APPENDIX B

TMPSUB2 AND SUBSTRAT USER'S GUIDE

General Information

SUBSTRAT and two helper programs are available on a diskette for IBM PC compatible computers. The distribution diskette includes both executable and source code for SUBSTRAT, executable code for the other two programs, and sample input files. The general relationship of programs and files is illustrated in Figure B-1. The TSDATA program is used to prepare data files for SUBSTRAT which in turn creates two types of output files. The plot file is used by the TSPLOT program to display contour plots of substrate temperatures. The list file includes a step-by-step record of the highest temperature in the substrate.

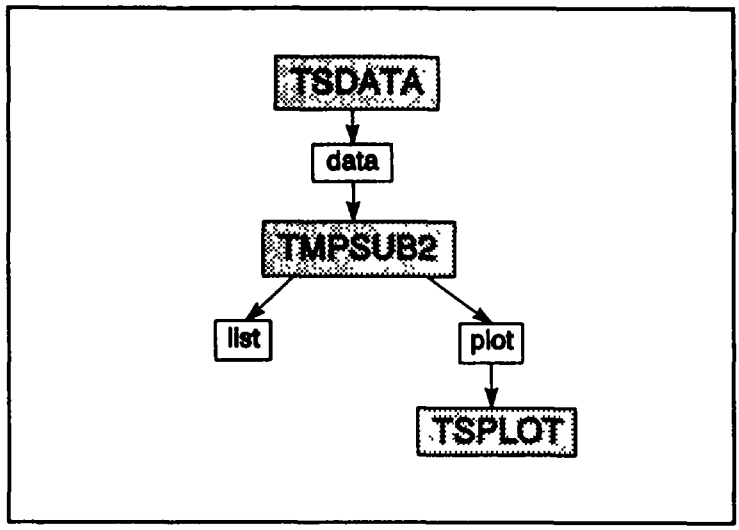


Figure B-1. TMPSUB2 Programs and Files

TSDATA and TSPLOT must be run using MS-DOS on IBM PC compatible computers with VGA graphics. SUBSTRAT requires a 386 class PC with math coprocessor or 486 class PC (no graphics needed) in order to achieve satisfactory performance. Typical execution times are 20 to 30 minutes on a 33Mhz 486 computer.

The SUBSTRAT source code (file SUBSTRAT.CCC) can be compiled using any ANSI C compiler. All SUBSTRAT input and output files are ASCII files. Therefore, SUBSTRAT can be recompiled and run on a different computer, while still using TSDATA and TSPLOT on a PC and transferring files between the computers. A different computer may allow SUBSTRAT to execute faster and/or handle more cells for more accurate simulation.

Be sure to inspect the README file on the distribution diskette. One way to read this file is to place the diskette in drive A: (or drive B:) and type

MORE < A:README (or MORE < B:README)

A permanent copy may be made with

PRINT < A:README

The README file contains a list of all files on the diskette, instructions for installing the necessary files on your hard disk, and information on any changes or additions to the program.

There should be at least 1,000,000 bytes available on your hard disk. It is best to create a single subdirectory for the executable programs and related data files. This will allow you to easily delete all

the files related to this program when you are finished with it. In general, when running on a PC, *keep all files in the current working directory.*

The following sections give details of the operation of SUBSTRAT, TSDATA, and TSPLOT.

SUBSTRAT

All input for SUBSTRAT must be placed in a data file. This file is read as the "standard input stream," so SUBSTRAT executes on MS-DOS and UNIX computers by redirecting the input file. For example, if there already exists an input data file, *e.g.*, TEST1.DAT, one can begin a run by typing

SUBSTRAT < TEST1.DAT

Note: SUBSTRAT can be aborted at any time by simultaneously pressing CTRL and C.

Sample run

If you have not already done so, install the SUBSTRAT program following the instructions in the README file. For example, from the directory on the hard disk where you want SUBSTRAT installed and with the diskette in drive A:, type

A:INSTALL A:

At the present time you only need to install in response to the first question you will be asked.

During installation a program will determine the "initial unallocated memory." If the required memory is greater than this amount, follow the instructions under memory requirements below before proceeding.

Should you wish to examine the directory at this point, a DIR command should indicate the presence of at least the following files: SUBSTRAT.EXE, TEST1.DAT, TEST2.DAT, and MEMREM.EXE. As mentioned above, begin the sample run by typing

SUBSTRAT <TEST1.DAT

SUBSTRAT will then (1) indicate that it is reading the data file, (2) echo the simulation title to the screen, (3) initialize the data in all cells, and (4) report the amount of unallocated memory. If there is "insufficient memory," an error message will be displayed and the run aborted. See the memory requirements section below for corrective action.

Every time SUBSTRAT completes a time step during the simulation, it displays the time (in seconds) and peak temperature (degrees C) on the screen. This allows you to monitor the progress of the simulation.

This same information is included on the list file, TEST1.LST, thus providing a permanent record of the primary value computed during the simulation. The list file also includes an echo of the input file which helps to identify the simulation and is especially useful in identifying any errors in the input which are also written to the list file.

The plot file, TEST1.PLT, contains all temperatures in the Y=0 and Z=0 planes at the times specified plus data to identify the simulation and the coordinate values.

Memory Requirements

SUBSTRAT has been written to handle an arbitrary number of cells up to some limit imposed by available memory or by the operating system. MS-DOS limits available random access memory (**RAM, not disk memory**) to 640,000 bytes which is shared by the program, the data in the program, a portion of the operating system, and perhaps various TSR (Terminate & Stay Resident) programs. TMPSUB allocates memory for its data arrays from available RAM. When there is insufficient memory to run a particular simulation, you must either make more memory available or reduce the memory required by the simulation. One way to make more memory available is to remove TSR programs, such as network connections. This usually requires rebooting the computer in such a manner that these programs are not automatically accessed. MS-DOS 5.0 uses somewhat less memory than previous versions. See your PC consultant for assistance. Run MEMREM to determine approximately the memory available for data.

The memory required by the simulation is determined primarily by the total number of cells which in turn is determined by the values on line 4 of the data file (see below). The total number of cells can be reduced to an arbitrarily small value, but accuracy will suffer. If you must search for the number of cells than can be run on your machine, begin with a relatively small number and increase it until the unallocated memory reported by SUBSTRAT is small.

With minimal other uses of memory, SUBSTRAT is limited to less than 20,000 cells under MS-DOS. The only way to simulate more cells is to recompile SUBSTRAT for a different operating system and/or a different computer.

