with successive displacement.
- c. Iterative method (successive displacement) solving for all timesteps simultaneously.

It was found that even with the use of an optimal over relaxation factor the matrix decomposition method is substantially faster than the iterative methods.

Therefore, the matrix decomposition method was chosen.

A description of the computer program using this method along with a flow chart is presented in Appendix A. Appendix B contains the complete computer program.

7 RESULTS

Two different boundary conditions were examined:

- a. constant heat flux
- b. a convective boundary

In both cases, the original specific gravity was 0.75 and the reference temperature was the initial temperature of 300 K. The slab was 25 mm thick and insulated on the unheated side (this is equivalent to a 50 mm thick slab heated from both sides symmetrically). A specific gravity of 0.75 was chosen so that the results may be compared with temperature profiles measured by C. K. Lee, R. F. Chaiken, and J. M. Singer (Ref. 9). Density and temperature profiles for each case are shown.

7.1 CONSTANT HEAT FLUX

A 25 mm thick slab of wood was heated by a constant heat flux of $80000 \text{ J} / \text{m}^2 \text{ s}$. This heat flux corresponds to real fire conditions (Ref. 9). Initially the wood was at 300 K and had a specific gravity of 0.75 (i.e. a density of $7.5 \cdot 10^5 \text{ g} / \text{m}^3$). It took 198 seconds to burn the whole slab. The boundary temperature (i.e. the temperature of the char before it was totally burnt) was around 1400 K. Graphs showing the temperature profiles and

the density profiles in the slab are shown in Figures 12-16.

Generally the boundary temperatures were much higher than the temperatures measured by Ref. 9. The reason for that is, that at high temperatures the reradiation of wood is fairly high. Therefore, the actual heat flux absorbed by the wood is much lower.

As it can be seen from the Figures 12-16, the chemical reaction takes place only in a very thin part close to the surface. Due to the high heat flux and relative low conductivity of wood the temperature increases only in an approximately 1 to 2 mm thick layer. This "reaction zone" moves inwards with a velocity of approximately 6 to 8 mm/min. On one side of the "reaction zone" the surface is ablating, while on the other end the temperature is still close to the initial temperature. Parallel to the rise in temperature, a loss in density due to the chemical reactions is taking place. The main drop in density occurs around 700 to 800 K when reactions 1 and 2 are taking place. Due to the fast reaction and low conductivity the velocity of the "reaction zone" is nearly constant over the whole time period and independent of the thickness of the slab. (i.e. the reaction is only taking

place at the surface)

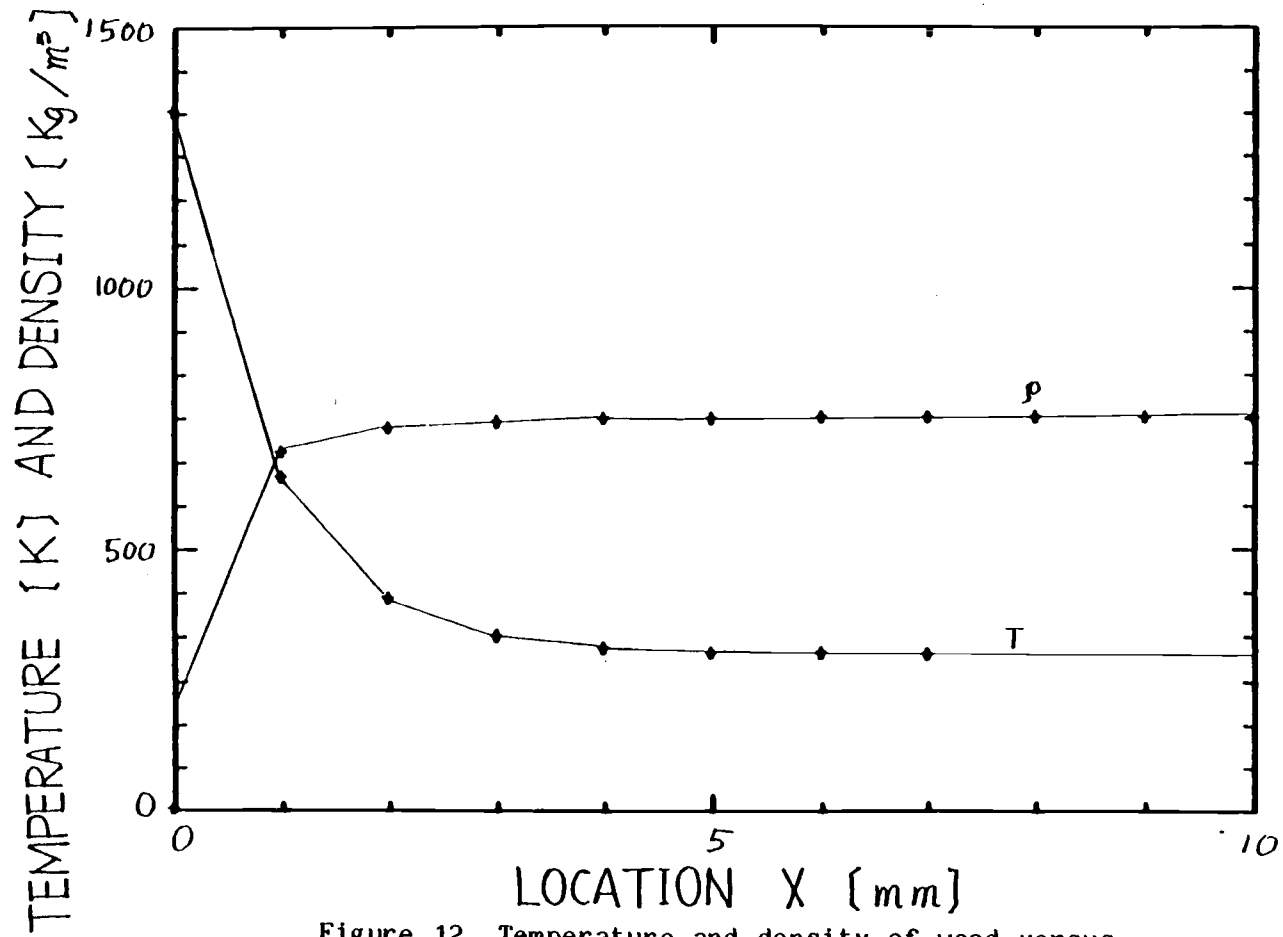


Figure 12. Temperature and density of wood versus location at time $t=10$ s and constant heat flux $Q=80000$ J/m² .

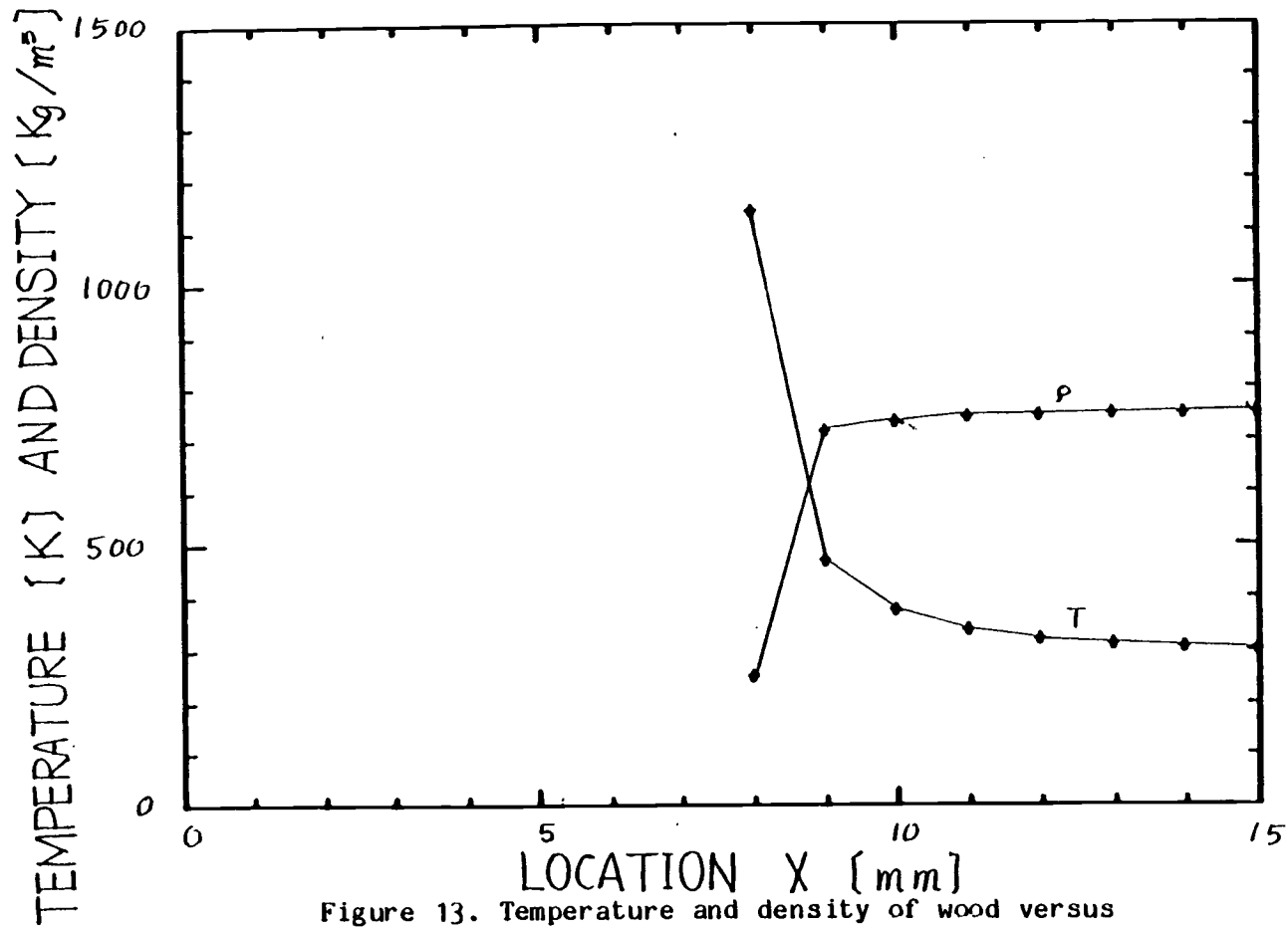


Figure 13. Temperature and density of wood versus location at time $t=60$ s and constant heat flux $Q=80000$ J/m^2 .

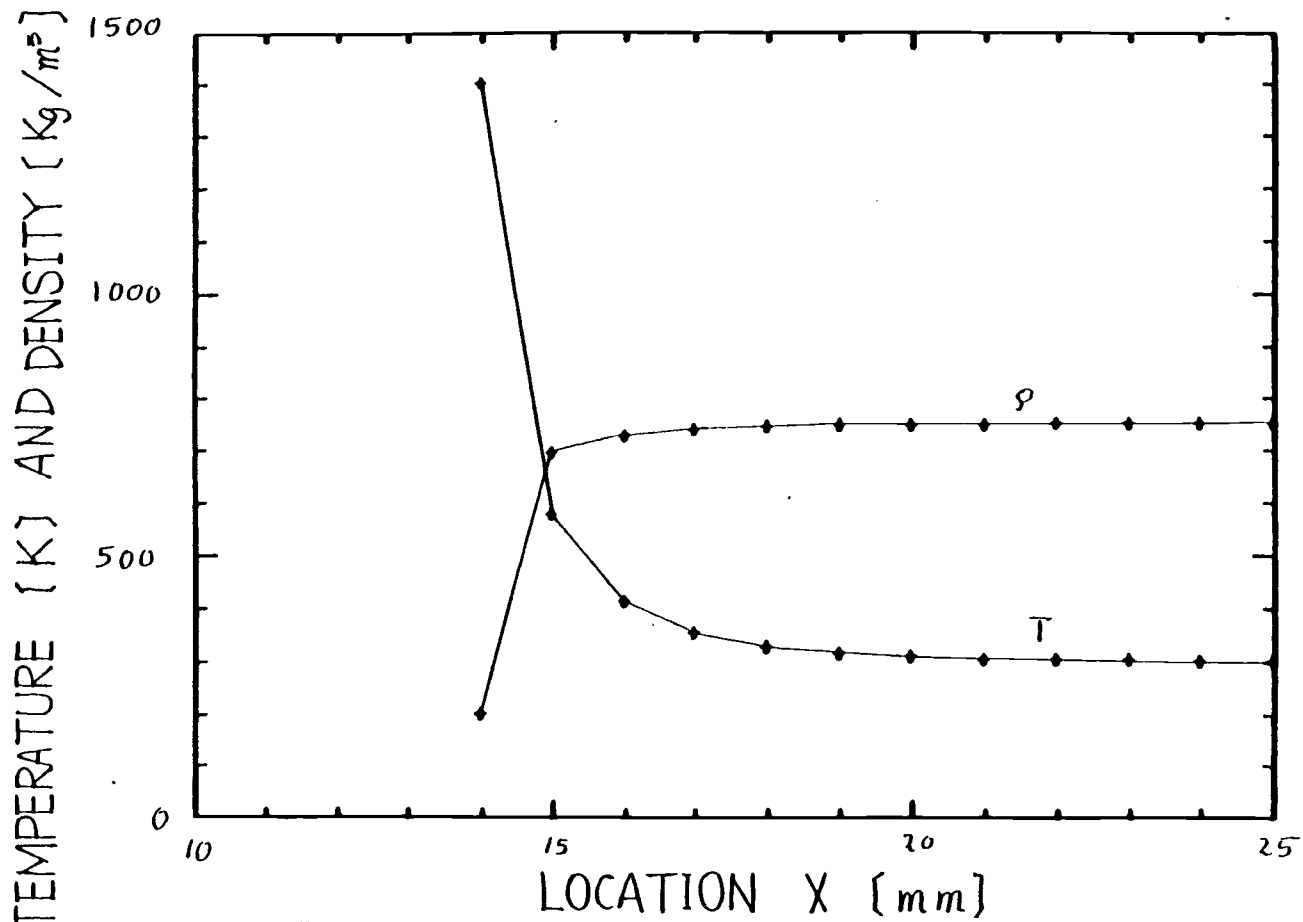


Figure 14. Temperature and density of wood versus location at time $t=120$ s and constant heat flux $Q=80000$ J/m² .

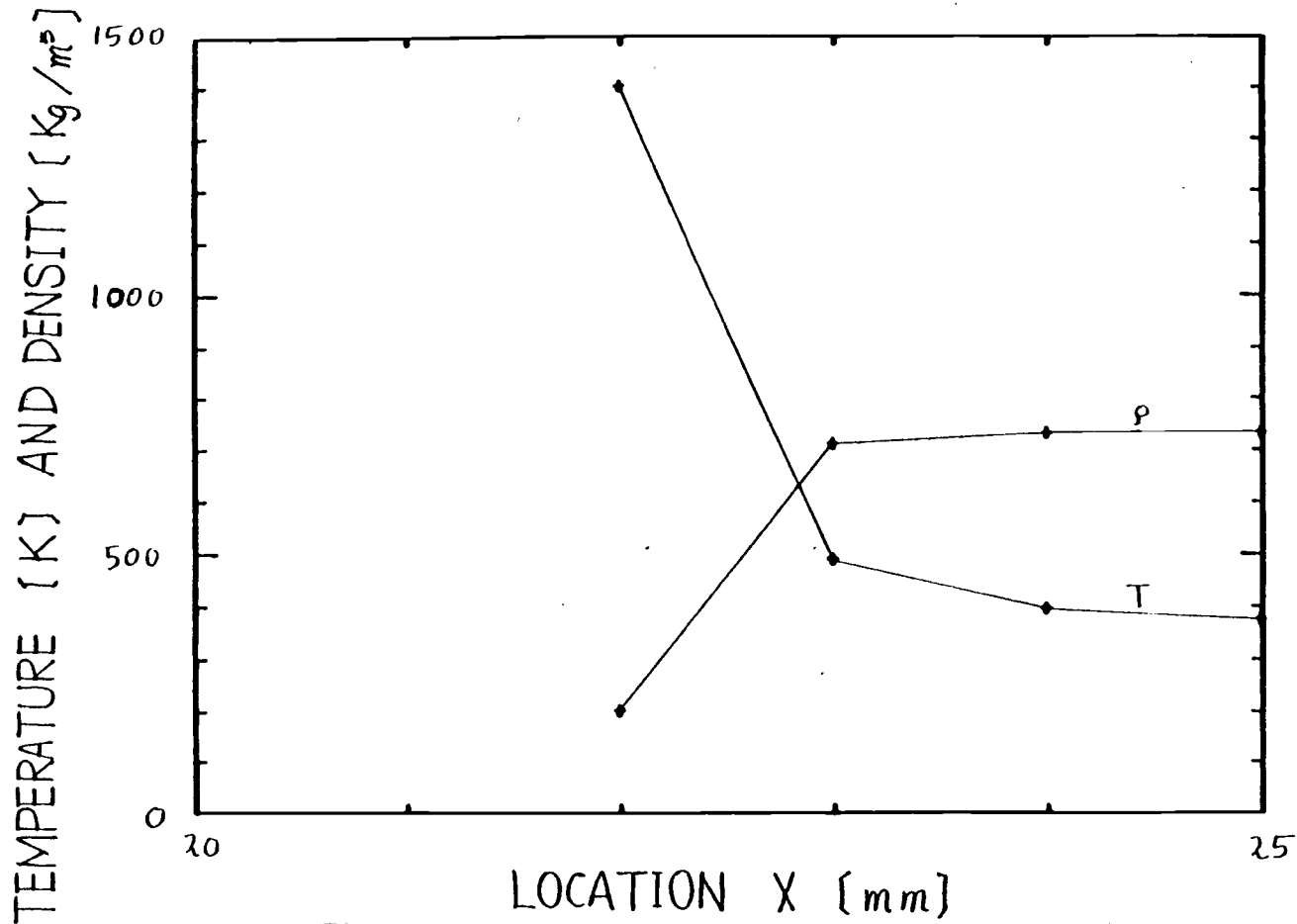


Figure 15. Temperature and density of wood versus location at time $t=180$ s and constant heat flux $Q=80000$ J/m².

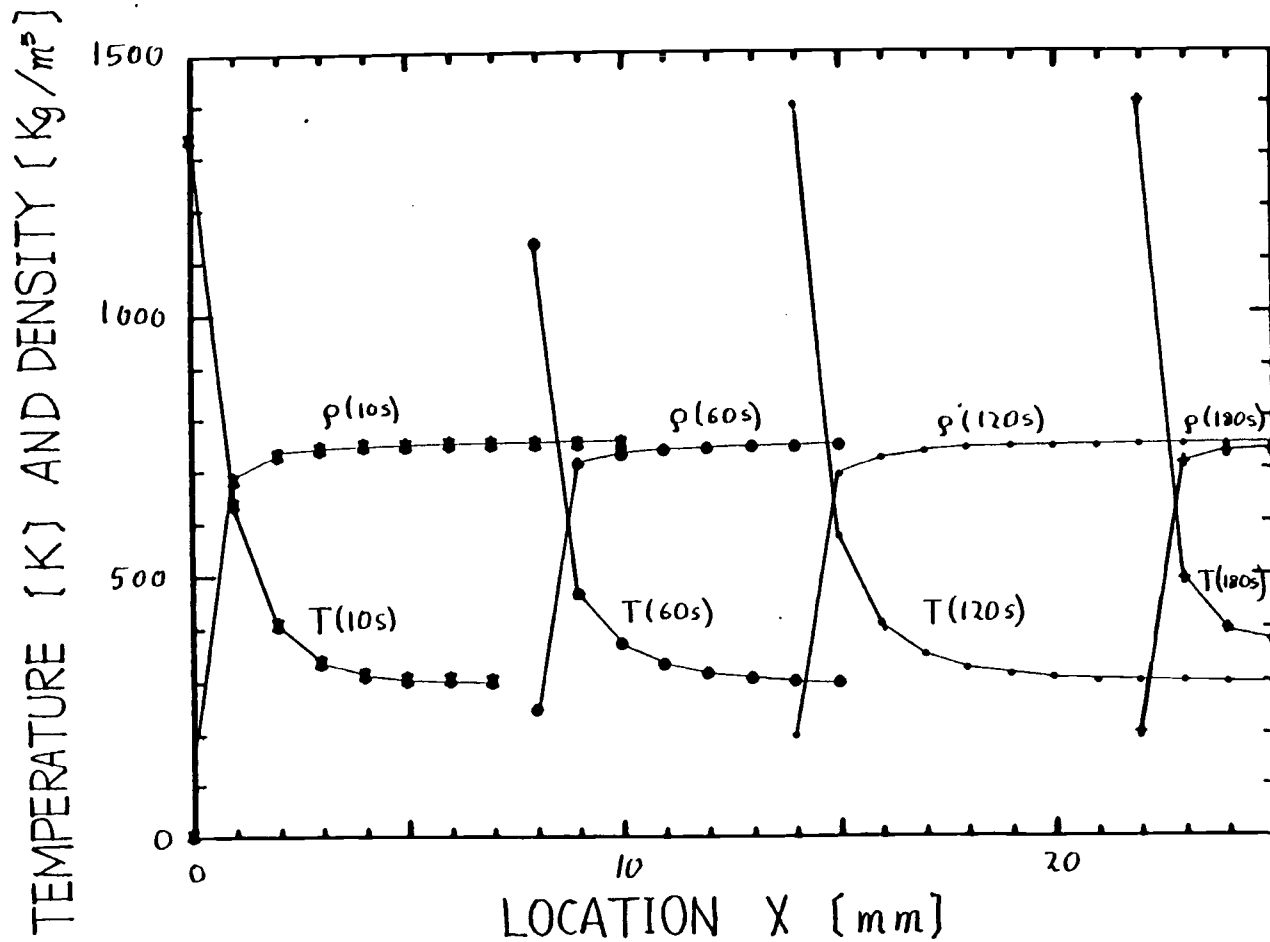


Figure 16. Temperature and density of wood versus location for time $t = 10, 60, 120, 180$ s and constant heat flux $Q = 80000 \text{ J/m}^2$.

The reasons for different temperatures at the boundary at different times in Figure 16 are:

- a. The actual boundary is not exactly at this location.
- b. Due to the treatment of the ablating nodes in the computer program, different nodes were directly exposed to the heat source for a different amount of time.

7.2 CONVECTIVE BOUNDARY

The same physical properties and the same initial conditions were chosen as in the constant heat flux case. A heat transfer coefficient of $18.4 \text{ J} / \text{m}^2 \text{ s}$ was chosen. This is the value used by Hohoku and Akita (Ref. 17). An ambient temperature of 1300 K was chosen, which is slightly lower than the boundary temperature under constant heat flux conditions. Density and temperature profiles are shown in Figures 17-29.

In contrast to the constant heat flux case, the boundary temperatures are not constant, they increase with time. The reason is that the reaction is much slower. As a result the influence of conduction within the wood slab can be seen. The boundary temperatures turn out to be around 850 to 900 K which is lower than the value of 1000 K in Ref. 9. The reason is that the heat source used in their experiment is a laser radiation source and not convection to an ambient temperature.

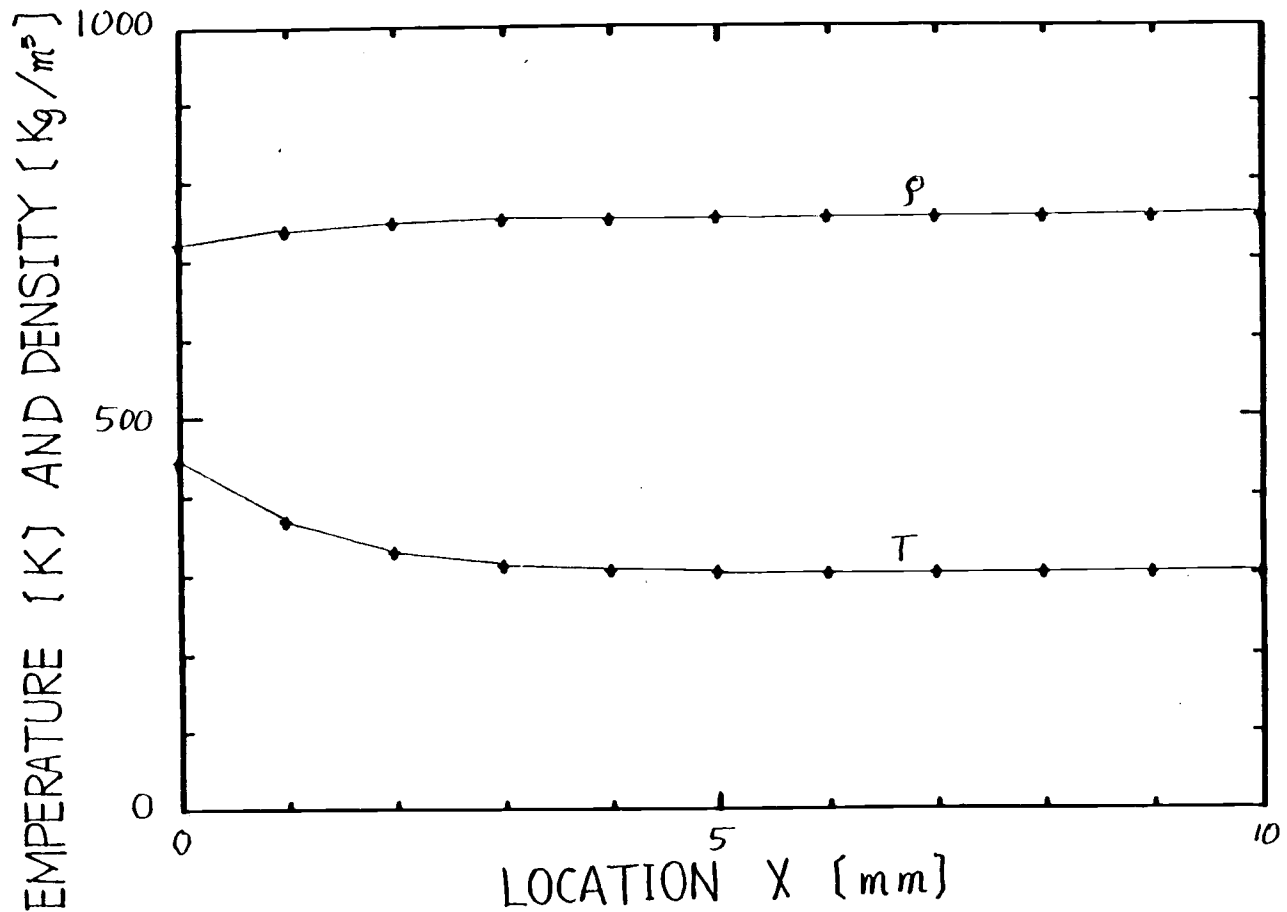


Figure 17. Temperature and density of wood versus location for time $t=10$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