Contents of SUBSTRAT Data File

line	variables	brief description
1	LIST	Name of the output file
2	PLOT	Name of the plot file
3	TITLE	Project title; echoed to output
4	NX NY NZ	number of cells in the X, Y, and Z directions (total number of cells = NX × NY × NZ)
5	NCX DX0 XW X0	X-coordinate data[1]: NCX number of constant length nodes in both directions from X0 DX0 length [mm] of constant length nodes XW total length [mm] of X axis X0 location of center of region of constant length nodes = initial position of peak flux from cigarette
6	NCY DY0 YW	Y-coordinate data[1]: NCY number of constant width nodes from Y = 0 DY0 width [mm] of constant width nodes YW total width [mm] of Y axis
7	NCZ DZ0 ZW FT	Z-coordinate data[1]: NCZ number of constant depth nodes from Z = 0 DZ0 width [mm] of constant depth nodes ZW total depth [mm] of Z axis FT fabric thickness [mm][2]
8	SEP	Width of air gap between fabric and padding [mm]
9	E TM NCF	Fabric data: E emittance TM maximum temperature[3] [°C] NCF number of data points for T, K, C (NCF <= 10)
10	T K C	Fabric thermal properties[4]: T temperature [°C] K conductivity [W/mK] C specific heat [kJ/kgK] Repeat line 10 up to NCF times.
11	DV DC DA	Densities: DV virgin material [kg/m^3] DC char [kg/m^3] DA ash [kg/m^3]
12	A N1 N2 T H	Fabric non-oxidative pyrolysis data: A reaction rate coefficient [1/min] N1 fabric mass exponent N2 oxygen concentration exponent (must be zero) T activation temperature [K] H heat of pyrolysis [kJ/kg]
13	A N1 N2 T H	Fabric oxidative pyrolysis data: A reaction rate coefficient [1/min] N1 fabric mass exponent N2 oxygen concentration exponent T activation temperature [K] H heat of pyrolysis [kJ/kg]

```
14      A N1 N2 T H     Fabric char pyrolysis data (similar to 13)

15      E TM NCP        Padding data:
                        E     emittance
                        TM    maximum temperature[3] [°C]
                        NCP   number of data points for T, K, C  (NCP <= 10)

16      T K C           Padding thermal properties[4]:
                        T     temperature [°C]
                        K     conductivity [W/mK]
                        C     specific heat [kJ/kgK]
                        Repeat line 16 up to NCP times.

17      DV DC DA        Densities:
                        DV    virgin material [kg/m3]
                        DC    char [kg/m3]
                        DA    ash [kg/m3]

18      A N1 N2 T H     Padding non-oxidative pyrolysis data (similar to 12)

19      A N1 N2 T H     Padding oxidative pyrolysis data (similar to 13)

20      A N1 N2 T H     Padding char pyrolysis data (similar to 13)

21      BC TA T0 OX     Boundary & initial conditions:
                        BC    0 = adiabatic outer boundaries[5],
                              1 = constant temperature outer boundaries
                        TA    ambient temperature [°C]
                        T0    initial substrate temperature [°C]
                        OX    oxygen concentration [fraction]

22      Q0 V Y X+ X-    Moving radiant flux distribution on surface:
                        Q0    peak flux [kW/m2]
                        V     velocity [mm/min]
                        Y     standard deviation in Y direction [mm]
                        X+    std dev in positive X direction [mm]
                        X-    std dev in negative X direction [mm]

23      HC HG           Heat transfer coefficients[6]
                        HC    for quiescent air [W/m2K]
                        HG    for impinging air [W/m2K]

24      dt DT TT        Simulation control:
                        dt    maximum time step [s]
                        DT    maximum temperature change [°C]
                        TT    total simulation time [s]

25      LIST I J K      Debug reports (SUBSTRAT compiled with DEBUG defined):
                        LIST  1 = activate data dumps (default 0)
                        I J K are the indices of the cell to be studied

26      PLOT            Time at which to write temperatures to the plot file;
                        repeat line 26 up to 10 times.
```

Notes:

[1] The relationship between the number of nodes, number of constant size nodes, size of constant size nodes and total length of an axis must be such that the variable width nodes are increasing in size.

[2] The fabric thickness and the depth of the constant depth cells are related: the fabric/padding boundary must be halfway between two cells. Therefore, the fabric thickness must be 0.5, or 1.5, or 2.5, etc., times the depth of the constant depth cells, or the constant depth cells must be 2, or 2/3, or 2/5, etc. times the thickness of the fabric. The boundary between the fabric and padding must be within the region of constant depth cells.

[3] When the temperature of any fabric (or padding) cell reaches the "maximum" fabric (or padding) temperature, the simulation is terminated.

[4] The way that k(T) and c(T) are input is by entering the values for each at a number of temperatures; the program then carries out a cubic spline fit to those points, to obtain the values at any other temperature. Even if k(T) and c(T) are given by explicit equations, this is still the way that the program "knows" the values.

[5] The "outer boundaries" of the substrate consist of the X = 0, X = XW, Y = YW, and Z = ZW planes (see items 5, 6, & 7).

[6] These coefficients refer to cases A and B in Section II.B.6. When using HC set HG to zero and vice versa.

The contents of the data file are described further in the description of the TSDATA program. It will generally be easier to check a data file by processing it with TSDATA, than to compare it line by line with the description given above.

TSDATA

The SUBSTRAT data file can be created with any ASCII line editor. However, the contents of the file are quite cryptic and thus prone to error; far better is to use TSDATA. TSDATA is an interactive program for creating data files. Because it is interactive, it uses certain commands which restrict its operation to IBM PC compatible computers. It includes extensive checking of the input data. TSDATA is especially useful for creating a data file which is only slightly different from another data file. This is useful in performing the parametric studies for which SUBSTRAT was designed.

Two special files are used by TSDATA. The help file, TSDATA.HLP, contains the text of the interactive help messages. Help is activated by pressing the F1 function key. If the help file is not available in the current working directory, no interactive help will be available. The configuration file, TSDATA.CFG, sets the colors of the display. The file included on the distribution diskette assumes that a standard VGA monitor is being used. If the configuration file is not in the current working directory, a set of default colors will be used. A new configuration file can be made by using the MAKECFGT program. See the README file for instructions.

The operation of TSDATA is explained on the following pages which show the messages and input screens which will appear as the program is run. After reading through these pages, try using TSDATA with one of the sample data files. Begin the program by typing TSDATA. Abort the program by pressing CTRL and C.

Sample Runs

At this point the following files should be available in the current working directory: TSDATA.EXE, TSDATA.HLP, TSDATA.CFG, and TEST1.DAT. If they are not, use the INSTALL procedure.