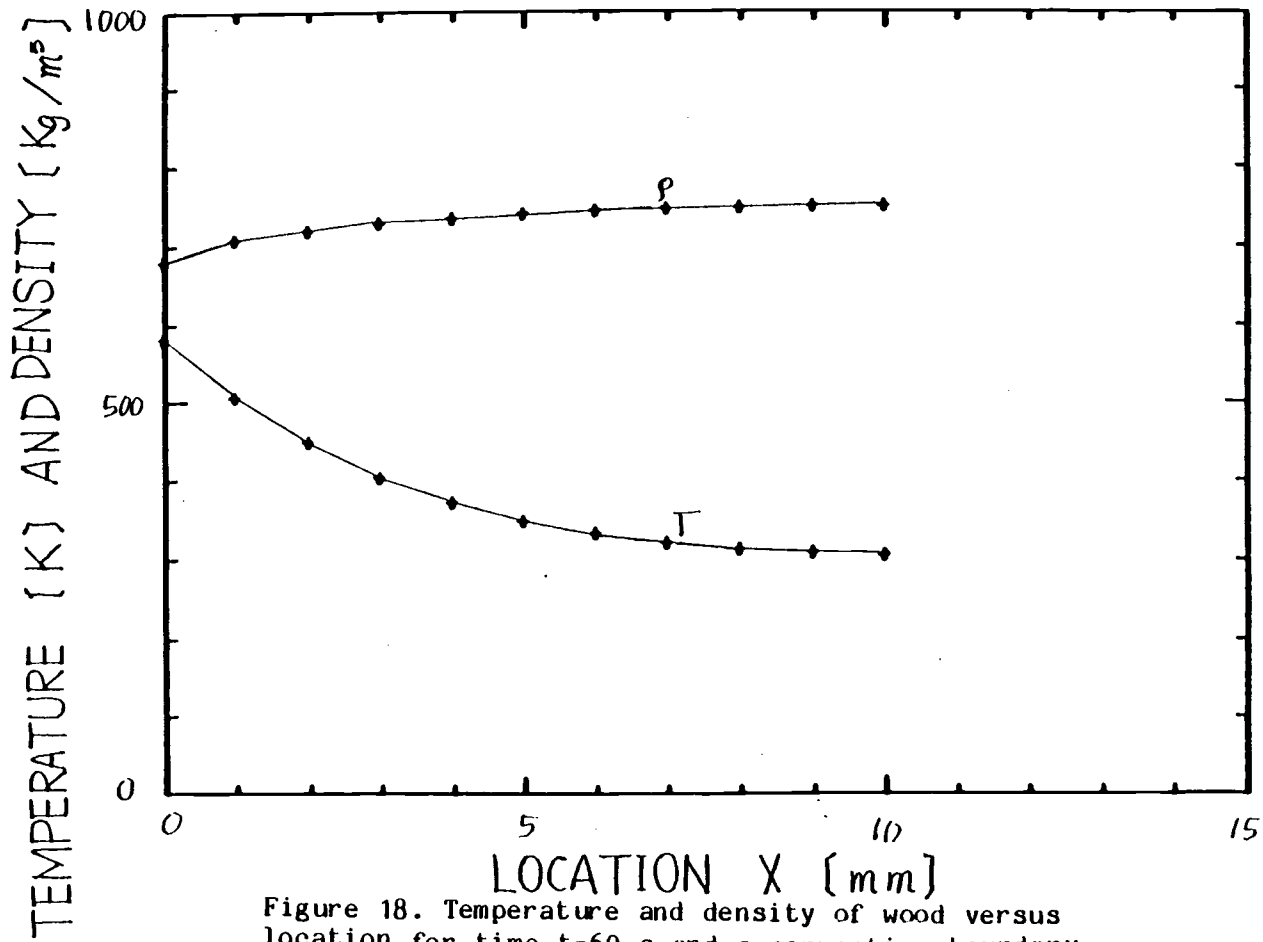


Figure 18. Temperature and density of wood versus location for time $t=60$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

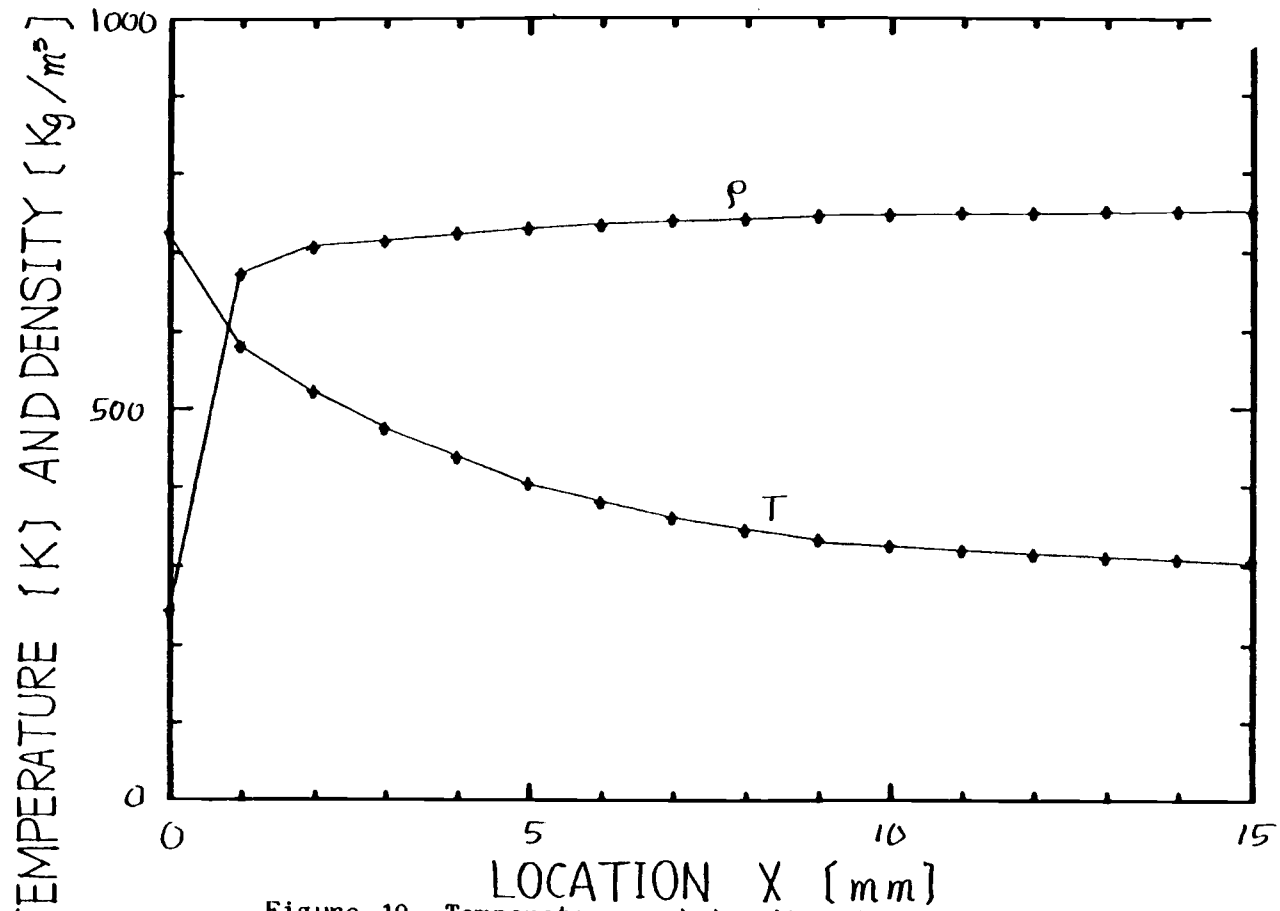


Figure 19. Temperature and density of wood versus location for time $t=120$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

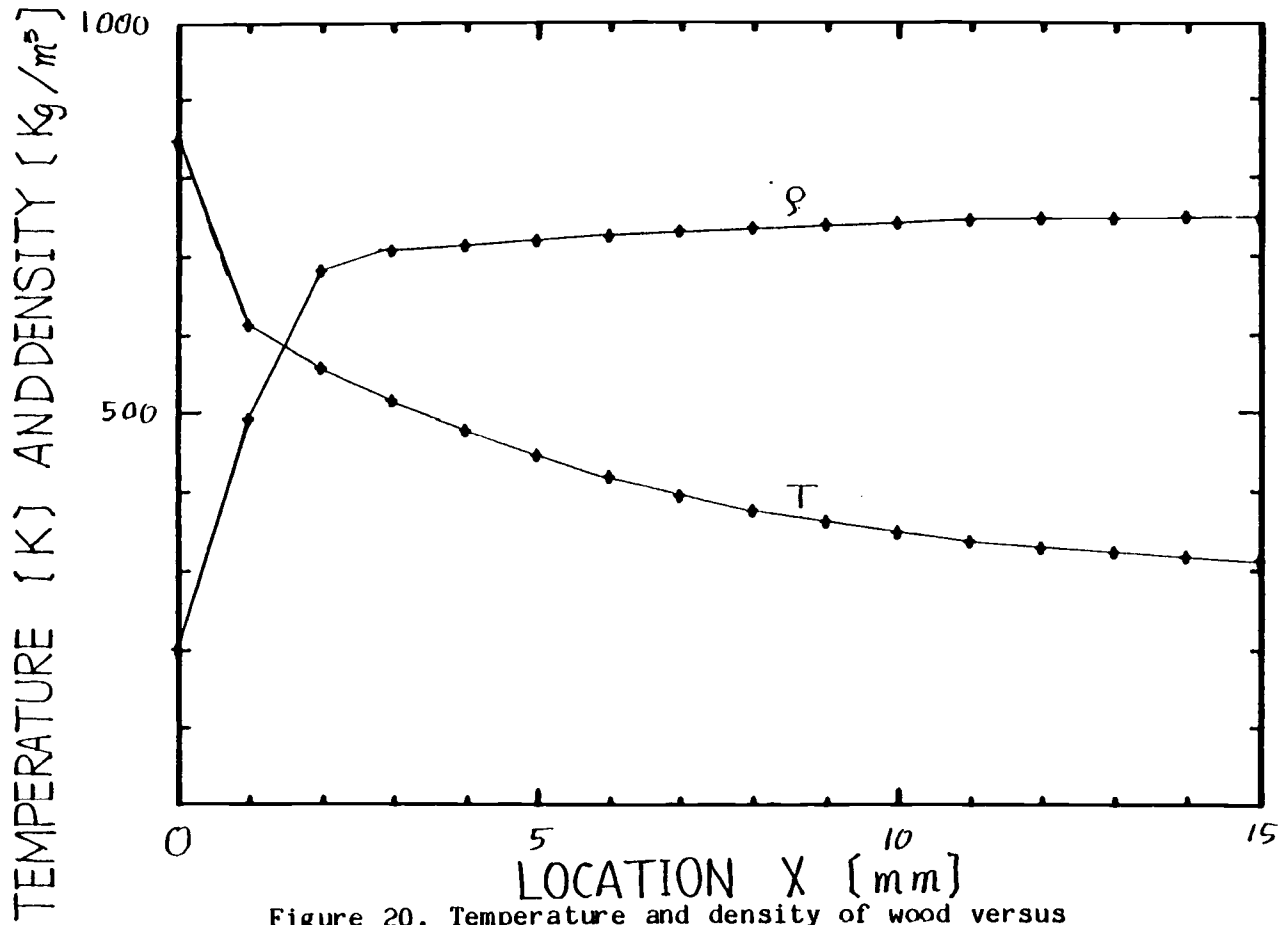


Figure 20. Temperature and density of wood versus location for time $t=180$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

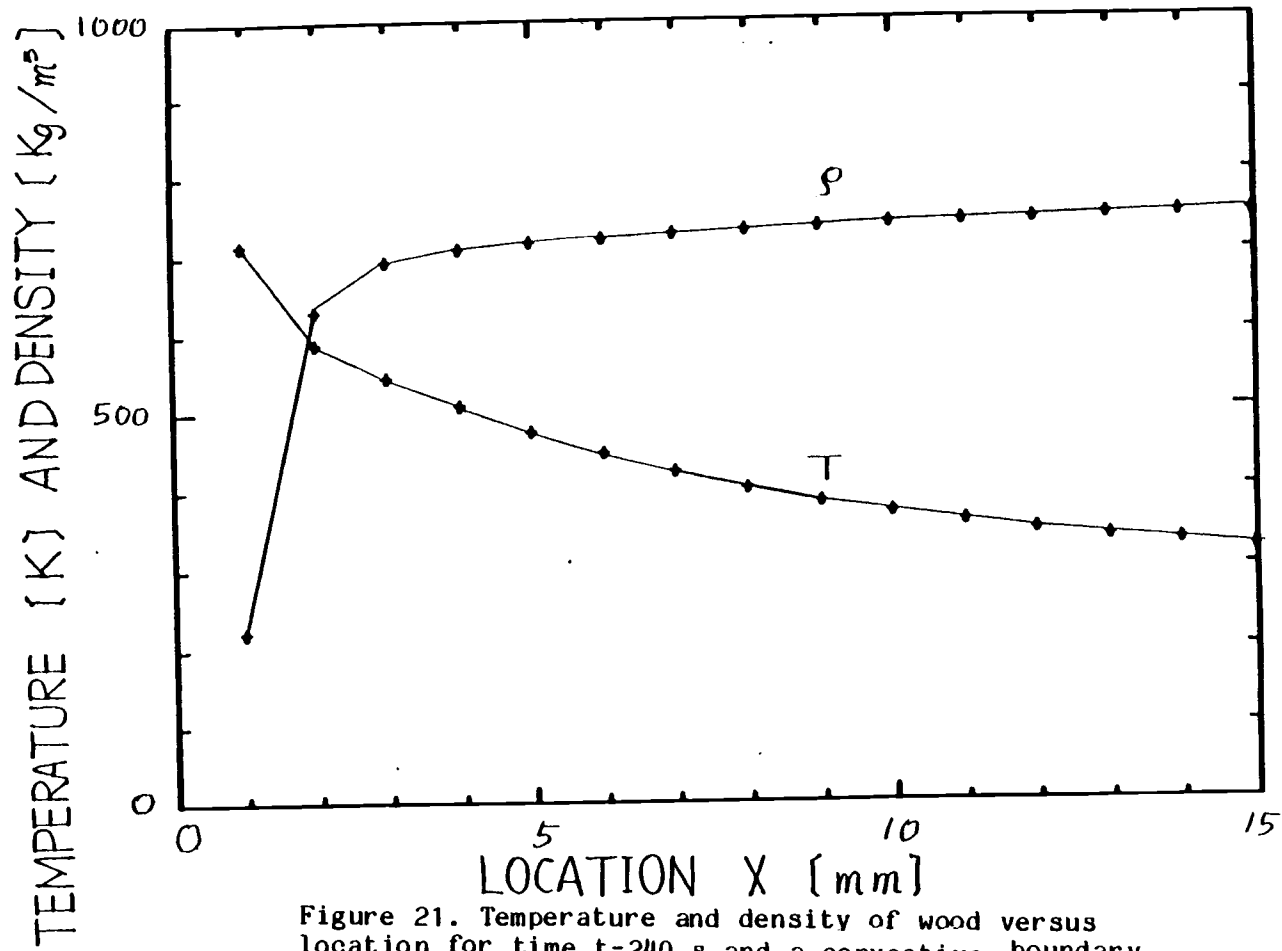


Figure 21. Temperature and density of wood versus location for time $t=240$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

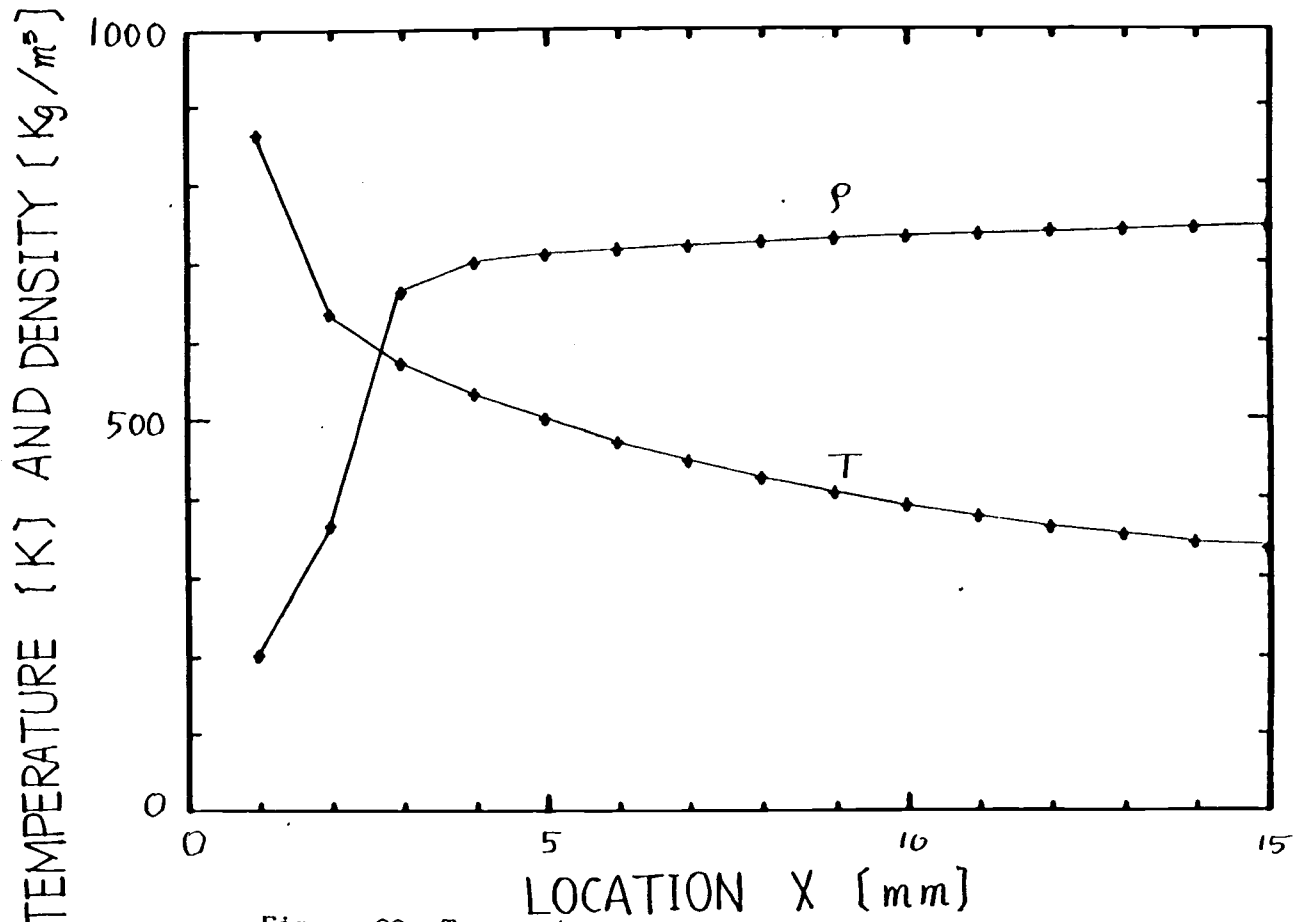


Figure 22. Temperature and density of wood versus location for time $t=300$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

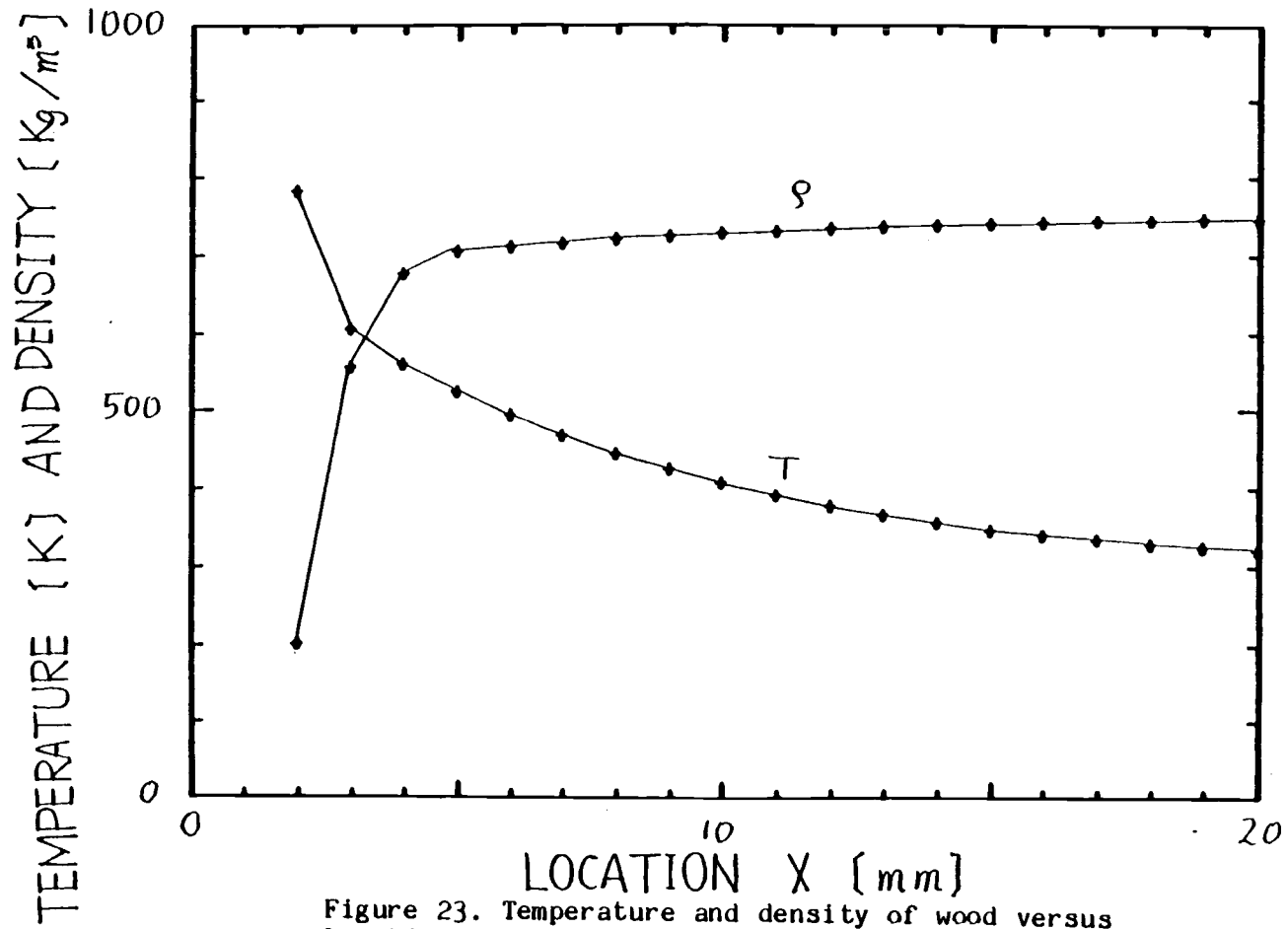


Figure 23. Temperature and density of wood versus location for time $t=360$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

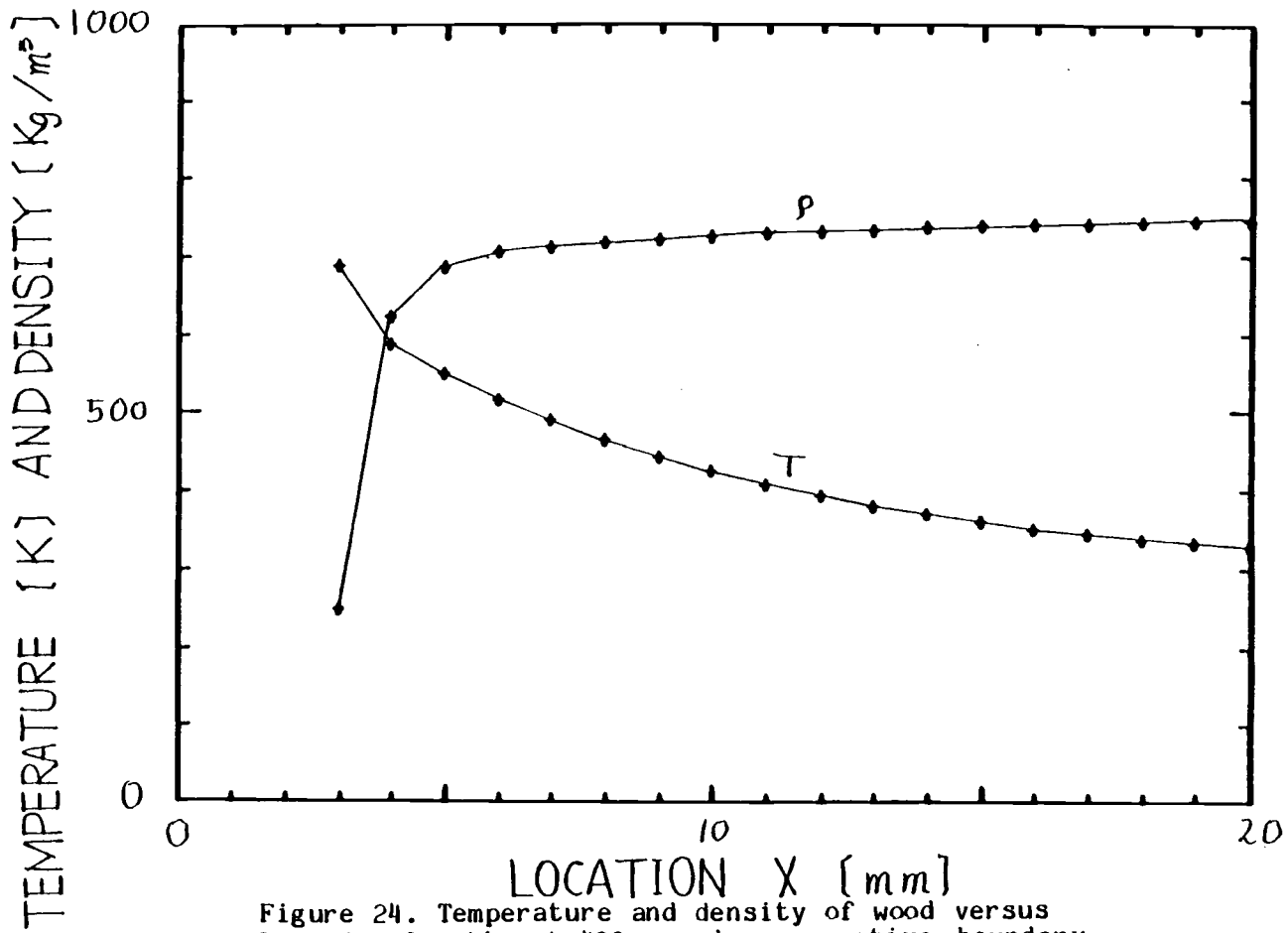


Figure 24. Temperature and density of wood versus location for time $t=420$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

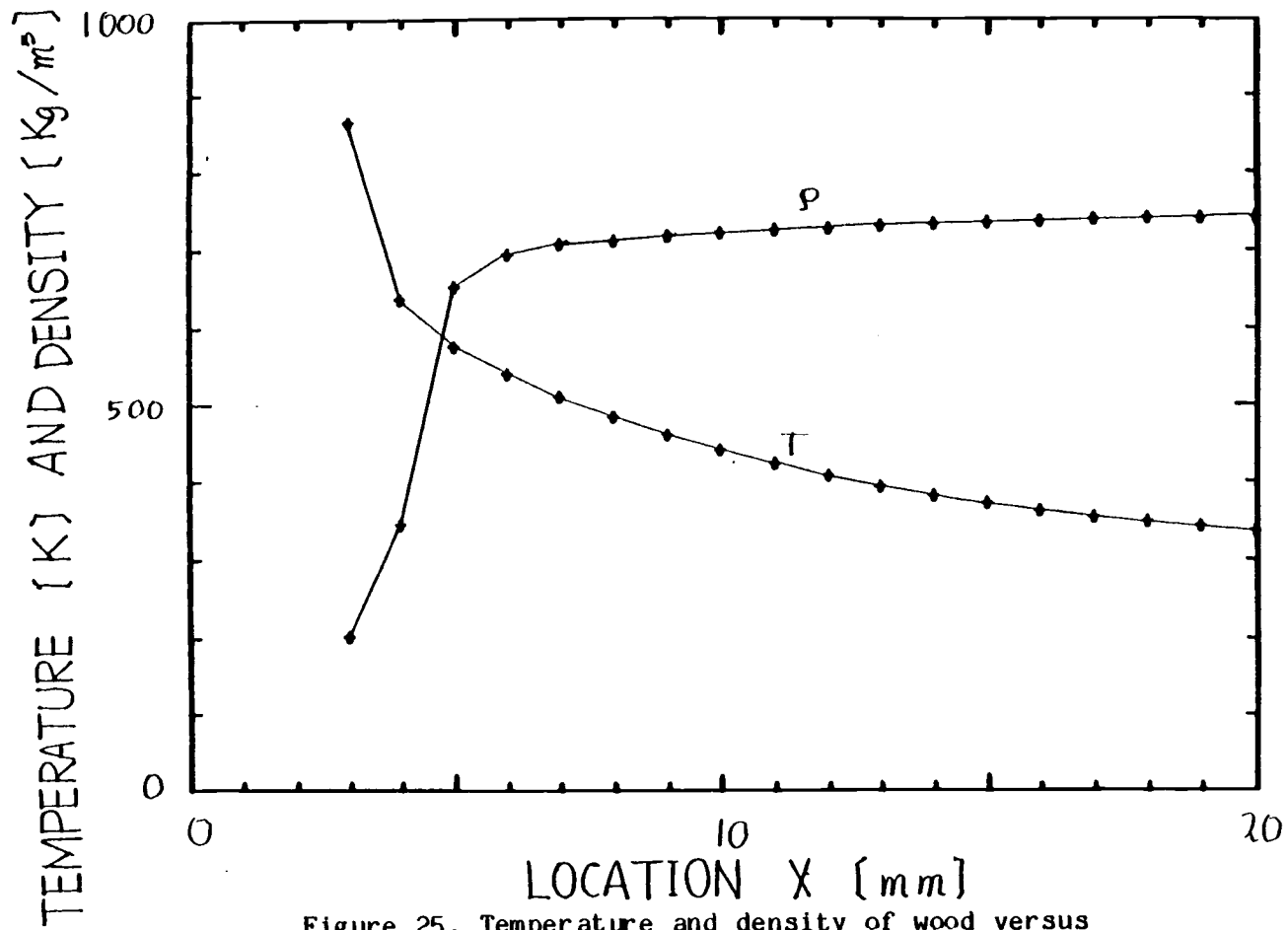


Figure 25. Temperature and density of wood versus location for time $t=480$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