First use TSDATA to view the contents of the TEST1.DAT file. Type:

TSDATA

Press ENTER until the main menu appears; press ENTER again to set up the file information. Enter TEST1.DAT as the name of the previous data file. Press ENTER to cycle through file names (respond Y to the warning message about a duplicate file). Press ESC to return to the main menu. Press ENTER to view each section of data in turn; press ESC to return. When you reach the Save option, press CTRL and C to abort the program. This process will not have changed TEST1.DAT.

Now create a new data file, TEST3.DAT, similar to TEST1.DAT but with a peak flux of 20kW/m^2. Proceed as above until you reach "Name of new data file:". At this point move the cursor to the "1" in the file name and press 3 and then press ENTER. Revise the other two file names and the title accordingly. Press ESC to return to the main menu, and move to the boundary conditions option. Press ENTER and move (using cursor keys) to the peak heat flux. Change the value to 20, press ENTER, press ESC. Now enter the save option, and respond Y to save the file TEST3.DAT. Then enter the exit option, respond Y to exit, and respond Y to create a batch file. After this you should have exited TSDATA. Now type RUN to start SUBSTRAT using TEST3.DAT as input data.

TSDATA Input Screens and Help Messages

Standard title page with disclaimer at start of TSDATA program.

```
==================================================

   TSDATA -- interactive program to prepare data files for SUBSTRAT

                          Version 1.0

        Developed at the National Institute of Standards and Technology.
                    Program author:  George Walton

    This program is furnished by the government and is accepted by any
    recipient with the express understanding that the United States
    Government makes no warranty, expressed or implied, concerning the
    accuracy, completeness, reliability, usability, or suitability for
    any particular purpose of the information and data contained in
    this program or furnished in connection therewith, and the United
    States shall be under no liability whatsoever to any person by reason
    of any use made thereof.  This program belongs to the government.
    Therefore, the recipient further agrees not to assert any proprietary
    rights therein or to represent this program to anyone as other than
    a government program.

==================================================
```

General description of input process:

```
==================================================
    This program assists you in preparing input data files for the SUBSTRAT
    program.  It operates best by reading an existing SUBSTRAT data file
    which is then modified to create a new data file.  A sample data file
    is distributed with the program.  It can also be used to enter data
    from scratch.  Several data files can be created in one TSDATA session.

    Data are processed interactively through a system of data entry menus.
    Keyboard input is required from the user whenever the cursor is in
    a data entry field.  A data entry field is designated by a special
    color as is shown in the lower right corner of this screen.  This is
    a standard pause allowing the user to read the screen.  Pressing any
    key in response will allow the program to continue.

    While the cursor is in a data entry field, it will often be possible
    to get help by pressing the F1 function key.  Help is intended to
    give additional information about the data.  For help to work, the
    TSDATA.HLP file must be in the same directory as the TSDATA.EXE file.
    Program execution may be terminated when the cursor is in a data
    entry field by pressing CTRL and C simultaneously.

==================================================
```

General description (continued):

There will usually be several data entry fields on a single screen. The field may be blank or it may present a default response. The contents of a data entry field (even all blank) may be edited. That is, characters may be overwritten, deleted, or inserted. It may or may not be necessary to make an entry depending on context.

These fields are ordered from top to bottom and left to right. Pressing the tab key or the down-arrow key moves the cursor to the next field to the right/down; The shifted-tab or up-arrow moves to the previous field to left/up. Control-home or page-up moves the cursor to the first field on the screen. Control-end or page-down moves to the last field. Movement between fields can be done only if an entry is not required and no other keys have been pressed.

Data entry begins in the exchange mode, i.e., the value of the key pressed replaces the character at the cursor. Pressing the insert key will switch to the insert mode (and from insert to exchange). The delete key will remove the character at the cursor. Control-x will clear the entire data entry field. Move the cursor left with the left-arrow, control-left-arrow, or home keys. Move the cursor right with the right-arrow, control-right-arrow, or end keys. When the data is satisfactory, press the ENTER key.

Various checks are usually made on each data entry. These may produce a warning or error message at the bottom of the screen. The first line of this message indicates the nature of the problem. The second line indicates the severity of the problem, the file and line in the TSDATA source code where the error message originated, and whether some help may be available by pressing the F1 key.

Most errors will return you to the data entry field to correct the input. Such errors include invalid characters or numeric values outside certain situation-dependent limits.

Some problems may generate a question:

```
Question? (y/n) ▒
```

The user can press the Y and then ENTER keys to indicate a positive (yes) response or N and then ENTER to indicate a negative (no) response.

Some errors are fatal causing the program to terminate.

Screen 1: (primary menu)

```
=====================================================

SUBSTRAT data preparation:

    ▌  File information

    ▌  Geometry description

    ▌  Fabric data

    ▌  Padding data

    ▌  Boundary conditions

    ▌  Simulation control

    ▌  Save this data file

    ▌  Exit data preparation

Use cursor keys to move between menu selections.
Press ENTER to activate the menu selection at the X.
Press ESC to return from a selection.  Press F1 for help.
=====================================================
```

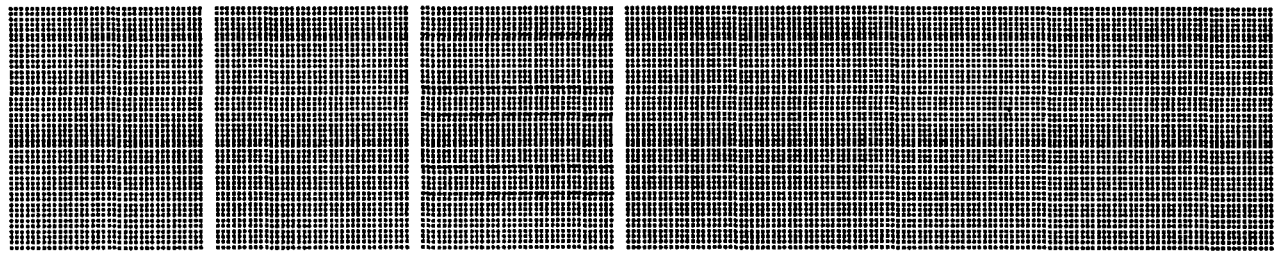
General help message:

```
This program assists you in preparing input data files for the SUBSTRAT
program.

This is the main menu.  It directs you to the different data
preparation subsections.

Begin each data file by entering the "file information".

Data relating to the geometry, fabric, padding, or boundary conditions
may be entered or changed in any order.

The data file is not created until you "save this data file".

Multiple data files can be created in one interactive session.
Terminate the session by entering "exit data preparation".
```

Note:
An X appears in the selection designator: ▌.