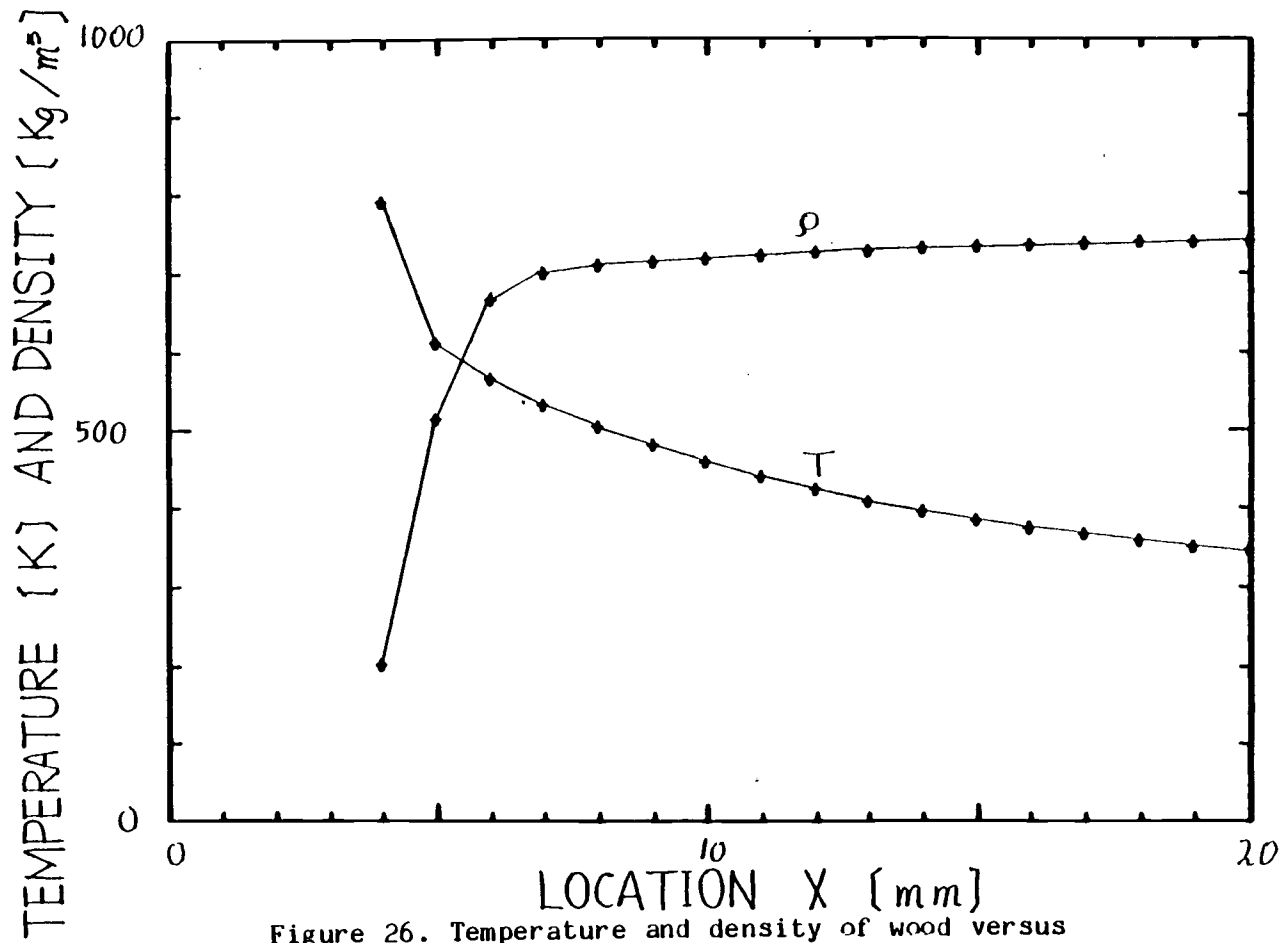


Figure 26. Temperature and density of wood versus location for time $t=540$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

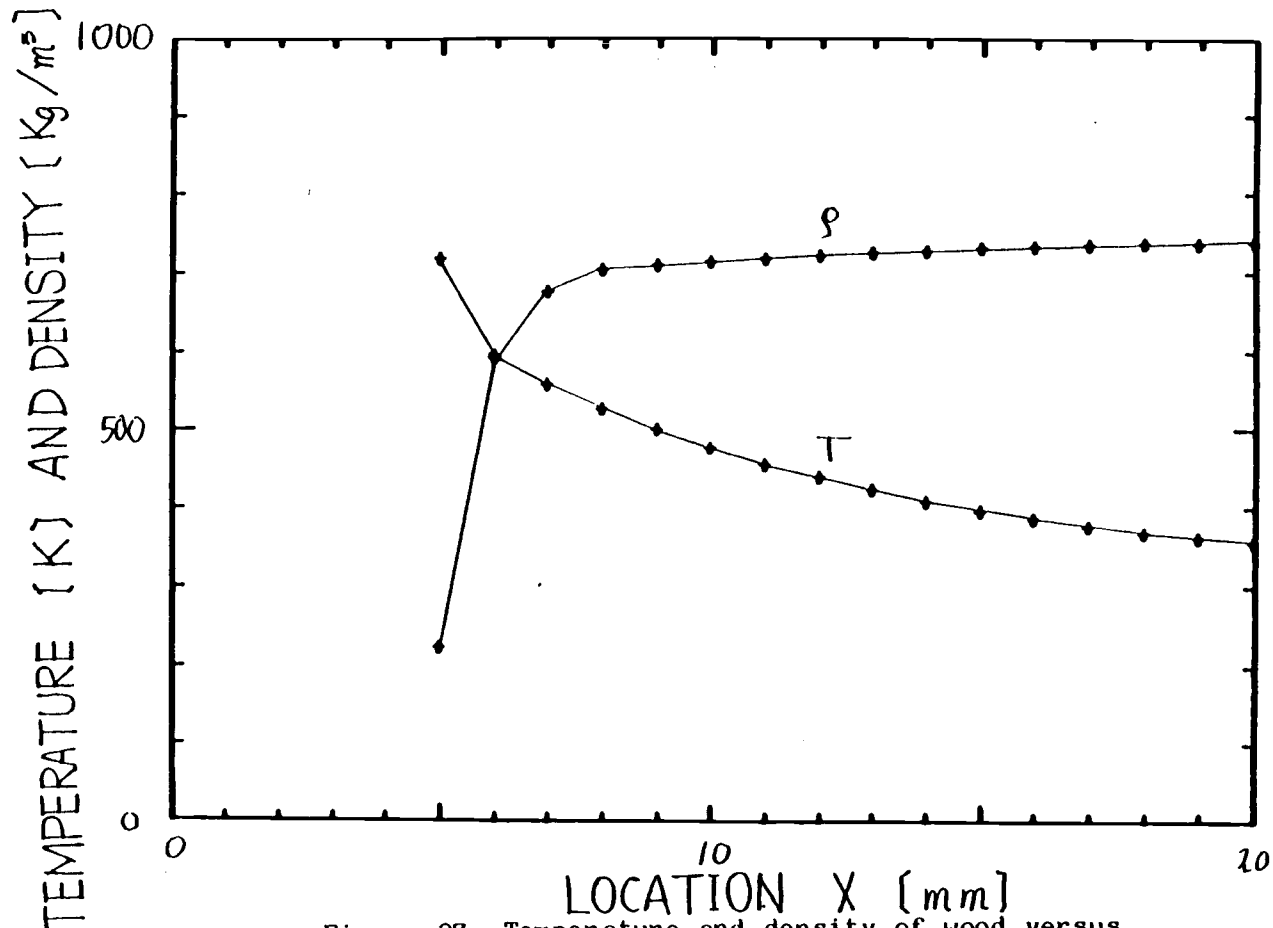


Figure 27. Temperature and density of wood versus location for time $t=600$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

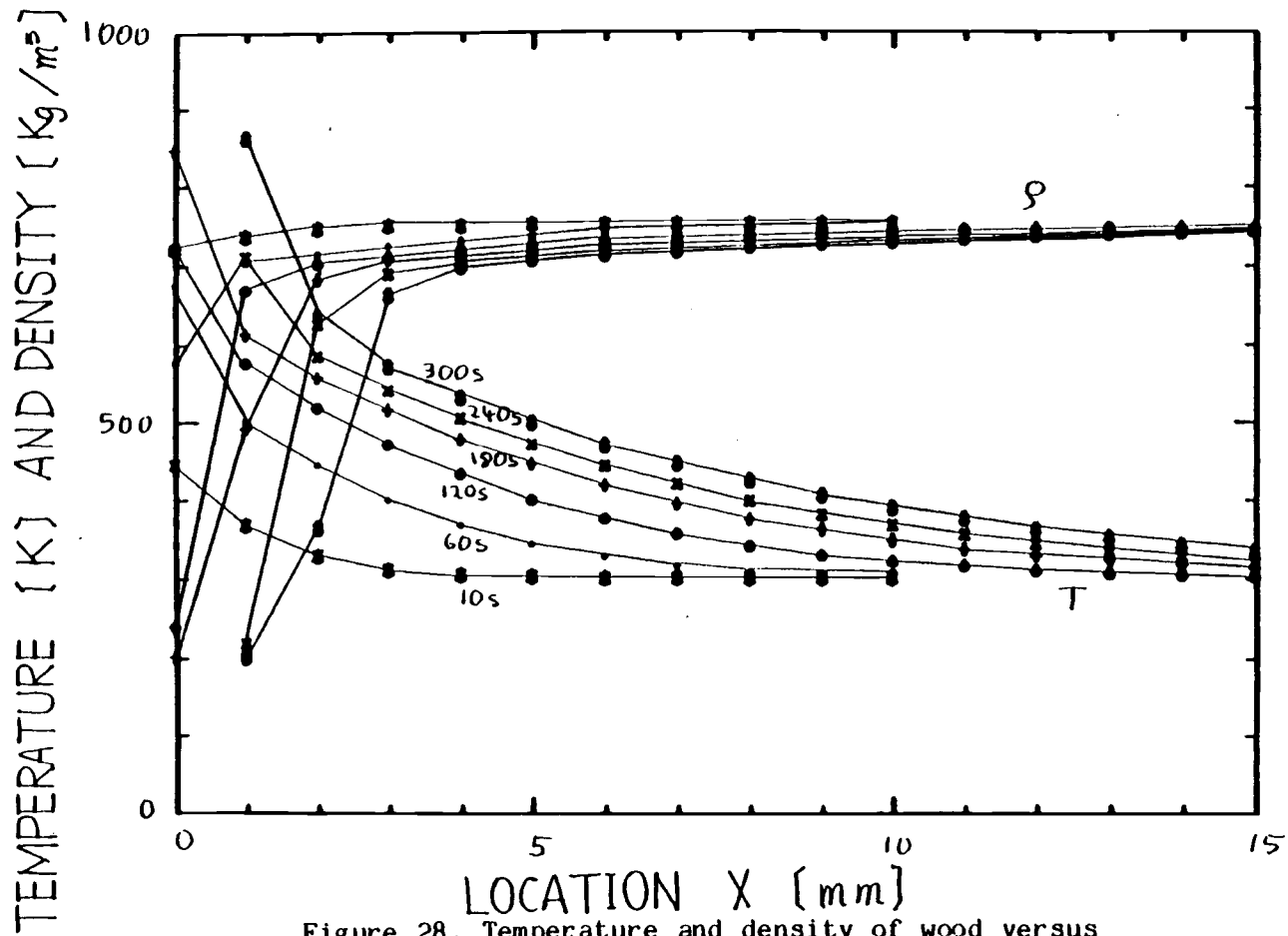


Figure 28. Temperature and density of wood versus location for time $t=10, 60, 120, 180, 240, 300$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

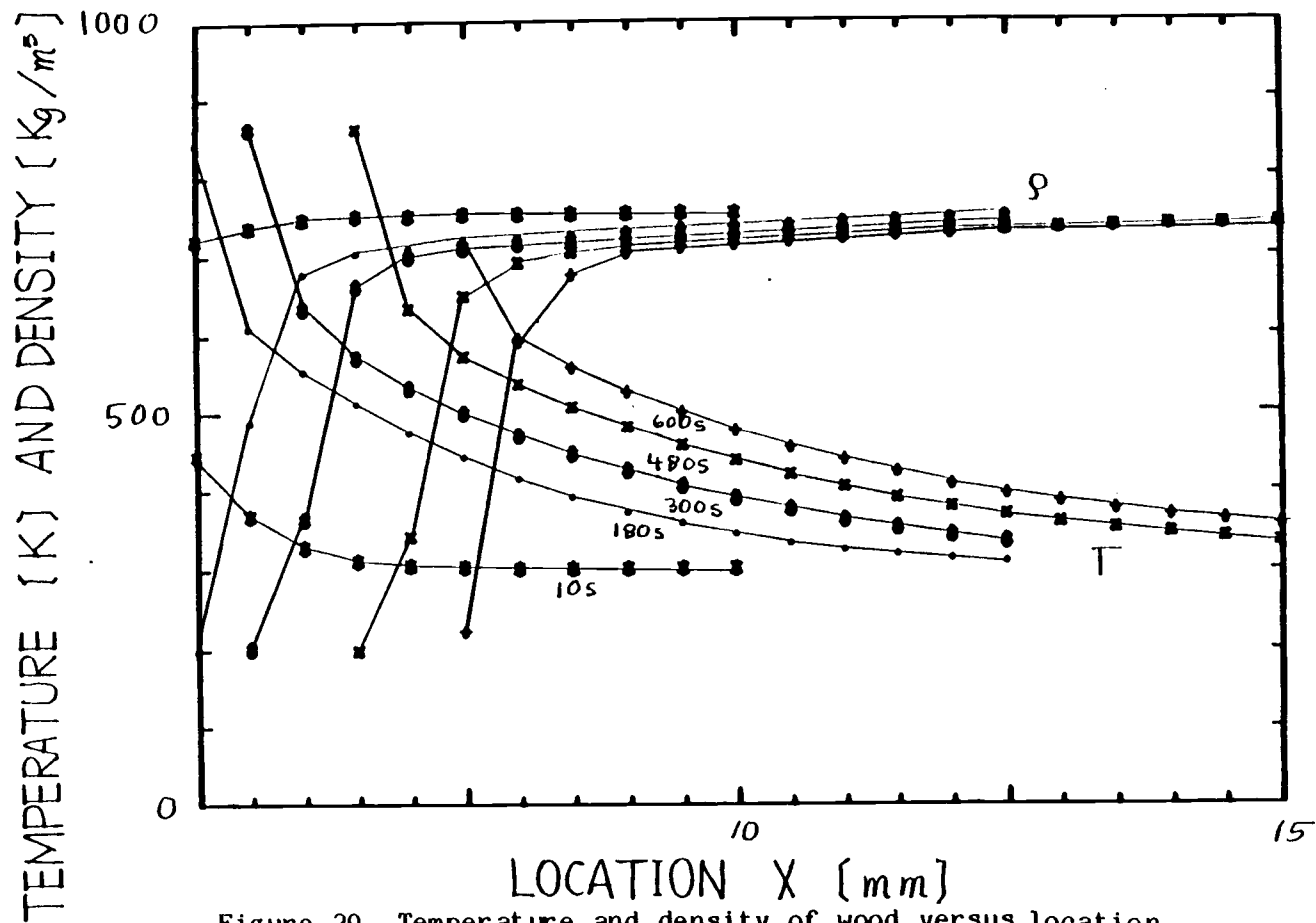


Figure 29. Temperature and density of wood versus location for time $t=10, 180, 300, 480, 600$ s and a convective boundary. ($T_{\text{ambient}} = 1300$ K)

A major density drop occurs at temperatures around 700 K which is slightly lower than in the constant heat flux case. The "reaction zone" is wider and not as distinctive as in the first case. The reason for that is, that due to the lower incoming energy, the heating of the slab is slower. Therefore, a part of the incoming energy is conducted into the slab where decomposition starts. The velocity with which the surface is ablating is not constant. At the beginning it is much slower (0.4 mm/min) where after about 6 minutes the velocity reaches a value of about 0.6 mm/min.

7.3 CONCLUSIONS

Decomposition of wood under fire-conditions takes place only at a thin area at the surface. This "reaction zone" depends on the boundary conditions between 1 and 3 mm thick. The temperature of the char before it is totally burnt depends also on the boundary condition. For high energy sources, values of 1400 K were found, while for low energy sources a value of 850 to 900 K was determined. In the second case the boundary temperature was also depending on time, while in the first case the time dependence was negligible. The velocity with which the

surface is ablating seems to be constant for a high incident heat flux (about 6 to 8 mm/min) while for a lower energy source the velocity is, due to conduction into the wood, time dependent.

The computer program was stable for even very large time intervals (3 seconds) and the the matrix inversion method made it possible to treat all the boundary conditions in one and the same program. The running time was mainly dependent on two factors, the number of intervals and the amount of output desired (both values could be changed).

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APPENDICES

APPENDIX A

What follows is a description of the computer program and a flow chart of the main program.

MAIN Program

- Reads information and data input
- Sets values according to the choice of the boundary conditions.
- Sets initial values and calculates parameters for the subroutines.
- Calls WOODPRO, GASPRO, CHARPRO, and SOURCE to obtain the physical properties for subroutines.
- Computes the parameters of the matrix.
- Calls MATDEC and MATSOL to get the temperature profile.
- Writes output.
- Stops program when maximum time is reached.
- Tests another case or calls exit.

SUBROUTINE MATDEC

- Decomposes the matrix into an upper and a lower triangular matrix.

SUBROUTINE MATSOL

- Forward solution to maintain Z
- Backward solution to maintain the temperatures.

SUBROUTINE WOODPRO

- Iterates on the specific gravity and the expansion coefficients of wood.
- Calculates the conductivity of wood.
- Calculates the specific heat of wood.

SUBROUTINE GASPRO

- Computes the specific heat of the gasmixture.
- Computes the density of the gasmixture.

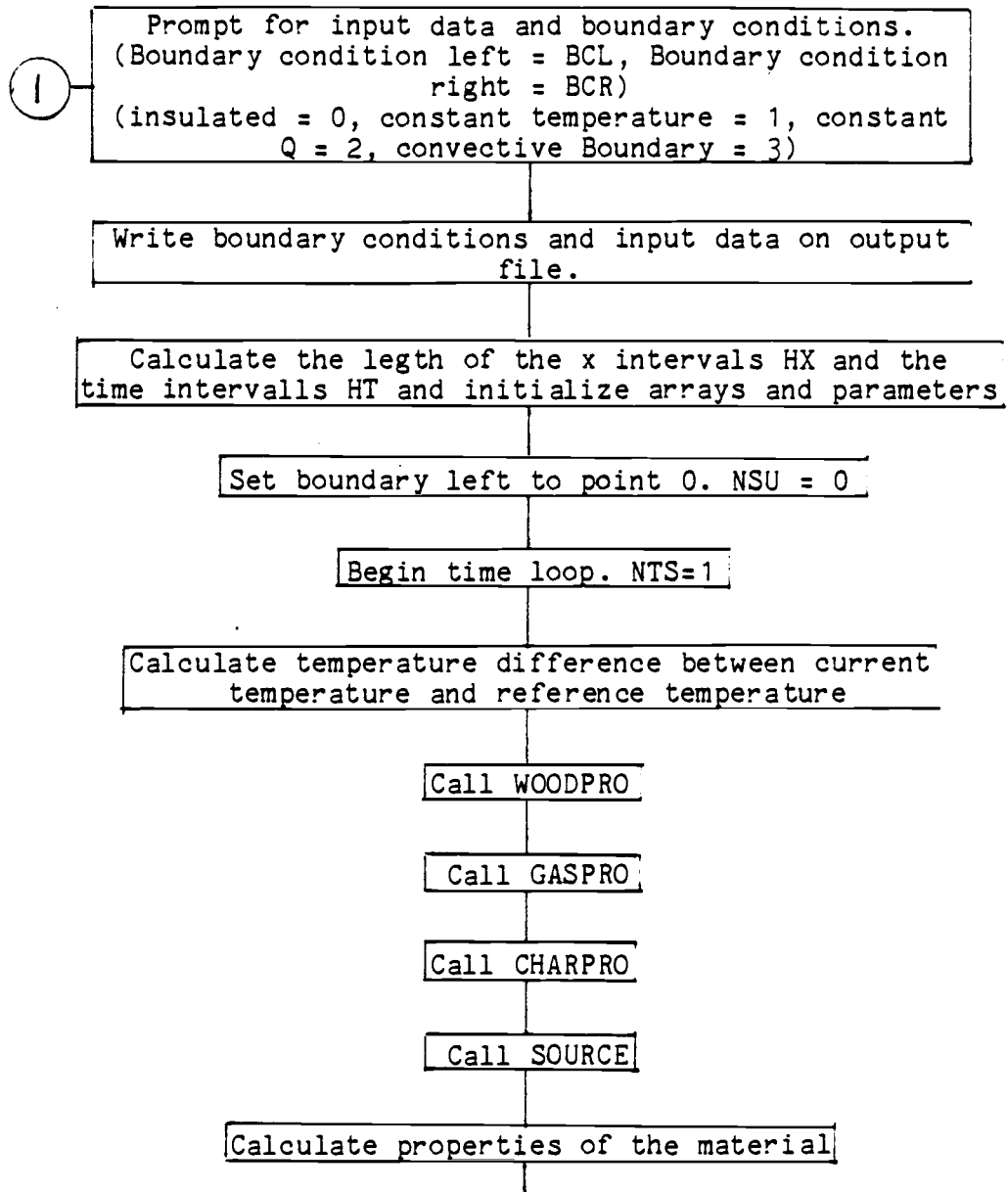
SUBROUTINE CHARPRO

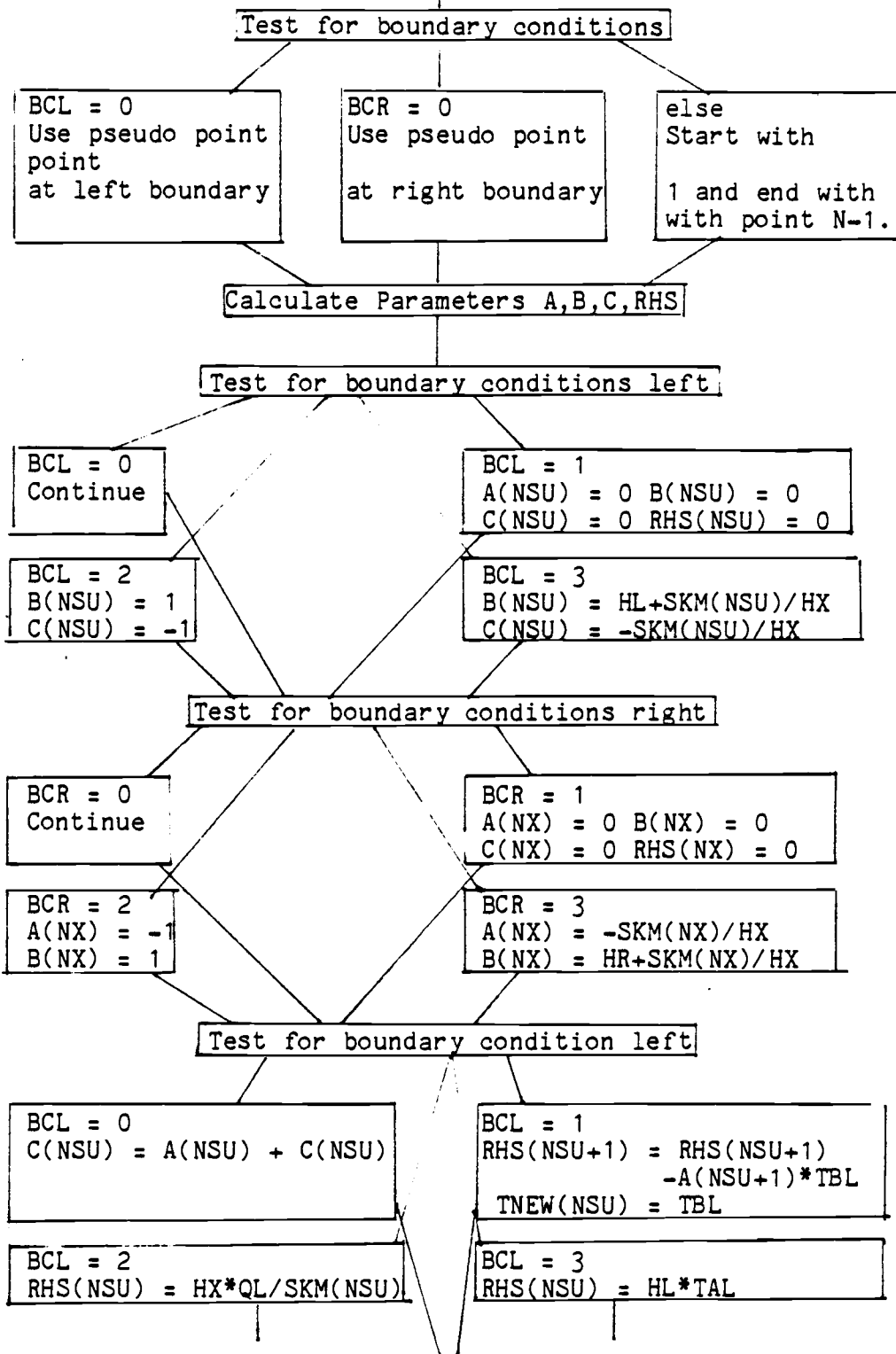
- Returns the specific heat, the conductivity and the density of char.