Screen 2:

```
=====================================================
  File information:                  press ESC when done;  press F1 for help.

Copy data from previous data file named:

Name of new data file:

Name of list file:

Name of plot file:

Title for this simulation:

Files previously defined in this session:
 data files   list files   plot files   titles (first 40 characters)
 ----------   ----------   ----------   ----------------------------
```



```
=====================================================
```

General help message:

The data files you create are stored in the current directory. If you want to make a data file which is similar to a previous data file, enter the name of the previous file. That file must also be in the current local directory.

SUBSTRAT creates two files when it is run:
(1) the list file (which echoes the input, saves any error messages, and notes the peak temperature of the substrate during the simulation),
(2) the plot file (which becomes the input file to the plotting program used to view the temperature distribution in the substrate).

Files should generally have different names. For example, consecutive SUBSTRAT runs with the same plot file names will save only the plot file from the last run (which will have replaced the previous plot files). Use identical names if you definitely want to replace existing files, including data files.

The title that you enter here is echoed in the list and plot files. Use the title as a reminder of the special features of a particular run.

Up to 10 data files created previously in this session are recorded at the bottom of the screen for your convenience.

Help messages in response to error messages:

(1) could not open file:

The file which you specified was not found. A typing error is the most likely problem, or the file is not in the current directory.

(2) duplicate file names:

This message indicates that a file name matches one in the local directory, or one previously set in this session, or that you have not pressed ENTER at each of the file names to complete the check of file names.

If you have copied an existing data file, the "new" file names are the ones that appeared in the existing data file.

Files should generally have different names. For example, consecutive SUBSTRAT runs with the same plot file names will save only the plot file from the last run (which will have replaced the previous plot files). Use identical names if you definitely want to replace existing files, including data files.

You may use a duplicate file name by responding 'Y' to the question about writing over the previous file.

Notes:

An entry for the previous data file causes its data to be copied.

The new data file will be created when "save this data file" is executed at the main menu. This save adds the new data, list and plot file names to the list displayed at the bottom of this screen.

There should be no duplicate file names. That would cause files to be overwritten during simulation. The program checks for duplicates.

The simulation title is echoed in the output files.

Note that upon entering the "Title for this simulation," the cursor jumps back to the first box and blanks it out. This is done only so that if the user has changed his mind (or an error has been made), new (or corrected) entries can be made immediately. If there has been no error, then simply press ESC.

Screen 3:

```
==========================================================
  Geometric description:              press ESC when done;  press F1 for help.

Fabric thickness:  [          ] mm

Width of air gap:  [          ] mm

X-coordinate data:
            Number of grid points:  [          ]      Rx = 1.xxx
         Total length of substrate:  [          ] mm
     Size of constant length cells:  [          ] mm
   Number of constant length cells:  [          ]

Y-coordinate data:
            Number of grid points:  [          ]      Ry = 1.xxx
          Half-width of substrate:  [          ] mm
      Size of constant width cells:  [          ] mm
    Number of constant width cells:  [          ]

Z-coordinate data:
            Number of grid points:  [          ]      Rz = 1.xxx
          Total depth of substrate:  [          ] mm
      Size of constant depth cells:  [          ] mm
    Number of constant depth cells:  [          ]
                                                  cells: xxxxx

==========================================================
```

General help message:

> The substrate consists of a thin fabric, padding, and possibly an air gap between them. An air gap width of 0.0 indicates no gap.
>
> The X direction is along the cigarette; the Y direction is along the fabric; the Z direction is into the padding.
>
> A variable grid is used. It consists of several constant width cells near the point of peak incident heat flux followed by increasingly larger cells out to the boundaries of the substrate. For example:
>
> ```
> |  |  |  |  |  |  |    |     |     |      |       |
> Y=0                                              Y=width
> ```
>
> Each variable width cell is R times longer than the preceding cell. Simulation is most accurate when R is only slightly greater than one. A value of R less than about 1.25 should be sufficiently accurate. Simulation will generally involve a trade-off of accuracy and run time.
>
> The fabric thickness and the depth of the constant depth cells are related: the fabric/padding boundary must be halfway between two cells. Therefore, the fabric thickness must be 0.5, or 1.5, or 2.5, etc., times the depth of the constant depth cells.

Other help messages:

> For the X-axis the following conditions should apply:
> $4 * NCX < NX$ and $(NX - 1) * DX0 <= XW$
> where NX = number of grid points, XW = total length of substrate, DX0 = size of const length cells, & NCX = number of const length cells.
>
> For the Y-axis the following conditions should apply:

```
    2 * NCY < NY   and   (NY - 1) * DY0 <= YW
where NY = number of grid points, 2YW = total width of substrate,
DY0 = size of const width cells, & NCY = number of const width cells.
Because of the assumed bilateral symmetry of the flux, it is only necesary
to make calculations between y = 0 and y = YW (half the width).  The number
of constant-width cells is that in the half-width section.

For the Z-axis the following conditions should apply:
    2 * NCZ < NZ   and   (NZ - 1) * DZ0 <= ZW
where NZ = number of grid points, ZW = total depth of substrate,
DZ0 = size of const depth cells, & NCZ = number of const depth cells.

The fabric thickness and the depth of the constant depth cells are
related:  the fabric/padding boundary must be halfway between two cells.
Therefore, the fabric thickness must be 0.5 or 1.5 or 2.5, etc., times
the depth of the constant depth cells, or the constant depth cells must
be 2 or 2/3 or 2/5, etc. times the thickness of the fabric.

The boundary between the fabric and padding must be within the region
of constant depth cells.
```

Notes:

"Rx", "Ry", and "Rz" are the geometric progression rates. The sample problems have a relatively high value in the Z direction. Tests have indicated this is satisfactory because the low conductivity of the padding permits less heat transfer in this direction.

"cells:" gives the total number of cells used to model the substrate. It equals NX × NY × NZ. This value is critical to the total memory required for a simulation.