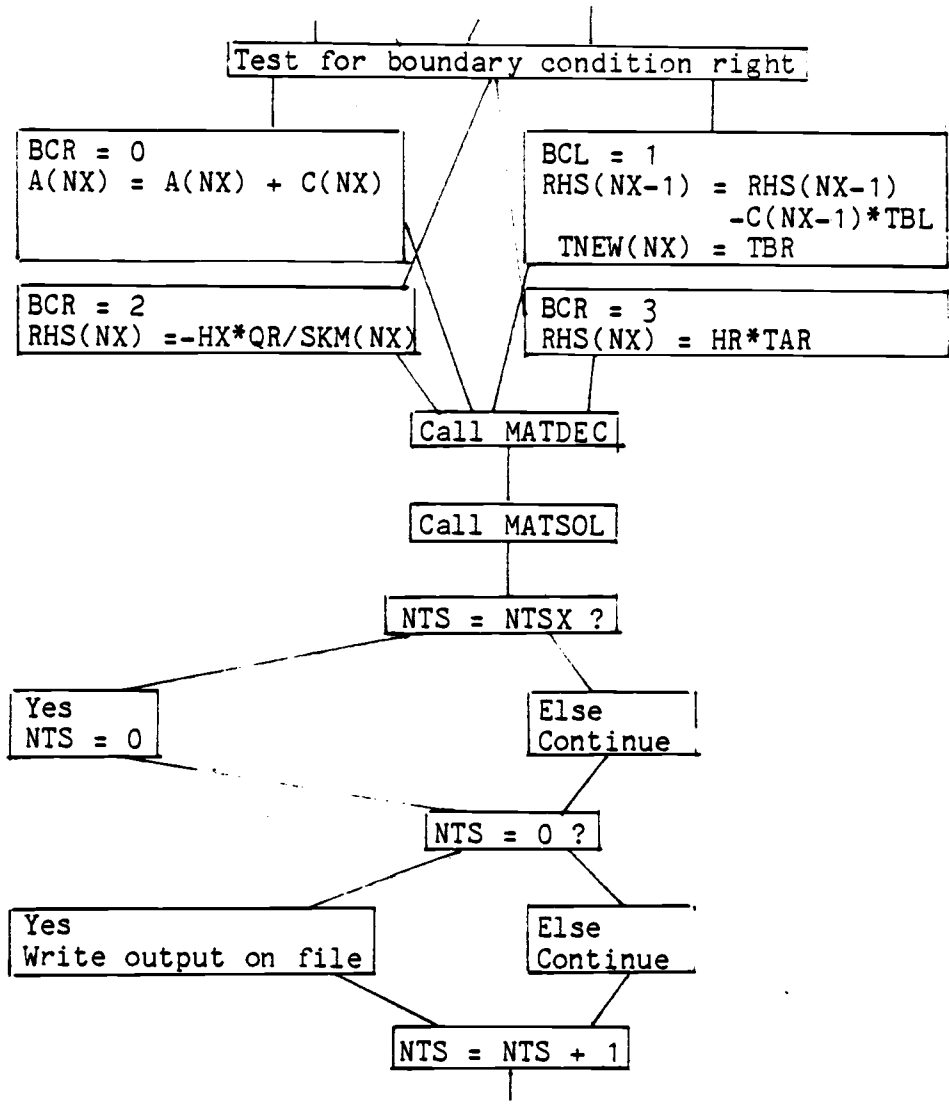
SUBROUTINE SOURCE

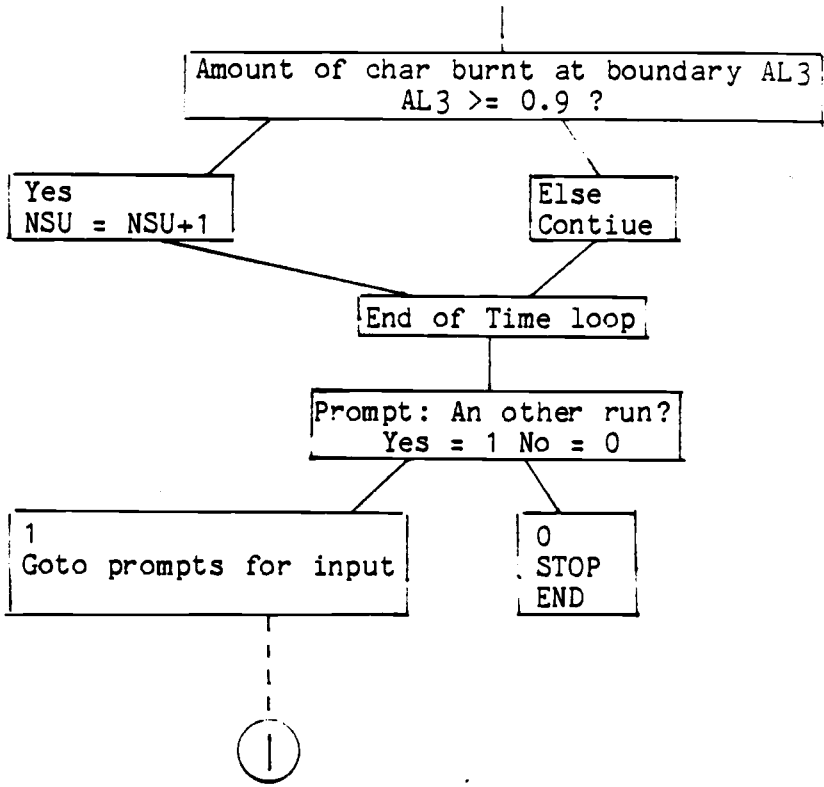
- Calculates the burnt mass of each reaction.
- Computes the overall heat source.
- Calculates the gasflow.

FLOW DIAGRAM OF THE MAIN PROGRAM









APPENDIX B

What follows is a listing of the computer programs.

MAIN PROGRAM

```

PROGRAM THESIS (INPUT,OUTPUT)
REAL A(0:100),R(0:100),C(0:100),AL(0:100),RE(0:100),FA(0:100)
REAL SKM(0:100),SKG(0:100),POG(0:100),ROM(0:100),SHM(0:100)
REAL SHG(0:100),S(0:100),RHS(0:100),TNEW(0:100),VG(0:100)
REAL SPGFC(0:100),SPG(0:100),DT(0:100),SK(0:100)
REAL SHC(0:100),MR1(0:100),MR2(0:100),MR3(0:100)
REAL SH(0:100),SKC(0:100),ROC(0:100),ALFAM(0:100)
REAL AL1(0:100),AL2(0:100),AL3(0:100)
REAL RM1(0:100),RM2(0:100),RM3(0:100),TOLD(0:100)
C
C
3000 KOR=0
1 PRINT*,*ENTER INITIAL TEMPERATURE,INITIAL SPEC. GRAVITY*
PRINT*,*OF THE WOOD AT REF. TEMP. AND THE REF. TEM.(K)*
READ*,TI,SPGO,TREF
IF (KOR.NE.0)GOTO 20
2 PRINT*,*ENTER THICKNESS AND # OF INTERVALLS*
READ*,XL,NX
IF (KOR.NE.0)GOTO 20
3 PRINT*,*ENTER MAX. TIME AND # OF TIME INTERVALLS*
READ*,TM,NT
IF (KOR.NE.0)GOTO 20
4 PRINT*,*SELECT LEFT BOUNDARY CONDITION*
PRINT*,*INSUL.=0,CON.TEMP.=1,CON.Q=2,CONVEC.=3*
READ*,BCL
5 IF (BCL.EQ.1) THEN
PRINT*,*ENTER LEFT HAND BOUNDARY TEMP.*
READ*,TBL
IF (KOR.NE.0)GOTO 20
ENDIF
6 IF (BCL.EQ.2) THEN
PRINT*,*ENTER CONST. Q LEFT*
READ*,QL
IF (KOR.NE.0)GOTO 20
ENDIF
7 IF (BCL.EQ.3) THEN
PRINT*,*ENTER LEFT HEAT TRANS. COEF. AND AMBI. TEMP.*
READ*,HL,TAL
IF (KOR.NE.0)GOTO 20
ENDIF
8 PRINT*,*SELECT RIGHT BOUNDARY CONDITTON*
PRINT*,*INSUL.=0,CON.TEMP.=1,CON.Q=2,CONVEC.=3*
READ*,BCR
9 IF (BCR.EQ.1) THEN
PRINT*,*ENTER RIGHT HAND BOUNDARY TEMP.*
READ*,TBR
IF (KOR.NE.0)GOTO 20
ENDIF
10 IF (BCR.EQ.2) THEN
PRINT*,*ENTER CONST. Q RIGHT*
READ*,QR
IF (KOR.NE.0)GOTO 20
ENDIF
11 IF (BCR.EQ.3) THEN
PRINT*,*ENTER RIGHT HEAT TRANS.COEF. AND AMBI.TEMP.*
READ*,HR,TAR
IF (KOR.NE.0)GOTO 20
ENDIF
12 PRINT*,*ENTER EPST,EPSTW*
READ*,EPST,EPSTW
IF (KOR.NE.0) GOTO 20
13 PRINT*,*ENTER # OF X INTERVALLS AND TIMEINTERVALLS SKIPPED*
READ*,NXSX,NTSX

```

```

      IF(KOR.NE.0) GOTO 29
      CONTROL INPUT
C
C
20  WRITE(1,100) TI,SPGO,TREF
      WRITE(1,101) XL,NX
      WRITE(1,102) TM,NT
      IF(RCL.EQ.0) WRITE(1,103)
      IF(RCL.EQ.1) WRITE(1,104) TRL
      IF(RCL.EQ.2) WRITE(1,105) QL
      IF(RCL.EQ.3) WRITE(1,106) HL,TAL
      IF(BCP.EQ.0) WRITE(1,107)
      IF(BCP.EQ.1) WRITE(1,108) TRP
      IF(BCP.EQ.2) WRITE(1,109) QR
      IF(BCP.EQ.3) WRITE(1,110) HR,TAR
      WRITE(1,111) EPST,EPSTW
      WRITE(1,112) NXSX,NTSX
      PRINT*,*OK=0,IF NOT INPUT # OF INCORRECT LINE*
      READ*,KOR
      IF(KOR.NE.0) GOTO(1,2,3,4,5,6,7,8,9,10,11,12,13) KOR
      FORMATS
C
C
100  FORMAT(1X,*1: TI= *,F6.2,2X,*SPGO= *,F6.4,2X,*TREF= *,F6.2)
101  FORMAT(1X,*2: THICKNES= *,F10.5,2X,*# OF XINTFPV.= *,I4)
102  FORMAT(1X,*3: MAX.TIME= *,F10.4,2X,*# OF TIME INT= *,I4)
103  FORMAT(1X,*4: LEFT HAND SIDE INSULATED*)
104  FORMAT(1X,*4: FIXED LEFT TEMP.*,/1X,*5: TRL= *,F10.4)
105  FORMAT(1X,*4: CONST.Q LEFT*/,1X,*6: LEFT Q= *,F11.3)
106  FORMAT(1X,*4: CONVECTION ON LEFT SIDE*/,1X,*7: HL
      C= *,F8.3,2X,*TAML= *,F10.4)
107  FORMAT(1X,*8: RIGHT HAND SIDE INSULATED*)
108  FORMAT(1X,*8: FIXED RIGHT TEMP.*,/1X,*9: TRR= *,F10.4)
109  FORMAT(1X,*8: CONST.Q RIGHT*/,1X,*10: RIGHT Q= *,F8.3)
110  FORMAT(1X,*8: CONVECTION ON RIGHT SIDE*/,1X,*11: HR
      C= *,F8.2,2X,*TAMR= *,F10.4)
111  FORMAT(1X,*12: EPST= *,F6.4,2X,*EPSTW= *,F6.4)
112  FORMAT(1X,*13: NXSX= *,I4,2X,*NTSX= *,I4)
C
C
      CALCULATION OF THE MATRIX
C
      HT=TM/NT
      HX=XL/NX
      NSU=0
      NTS=1
C
C
      CALCULATION OF THE PROPERTIES
C
      DO 50 I=0,NX
      MB1(I)=0
      MB2(I)=0
      MB3(I)=0
      AL1(I)=0
      AL2(I)=0
      AL3(I)=0
      BM1(I)=0
      BM2(I)=0
      BM3(I)=0
      ALFAW(I)=1
      TOLD(I)=TI
50  SPGFO(I)=SPGO
C
C
      BEGINNING OF THE TIME LOOP
      DO 2000 IJ=1,NT
      TIME=HT*IJ
      DO 51 I=NSU,NX

```

```

51 DT(I)=TOLD(I)-TPEF
C
CALL WOODFRD(NX,SPGO,SPGFO,DT,TOLD,EPHW,SPG,SK,SH)
CALL GASPRO(NX,TOLD,SHG,POG)
CALL CHAPFRD(NX,SYC,SHC,POC)
CALL SOURCE(AL1,AL2,AL3,TOLD,NX,HT,HX,SPG,S,VG,ALFAW,
CMR1,MB2,MB3,ROG,RM1,RM2,RM3)
C
C
C      CALCULATION OF THE PARAMETERS
C
DO 52 I=NSU,NX
ROW=SPG(I)*1E6
ROM(I)=ALFAW(I)*ROW+(1-ALFAW(I))*POC(I)
SKM(I)=ALFAW(I)*SK(I)+(1-ALFAW(I))*SKC(I)
SHM(I)=ALFAW(I)*SH(I)+(1-ALFAW(I))*SHC(I)
52 SPGFO(I)=SPG(I)
C
DO 70 III=NSU,NX
IF(III.EQ.(NSU+1)) THEN
UL=(1-ALJ(NSU))
IF(UL.LE.0.?) UL=0.9
ELSE
UL=1
ENDIF
IIII=III
I=III
II=I-1
IIII=II
IF(I.EQ.NSU) THEN
IF(RCL.EQ.0) THEN
II=I
IIII=NSU
VG(NSU)=0
ELSE
GOTO 70
ENDIF
ENDIF
IF(I.EQ.NX) THEN
IF(RCR.EQ.0) THEN
I=II
IIII=NX
VG(NX)=0
ELSE
GOTO 70
ENDIF
ENDIF
ENDIF
A(III)=SKM(II)*HT/(HX*UL)+SHG(II)*ROG(II)*VG(IIII)*HT/2
C+SHG(II)*(MB1(II)*0.6+MB2(II)*0.6+MB3(II))/2
B(III)=(-SKM(I)/HX-SKM(II)/(HX*UL))*HT-(POG(I)*VG(IIII)*SHG(I)/2
C-POG(II)*VG(IIII)*SHG(II)/2)*HT-HX/2*(POG(II)*SHG(I)+
CPOM(I)*SHM(I)+(POG(II)*SHG(II)+ROM(II)*SHM(II))*UL)
C+SHG(II)*(MB1(II)*0.6+MB2(II)*0.6+MB3(II))/2
C(III)=SKM(I)*HT/HX-POG(I)*VG(IIII)*HT*SHG(I)/2
RMS(II)=-HX/2*(S(I)+S(II)*UL)*HT-HX/2*(POG(II)*SHG(II)+ROM(II)
C*SHM(I)+(POG(II)*SHG(II)+ROM(II)*SHM(II))*JL)*TOLD(III)
70 CONTINUE
IF(RCL.EQ.2) THEN
B(NSU)=1
C(NSU)=-1
ENDIF
IF(RCL.EQ.3) THEN
B(NSU)=HL+SKM(NSU)/HX