The following figure illustrates the substrate coordinate system and the variable grid:

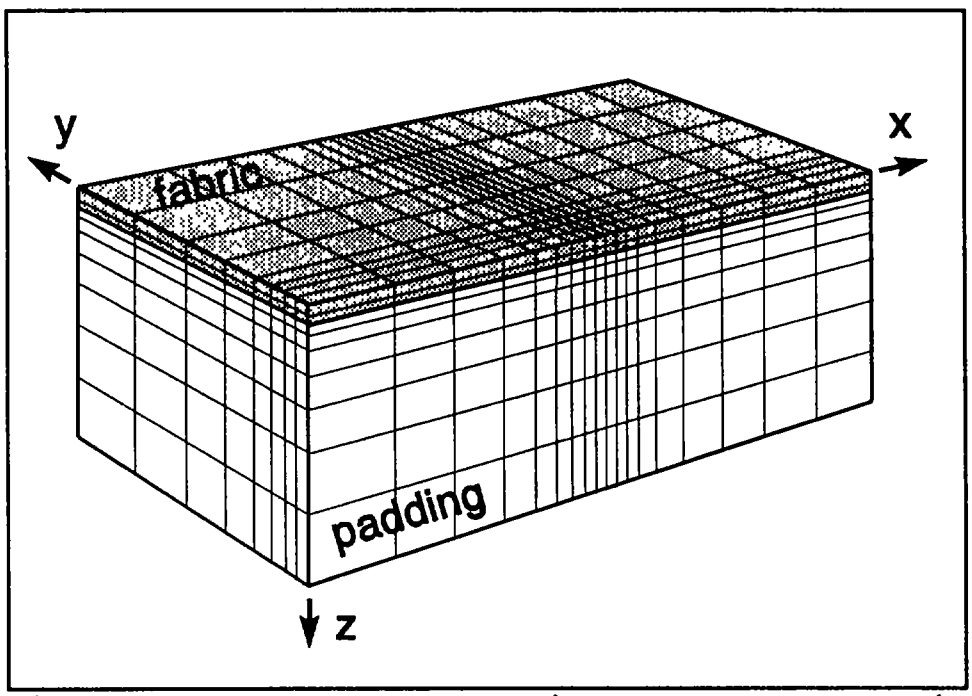


Figure B-2. Substrate Coordinate System and Variable Grid

Screen 4:

```
==========================================================
  Fabric Properties:                  press ESC when done;  press F1 for help.

Emittance:                Maximum temperature:              °C

  #        T [°C]          K [W/m K]          C [kJ/kg K]
  1
  2
  3
  4
  5
  6
  7
  8
  9
 10

Densities: ( kg/m3 )
    Virgin material:              char:              ash:

Reactions:
  #          A              n1              n2              Ta              Hc
  1
  2
  3

==========================================================
```

General help message:

Emittance is used in computing radiant heat loss from the fabric to ambient and radiant heat transfer across the air gap.

The simulation stops when the temperature of any fabric cell reaches the prescribed maximum temperature.

Thermal conductivity (K) and heat capacity (C) can be specified at up to 10 temperatures. SUBSTRAT uses a cubic spline curve fit for K and C. As fabric mass is lost by pyrolysis, K is also reduced in proportion to the current density. Values are required at least two temperatures even if K and C are constant.

A two-stage, three-reaction pyrolysis model is used: the virgin material is converted to char in stage 1 and then to ash. The char density is the value for completely converting the virgin material to char with no conversion to ash. The ash density is what's left after total pyrolysis.

The pyrolysis equations are of the form:

$$R = A * Dm^{n1} * Cx^{n2} * \exp(Ta/T) \quad \text{and} \quad Q = R * Hc$$

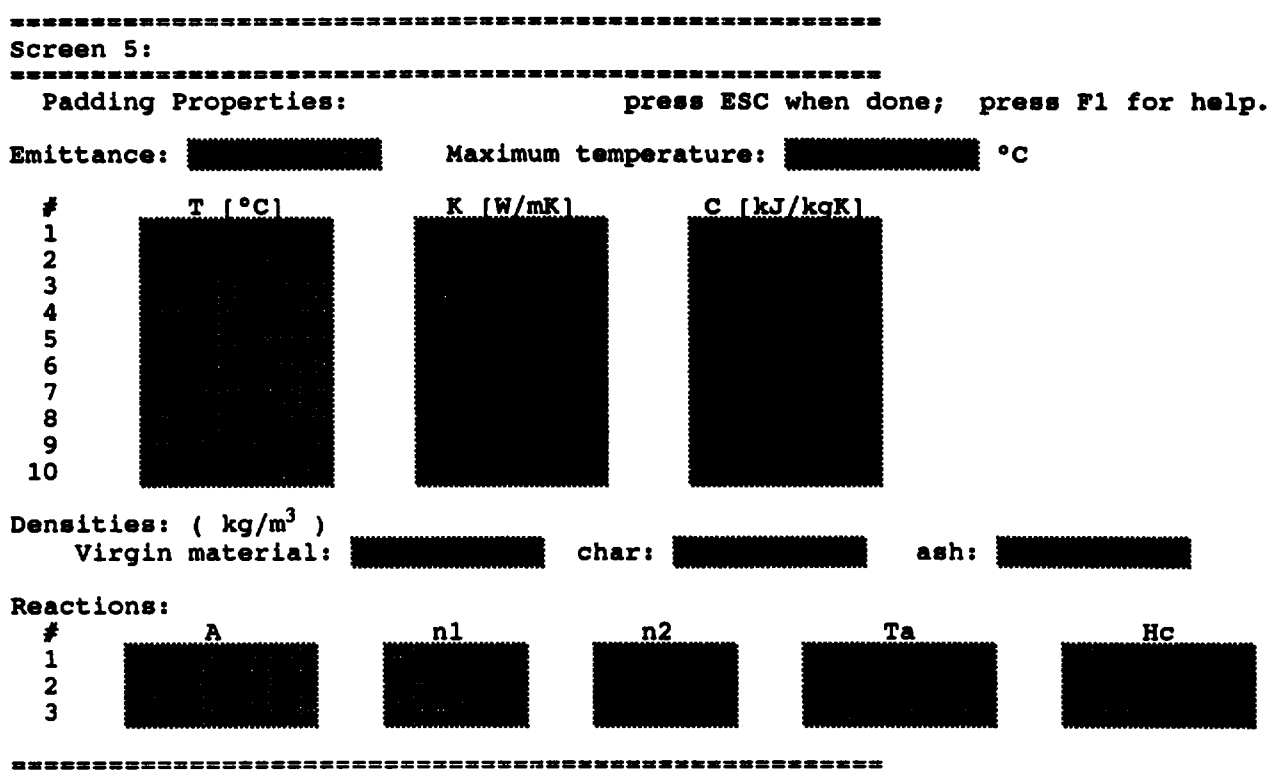
where

- R = rate of pyrolysis
- A = reaction coefficient [1/min]
- Dm = density of material (virgin or char)
- n1 = related exponent
- Cx = oxygen concentration
- n2 = related exponent
- Ta = activation temperature [K]
- T = current cell temperature [K]
- Hc = heat of pyrolysis [kJ/kg]

```
The first reaction is thermal degradation (n2 = 0 and Hc < 0) of virgin
material.  The second reaction is oxidation of the virgin material.
These two reactions produce char.  The third reaction is oxidation
of the char to produce ash.
```

Help message in response to error message:

```
Temperatures must be given in increasing order.
The lowest temperature should be several degrees less than any
possible substrate temperature.  The highest temperature should
be several degrees higher than the maximum temperature.
```



Padding help messages are similar to fabric messages.