```

```

C(NSU)=-SKM(NSU)/HX
ENDIF
IF(RCL.EQ.1) THEN
A(NSU)=0
B(NSU)=0
C(NSU)=0
RHS(NSU)=0
ENDIF
C
IF(QCR.EQ.2) THEN
A(NX)=-1
B(NX)=1
ENDIF
IF(BCR.EQ.3) THEN
B(NX)=HP+SKM(NX)/HX
A(NX)=-SKM(NX)/HX
ENDIF
IF(QCR.EQ.1) THEN
A(NX)=0
B(NX)=0
C(NX)=0
RHS(NX)=0
ENDIF
C
DECOMP(SITION OF THE MATRIX AND THE SOLUTION FOR THE TEMPERATURE
C
DO=0
ONX=0
NS=NSU
NE=NX
C
IF(RCL.EQ.0) THEN
C(NSU)=A(NSU)+C(NSU)
ENDIF
C
IF(QCR.EQ.0) THEN
A(NX)=A(NX)+C(NX)
ENDIF
C
IF(RCL.EQ.1) THEN
RHS(1)=RHS(1)-A(1)*TBL
TNEW(NSU)=TBL
NS=1+NSU
ENDIF
C
IF(QCR.EQ.1) THEN
RHS(NX-1)=RHS(NX-1)-C(NX-1)*TBR
TNEW(NX)=TBR
NE=NX-1
ENDIF
C
IF(RCL.EQ.2) THEN
RHS(NSU)=HX*QL/SKM(NSU)
DO=0
ENDIF
C
IF(QCR.EQ.2) THEN
RHS(NX)=-HX*QR/SKM(NX)
ONX=0
ENDIF
C
IF(RCL.EQ.3) THEN
DO=0
RHS(NSU)=HL*TAL

```

```

      ENOIF
C
      IF(PCP,PO,3) THEN
      ONX=0
      PHS(NX)=HP*TAJ
      ENOIF
C
      CALL MATDEC(A,R,C,DO,ONX,NS,NE,AL,RE,GA,DEQ,DFN)
      CALL MATSOL(NS,NF,AL,RE,GA,DEQ,DFN,PHS,TNEW)
      IF(NTS.EQ.NTSX) NTS=0
      IF(NTS.EQ.0) THEN
      SUP=NSU*HX
      WRITE(1,200) TIME,SUP
      WRITE(1,201) (TNEW(I),I=0,NX,NXSX)
      WRITE(1,202)
      WRITE(1,204) (RDM(I),I=0,NX,NXSX)
      WRITE(1,203)
      WRITE(1,201) (AL3(I),I=0,NX,NXSX)
      ENOIF
      NTS=NTS+1
      DO 1001 I=NSU,NX
      IF (AL3(I).GT.0.0) THEN
      NSU=NSU+1
      ENDTF
1001 TOLD(I)=TNEW(I)
2000 CONTINUE
200  FORMAT(1X,'TIME= ',F10.6,1X,' S',1X,'DUMP MATERIAL = ',
      F10.6,1X,'**')
201  FORMAT(1X,11F10.4)
202  FORMAT(1X,'RDM')
203  FORMAT(1X,'AL3')
204  FORMAT(1X,11E10.4)
      PRINT*,*AN OTHER RUN? YES=L,NO=0*
      READ*,AAA
      IF(AAA.EQ.1) GOTO 3000
      STOP
      END
      SUBROUTINE MATDEC(A,R,C,DO,ONX,NS,NE,AL,RE,GA,DEQ,DFN)
      REAL A(0:100),R(0:100),C(0:100),AL(0:100),RE(0:100),GA(0:100)
      DO 1 I=NS+1,NF-1
      AL(I)=A(I)
      RE(NS)=R(NS)
      GA(NS)=C(NS)/RE(NS)
      DEQ=DO/RE(NS)
      DFN=ONX
      RE(NS+1)=R(NS+1)-AL(NS+1)*GA(NS)
      GA(NS+1)=(C(NS+1)-AL(NS+1)*DEQ)/RE(NS+1)
      DO 2 I=NS+2,NF-1
      RE(I)=R(I)-AL(I)*GA(I-1)
      GA(I)=C(I)/RE(I)
2    AL(NE)=A(NE)-DFN*GA(NE-2)
      BE(NE)=R(NE)-AL(NE)*GA(NE-1)
      RETURN
      END
      SUBROUTINE MATSOL(NS,NE,AL,RE,GA,DEQ,DFN,PHS,T)
      REAL AL(0:100),RE(0:100),GA(0:100),PHS(0:100),T(0:100),Z(0:100)
C
C      FORWARD SOLUTION TO MAINTAIN Z
C
      Z(NS)=PHS(NS)/RE(NS)
      DO 1 I=NS+1,NE-1
1    Z(I)=(PHS(I)-AL(I)*Z(I-1))/RE(I)
      Z(NE)=(PHS(NE)-AL(NE)*Z(NE-1)-DFN*Z(NE-2))/RE(NE)

```

```
C
C   BACKWARD SOLUTION
C
      T(NF) = Z(NF)
      DO 2 I = NF - 1, NS + 1, -1
2     T(I) = Z(I) - GA(I) * T(I + 1)
      T(NS) = Z(NS) - GA(NS) * T(NS + 1)
      RETURN
      END
```

SUBROUTINE SOURCE

```

SUBROUTINE SOURCE(AL1,AL2,AL3,TCLD,NX,HT,HX,SPG,S,VG,ALFAW,
  LM01,M02,M03,PLG,BM1,BM2,BM3)
  REAL TCLD(0:100),AL1(0:100),AL2(0:100),AL3(0:100)
  REAL Y3(0:100),SPG(0:100),M01(0:100),M02(0:100)
  REAL MG(0:100),ALFAW(0:100),ALW1(0:100),ALW2(0:100)
  REAL VG(0:100)
  REAL POG(0:100),MB,M10,M20,M30,M
  REAL BM1(0:100),BM2(0:100),BM3(0:100)
  REAL Y1(0:100),Y2(0:100),M03(0:100),S(0:100)

```

```

THIS SUBROUTINE CALCULATES THE SOURCE TERM FOR BURNING WOOD

```

```

REACTION 1: CHARING OF HEMICELLULOSE AND LIGNIN

```

```

DO 1 I=0,NX
  IF(TCLD(I).LT.523) THEN
    ALW1(I)=1
    M01(I)=0
    GOTO 1
  ENDOF
  E1=4000
  RK1=1.425
  Y01=1
  YF1=0.4
  AL1(I)=AL1(I)+RK1*EXP(-E1/(8.314*TCLD(I)))*(1-AL1(I))*HT
  IF(AL1(I).GT.1) AL1(I)=1
  Y1(I)=Y01-AL1(I)*(Y01-YF1)
  M10=SPG(I)*HX*1E6/2
  M0=(1-Y1(I))*M10/0.6
  M01(I)=M0-BM1(I)
  BM1(I)=M0
  ALW1(I)=(M10-M0)/M10
  CONTINUE

```

```

REACTION 2: CHARING OF CELLULOSE

```

```

DO 2 I=0,NX
  IF(TCLD(I).LT.573) THEN
    ALW2(I)=1
    M02(I)=0
    GOTO 2
  ENDOF
  E2=250000
  RK2=0E19
  Y02=1
  YF2=0.4
  AL2(I)=AL2(I)+RK2*EXP(-E2/(8.314*TCLD(I)))*(1-AL2(I))*HT
  IF(AL2(I).GT.1) AL2(I)=1
  Y2(I)=Y02-AL2(I)*(Y02-YF2)
  M20=SPG(I)*HX*1E6/2
  M0=(1-Y2(I))*M20/0.6
  M02(I)=M0-BM2(I)
  BM2(I)=M0
  ALW2(I)=(M20-M0)/M20
  CONTINUE

```

```

REACTION 3: BURNING OF THE CHAR

```

```

DO 3 I=0,NX
  IF(TCLD(I).LT.623) THEN
    M03(I)=0
    GOTO 3
  ENDOF

```

```

E3=54000
RK3=1E6
Y03=6.4
YF3=0
AL3(I)=AL3(I)+RK3*EXP(-E3/(8.314*TOL0(I)))*(1-AL3(I))*HT
IF(AL3(I).GT.1) AL3(I)=1
Y3(I)=Y03-AL3(I)*(Y03-YF3)
M30=SPG(I)*HX*1E6
M0=(6.4-Y3(I))*M30
M03(I)=M0-0M3(I)
0M3(I)=M0
3 CONTINUE
C
C CALCULATION OF ALFAM
DO 4 I=0,NX
4 ALFAM(I)=(ALW1(I)+ALW2(I))/2
C
C SOURCE TERM
C
Q1=-168
Q2=1883
Q3=1465
DO 10 I=0,NX
10 S(I)=Q1*M01(I)+Q2*M02(I)+Q3*M03(I)
MG(I)=M01(I)*0.6+M02(I)*0.6+M03(I)
C
C CALCULATION OF THE VELOCITY
M=0
DO 20 I=NX,0,-1
M=M+MG(I)
20 VG(I)=-M/(HT*ROG(I))
200 FORMAT(1X,HT= ,F8.4)
201 FORMAT(1X,TOL0( ,I2,1X, )= ,F8.3)
202 FORMAT(1X,I= ,I2,1X,AL1= ,E12.4,1X,Y1= ,E12.4,2X,2E9.2)
RETURN
END

```


SUBROUTINE GASPRO

```

SUBROUTINE GASPRO(NX,TOLD,SHG,ROG)
REAL TOLD(0:100),MCO,MCO2,SHG(0:100),ROG(0:100)
C THIS SUBROUTINE CALCULATES THE PROPERTIES OF A
C CO AND CO2 GAS MIXTURE
C
C ENTERING THE CONSTANTS
MCO=28E-3
MCO2=44E-3
C CALCULATION OF THE SPECIFIC HEAT IN J/MOL*K
C
DO 1 I=0,NX
SHCO=26.881+6.971E-3*TOLD(I)-0.821E-6*TOLD(I)*TOLD(I)
SHCO2=26.018+43.528E-3*TOLD(I)-14.943E-6*TOLD(I)*TOLD(I)
C TRANSFORMATION OF THE SPECIFIC HEAT IN J/G*K
SHCO=SHCO/(1000*MCO)
SHCO2=SHCO2/(1000*MCO2)
SHG(I)=0.4*SHCO+0.6*SHCO2
1 CONTINUE
C
C CALCULATION OF THE DENSITIES, YJ=NJ/NM
RO IS IN G/M**3
YCO=0.4/(MCO*(0.4/MCO+0.6/MCO2))
YCO2=1-YCO
PCO=YCO*1E5
PCO2=YCO2*1E5
DO 2 I=0,NX
ROCO=PCO*MCO/(8.314*TOLD(I))
ROCO2=PCO2*MCO2/(8.314*TOLD(I))
ROG(I)=ROCO+ROCO2
2 ROG(I)=ROG(I)*1000
RETURN
END

```

SUBROUTINE WOODPRO

```

SUBROUTINE WOODPRO (NX,SPGO,SPGFO,DT,TOLD,EP SW,SPG,SK,SH)
REAL SPGFO(0:100),DT(0:100),TOLD(J:100),SPG(0:100)
REAL T(0:100),DTF(0:100),ALRA(C:100)
REAL SK(0:100),SH(0:100),ALTA(G:100),VOL(J:100)

```

```

THIS SUBROUTINE CALCULATES THE THERMAL PROPERTIES OF
DRY WOOD.

```

```

CALCULATION OF THE SPECIFIC GRAVITY. THE TEMPERATURE WAS
ORIGINALLY IN FahrenHEIT

```

```

ALGR=2.1E-6
DO 10 I=0,NX
1 ALRA(I)=(32*SPGFO(I)+99)*1E-6
  ALTA(I)=(33*SPGFO(I)+18.4)*1E-6
  DTF(I)=DT(I)*1.8
  VOL(I)=(1+DTF(I)*ALGR)*(1+DTF(I)*ALRA(I))*(1+DTF(I)*ALTA(I))
  SPG(I)=SPGO/VOL(I)
  SS=(SPG(I)-SPGFO(I))/SPG(I)
  SPGFO(I)=SPG(I)
  IF(ABS(SS).GT.EPSW)GOTO 1
10 CONTINUE

```

```

CALCULATION OF THE CONDUCTIVITY
ORIGINAL UNITS BTU*IN/HR*FT*FT, NOW W/M*K
DO 11 I=0,NX
11 SK(I)=SPG(I)*1.39+0.165
  SK(I)=SK(I)*0.14413

```

```

CALCULATION OF THE SPECIFIC HEAT
OLD UNITS BTU/LBM*F, NOW J/G*K
DO 12 I=0,NX
12 SH(I)=0.25+0.4066*(TOLD(I)*1.8-453.67)
  SH(I)=4.184*SH(I)
RETURN
END

```

SUBROUTINE CHARPRO

```
      SUBROUTINE CHARPRO(NX,SKC,SHC,ROC)
      REAL SKC(0:100),SHC(0:100),ROC(0:100)
      DO 1 I=0,NX
      SHC(I)=2
      SKC(I)=0.03
      ROC(I)=200000
1     CONTINUE
      RETURN
      END
```