Screen 6:

```
=====================================================
  Boundary Conditions:                press ESC when done;  press F1 for help.

At X=0, X=Xmax, Y=Ymax, Z=Zmax: (▒) adiabatic
                                (▒) constant temperature

 Initial substrate temperature: ▒▒▒▒▒▒▒▒▒▒ °C

           Ambient temperature: ▒▒▒▒▒▒▒▒▒▒ °C

          Oxygen mass fraction: ▒▒▒▒▒▒▒▒▒▒

Heat transfer coefficients:
                 Quiescent air: ▒▒▒▒▒▒▒▒▒▒ W/m2K
                 Impinging air: ▒▒▒▒▒▒▒▒▒▒ W/m2K

Moving heat flux pattern from the cigarette:
                Peak heat flux: ▒▒▒▒▒▒▒▒▒▒ kW/m2
    Initial X position of peak: ▒▒▒▒▒▒▒▒▒▒ mm
                  +X velocity: ▒▒▒▒▒▒▒▒▒▒ mm/min
     ±Y standard deviation (A): ▒▒▒▒▒▒▒▒▒▒ mm
     +X standard deviation (B): ▒▒▒▒▒▒▒▒▒▒ mm
     -X standard deviation (C): ▒▒▒▒▒▒▒▒▒▒ mm

=====================================================
```

General help message:

Select the condition of the outer boundaries (X=0, X=length, Y=width, Z=depth) by pressing ENTER in the appropriate place.

The incident heat flux from the cigarette is represented by a moving flux distribution on the surface of the substrate. This distribution has the shape of non-symmetric Gaussian curve which is described by six parameters:

(1) the X coordinate at the peak of the curve at the start of the simulation { the initial position of the peak is (Xo, 0, 0) },
(2) the speed, S, at which the peak moves along the X axis { the position P of the peak at time t is (Xo+S*t, 0, 0) },
(3) the maximum heat flux at the peak { at position (P, 0, 0) },
(4) the width of the curve in the Y direction { at position (P, ±A, 0), the heat flux is 0.37 times the flux at the peak },
(5) the width of the curve in front of the peak { at position (P+B, 0, 0), the heat flux is 0.37 times the flux at the peak }, and
(6) the width of the curve behind the peak { at position (P-C, 0, 0), the heat flux is 0.37 times the flux at the peak }.

Screen 7:

```
=======================================================
  Simulation Control:                press ESC when done;  press F1 for help.

              Maximum time step: [          ] s

     Maximum temperature change: [          ] °C

          Total simulation time: [          ] s

                 Plot times (s):
                               1 [          ] s
                               2             s
                               3             s
                               4             s
                               5             s
                               6             s
                               7             s
                               8             s
                               9             s
                              10             s

=======================================================
```

General help message:

SUBSTRAT uses a variable time step which is chosen so as not to exceed the maximum time step given and so that the maximum temperature change in any cell is not greater than the maximum given. This allows the program to run quickly when the temperatures are not changing rapidly. Smaller values for these two parameters will lead to more accurate simulations at the cost of longer execution times.

The simulation will stop at the total simulation time unless it has already stopped by exceeding a maximum fabric or padding temperature.

Plot times are entered in increasing order. When the simulation reaches a plot time, substrate temperatures are copied to the plot file. Leave later positions blank if you do not want to use all 10 times. A plot is automatically written when the simulation stops. The last plot time should be greater than the simulation time to satisfy a requirement in the SUBSTRAT program.

Screen 8:

```
=====================================================

Save this data file? (y/n) ▌

display any error message(s).

=====================================================
```

General help message:

> If you entered this area accidentally and are not ready to stop preparing the current data file, respond "N" to this question. This will return you to the main menu.

Help messages in response to error message:

(1) check data.

> Data in the indicated section may be incomplete or incorrect. Enter that section and check the data.

(2) temperature problem.

> The lowest temperature for fabric or padding thermal properties must be several degrees lower than either the initial or ambient temperature. You need to change (at least) one of those values.

(3) files limit.

> No more SUBSTRAT data files can be created in this session. You probably should exit TSDATA now. You may replace one of the data files already created.

Screen 9:

```
==================================================

Exit data preparation? (y/n) ▌                    (1)

display error messages, if applicable             (2)

prepare DOS batch file to run all cases (y/n)? ▌  (3)

==================================================
```

Help messages:

(1) initial message.

```
If you entered this area accidentally and are not ready to stop
preparing data files, answer "N" to this question.
```

(2) error messages.

```
This warning indicates that TSDATA may have data which you have not saved.
If you respond "Y" to the question about checking this data file, you
are returned to the main menu where you can check and then save the file.
If you respond "N", you will continue to exit the TSDATA program.
```

(3) batch file message.

```
A positive response will create a file RUN.BAT resembling:

SUBSTRAT <datafile.1
SUBSTRAT <datafile.2
SUBSTRAT <datafile.3
SUBSTRAT <datafile.4

This file can be used to run SUBSTRAT on computers using MS-DOS.
```

Notes:

Message (1) appears automatically.

Error message (2) may appear.

Message (3) appears after a Y to question (1).

TSPLOT

The TSPLOT program will display contour plots of substrate temperatures on the screen. It is an interactive program which uses the plot file from SUBSTRAT as input. Because it is interactive and graphic, it uses certain commands which restrict its operation to IBM PC compatible computers. A plot file contains the substrate surface (Z = 0 plane) and center-plane (Y = 0 plane, see Figure B-2) temperatures at various times set in the input data file.

Three special files are used by TSPLOT. The CHRSET.VGA file contains the bit patterns for the graphic display. This file is required. The help file, TSPLOT.HLP, contains the text of the interactive help messages. Help is activated by pressing the F1 function key. If the help file is not available in the current working directory, no interactive help will be available. The configuration file, TSPLOT.CFG, sets the colors of the display. The file included on the distribution diskette assumes that a standard VGA monitor is being used. If the configuration is not in the current working directory, a set of default colors will be used. These colors may not provide satisfactory contour plots. A new configuration file can be made by using the MAKECFGG program. See the README file for instructions.

The operation of TSPLOT is briefly explained on the following page. Because the screen interface is similar to TSDATA and relatively few options are available, a detailed description should not be necessary. After reading this description, try using TSPLOT with the sample plot files. Begin the program by typing TSPLOT. Abort the program by pressing CTRL and C.

Sample Run

At this point the following files should be available in the current working directory: TSPLOT.EXE, CHRSET.VGA, TSPLOT.HLP, TSPLOT.CFG, TEST1.PLT, and TEST2.PLT. If they are not, use the INSTALL procedure. If you ran TEST1 or TEST2 and aborted before completion, use INSTALL to replace the plot files with the original complete versions.

Type TSPLOT. Press ENTER until the main menu appears; press ENTER again to get the plot file. Enter TEST1.PLT as the name of the plot file. After returning to the main menu, press ENTER to display the next plot. Note that this plot is for t = 1 second, and the pattern is rather small. After viewing this plot, press any key to return to the main menu. Move (use cursor keys) to the set display parameters option and press ENTER. Change the Xmin value from "0" to "10", press ENTER, change Xmax from "60" to "50", press ENTER, and press ESC. Now press ENTER to display the prior plot. The limits of the display have been changed, and the heated area appears larger. Press ENTER to alternate between the main menu and the next plot. In the later plots note the discontinuity in the profiles in the padding caused by the air gap. After the last plot you will arrive at the exit option. Instead of exiting, move to the get plot file option, press ENTER, and enter TEST2.PLT as the name of the plot file. Return to the main menu and display the next plot which is the first plot from TEST2.PLT. Note that the limits of the X-axis have not been reset for this new plot. As you continue by displaying successive plots note how the point of peak temperature is moving along the X-axis. When you reach the exit option, press ENTER, and respond Y to exit the program.

TSPLOT Main Menu

This is the main menu screen. It directs you to the different options.

```
=====================================================

TSPLOT program:

   ▌  Get plot file

   ▌  Display next plot

   ▌  Redisplay

   ▌  Set display parameters

   ▌  Exit


Use cursor keys to move between menu selections.
Press ENTER to activate the menu selection at the X.
Press ESC to return from a selection.  Press F1 for help.
=====================================================
```

The first option is "Get plot file". You must get a (enter the name of an existing) plot file before any plots can be displayed.

The plot file is read sequentially. You may display the data at the next plot time (option two), or you may redisplay the last plot shown (option three).

The graphic display consists of three parts: the temperature scale (in °C) to the right, the substrate surface temperature contours in the upper left of the screen, and the center-plane temperatures in the lower left. In other words, the temperature contours for the $Z=0$ and $Y=0$ planes are displayed together as if they have been folded along the X-axis so as to both be flat on the screen. The display also shows the time and the X-axis with coordinates at the left and right edges and tic marks every millimeter.

The fourth option lets you reset the display parameters. You may set the coordinates of the left and right edges of the display. These values change both the position and the scale of the regions being displayed thus enlarging or shrinking the plot. The initial limits of the X-axis are for the entire region simulated. You may also change the temperature contours which are initially set at 25 °C intervals. Changes must be made so that each temperature is always less than the one above and more than the one below. You will then probably want to redisplay the last plot.

After displaying one set of plots, you may get a new plot file without exiting this program. This is the only way to go back in time on the plot file: get the plot file again and start at the beginning.

When you reach the end of the plot file, TSPLOT automatically takes you to the exit option.

APPENDIX C

ANALYSIS OF NUMERICAL ERRORS PRODUCED BY A RUNAWAY REACTION RATE

We have made an effort to make a fine grid in the region where the fluxes and flux gradients are high. Nevertheless, when the reaction rates become very high, the gradients will become so steep that the approximation of constant temperature and constant reaction rate within a cell becomes questionable. In this appendix, we examine the magnitude of the errors thus committed by discretization. This analysis can also serve to make appropriate corrections in the program; this has not been done here, partly because the analysis should first be generalized to the non-symmetric case. (See the assumptions made just below equation (C1).

Consider the heat diffusion equation, equation (95). Suppose we have the (correct) temperature distribution T(x,y,z,t), with a peak at (x_o,y_o,z_o); the reaction rate is given by an expression such as equations (108) or (110). Let us simplify this form and assume that

$$R_p = R_\infty \exp(-T_A/T(r)) \tag{C1}$$

where all the preexponential factors are lumped together as the factor R_∞ and $\mathbf{r} = (x,y,z)$ is the position vector. Consider the terms in equation (12); we simplify the analysis by assuming that the temperature peak lies at the cell center (*i.e.*, at $\mathbf{r}_o$), and that the distribution is symmetric fore-and-aft. Then, since calculating R_p in that cell means calculating it at the center, and therefore the peak, that means we **overestimate** the reaction rate, since the rate falls off at the faces of the cell.

Symmetry implies that

$$\nabla\cdot(\kappa\nabla T) \approx \kappa\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right) \approx 3\kappa\frac{\partial^2 T}{\partial x^2} \tag{C2}$$

A second-order approximation to this derivative is

$$\nabla\cdot(\kappa\nabla T) \approx 3\kappa\frac{T_{i-1}-2T_i+T_{i+1}}{(\Delta x)^2} \tag{C3}$$

Because of the assumed symmetry, $T_{i-1} = T_{i+1}$, so that we finally have

$$\nabla\cdot(\kappa\nabla T) \approx 6\kappa\frac{T_{i-1}-T_i}{(\Delta x)^2} \tag{C4}$$

Inserting this into equation (12), that equation becomes

$$\rho c\frac{\Delta T_{i,j,k}}{\Delta t} \approx H_c R_p(r) - 2\kappa\frac{T_{i,j,k}-T_{i-1,j,k}}{(\Delta x)^2} - \ldots \tag{C5}$$

minus similar terms in Δy and Δz (as indicated by the ellipsis). Suppose further, for the sake of simplicity, that the temperature profile is Gaussian:

$$\theta(x,y,x,t) = \theta_m \exp\left[-\frac{(x-x_o)^2+(y-y_o)^2+(z-z_o)^2}{\sigma^2}\right] \tag{C6}$$

where $\theta = T - T_a$

and T_a = ambient (reference) temperature.

If we redefine the origin to be at (x_o,y_o,z_o), then

$$\theta(x,y,x,t) = \theta_m \exp(-r^2/\sigma^2) \tag{C7}$$

where $r^2 = x^2 + y^2 + z^2$.

Then if $x^2/\sigma^2 << 1$ everywhere within the cell, we can expand (C7). At the center of the cell,

$$\theta_i = \theta(r_0) = \theta_{max} \equiv \theta_m \tag{C8}$$

and

$$\theta_{i-1} = \theta_m \exp[-(\Delta x/\sigma)^2] \approx \theta_m[1-(\Delta x/\sigma)^2]. \tag{C9}$$

Define $\xi = (\Delta x/\sigma)^2$. Then

$$T_i - T_{i-1} = \theta_i - \theta_{i-1} \approx \theta_m \xi \tag{C10}$$

so that equation (C5) becomes

$$\rho c \frac{\Delta\theta}{\Delta t} \approx H_c R_p - \frac{2\kappa}{(\Delta x)^2}\left[\theta_m \frac{(\Delta x)^2}{\sigma^2}\right] - \ldots \tag{C11}$$

Assuming three-fold symmetry, the other two terms in (C11) are the same, and thus

$$\rho c \frac{\Delta\theta}{\Delta t} \approx H_c R_p - 6\kappa \frac{\theta_m}{\sigma^2} \tag{C12}$$

Note that the dependence on Δx has dropped out. Indeed, the last term is the exact diffusive loss rate, resulting from the distribution (C7).

Now let us examine the magnitude of the error made by using a <u>finite</u> value of Δx. From equation (C7),

$$\Delta\theta \equiv \theta_i - \theta_{i-1} = \theta_m[1 - \exp(-\xi)] \tag{C13}$$

Then expanding to the next higher order than was done in (C9),

$$\Delta\theta \approx \theta_m \xi(1 - \xi/2) \tag{C14}$$

and the second term in (C5) becomes

$$\frac{2\kappa\Delta\theta}{(\Delta x)^2} \approx \frac{2\kappa\theta_m}{\sigma^2}(1 - \xi/2) \tag{C15}$$

Thus the numerical calculation <u>underestimates</u> the loss rate. Since the correct heat loss rate is

$$\mathcal{L} = 6\kappa\theta_m/\sigma^2 \tag{C16}$$

and we have

$$L = \frac{6\kappa\theta_m}{(\Delta x)^2}[1-\exp(\xi)], \tag{C17}$$

we multiply L by the ratio

$$F = \frac{\xi}{[1-\exp(-\xi)]} \approx \frac{1}{1-\xi/2} \tag{C18}$$

in order to get the correct loss rate $\mathcal{L}$.

As the temperature "runs away," the distribution becomes increasingly peaked, and σ declines. As it does so, ξ increases, and so, therefore, does F; this helps to slow down, or moderate, the runaway. ξ is readily found to be

$$\xi = \ln(\theta_l/\theta_{l-1}) \tag{C21}$$

Next, consider the source term in equations (C5) and (C12), again. Define

$$f(x,y,z) = \exp[-T_A/T(x,y,z)] \tag{C22}$$

The correct power output in the elemental volume ΔV is, from equation (C1),

$$R_p \Delta V = 8R_m \int_0^{\Delta x/2} dx \int_0^{\Delta y/2} dy \int_0^{\Delta z/2} f(x,y,z)\, dz \tag{C21}$$

where we have again translated (x_o,y_o,z_o) to be at the origin, and have taken advantage of the 3-fold reflection symmetry. Again assume equation (C7) to hold. If $\xi << 1$, then within the cell we can Taylor expand and write

$$f(x,y,z) = \exp(-T_A/T_m) + x\left(\frac{\partial f}{\partial x}\right)_0 + \frac{x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_0 + \ldots \tag{C22}$$

plus similar terms in y and z. Since the peak is at the origin,

$$\left(\frac{\partial f}{\partial x}\right)_0 = \left(\frac{\partial f}{\partial y}\right)_0 = \left(\frac{\partial f}{\partial z}\right)_0 = 0, \tag{C23}$$

and dropping the higher-order terms,

$$f(x,y,z) \approx \exp(-T_A/T_m) + \frac{x^2}{2}\left(\frac{\partial^2 f}{\partial x^2}\right)_0 + \frac{y^2}{2}\left(\frac{\partial^2 f}{\partial y^2}\right)_0 + \frac{z^2}{2}\left(\frac{\partial^2 f}{\partial z^2}\right)_0 \tag{C24}$$

We find that

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_0 = -\frac{2T_A}{T_m^2}\frac{\theta_m}{\sigma^2}\exp(-T_A/T_m) \tag{C25}$$

Thus

$$f(x,y,z) \approx \exp(-T_A/T_m)\left[1 - \frac{T_A\theta_m}{T_m^2\sigma^2}r^2\right] \tag{C26}$$

and integration over the cell yields

$$R_p \Delta V \approx (\Delta x)^3 R_\infty f(0) \left[1 - \frac{T_A \theta_m}{4 T_m^2} \xi^2 \right] \tag{C27}$$

This is only valid for $\Delta x/\sigma << 1$. In that limit, however, (C26) is well approximated by

$$\bar{R}_p \approx R_\infty \exp(-T_A/T_m) \exp\left[-\frac{T_A \theta_m}{4 T_m^2} \xi^2 \right] \tag{C28}$$

which is a reasonable first approximation to the correct integral, even when $\Delta x/\sigma$ is not very small.

The numerical approximation is

$$R_p = R_p(r_0) \approx R_\infty \exp(-T_A/T_m) \tag{C29}$$

Thus (C28) shows that we must multiply this approximation by $\exp\left[-\frac{T_A \theta_m}{4 T_m^2} \xi^2 \right]$ in order to get a still better approximation to the source term.

APPENDIX D

ANALYSIS OF IGNITION EXPERIMENT

Among the things we wish to extract from this experiment is the heat transfer coefficient to the surface, h. Figure D-1 shows the total heating fluxes to the gauge, as a function of the power input, with and without a purging flow of nitrogen. Consider the 18 kW/m^2 case. **Without** the purge flow, the heating flux is purely radiative, and is measured to be $\phi_{rad}^* \approx 10$ kW/m^2. With the purge flow on, there is considerable convective heating of the surface as well, and the measured flux is $\phi_{tot} \approx 18$ kW/m^2, suggesting that the convective flux is $\phi_{con} = \phi_{tot} - \phi_{rad} = 18 - 10 = 8$ kW/m^2. However, when the purge flow is turned on, it cools off the heating element somewhat. How much it does so, however, is unknown. Assume that the purge flow reduces the hot-surface temperature such that ϕ_{rad} is reduced to some fraction F of the original. Then

$$\phi_{rad} \approx 10F \tag{D1}$$

and

$$\phi_{con} \approx 18 - 10F \tag{D2}$$

At the point P, on the heater axis but at the surface being heated (5.4 mm below), the heater subtends a solid angle such that the view factor is Ω. Hence the impinging radiative flux is

$$\phi_{rad} = \Omega \epsilon_d \sigma T_d^4 + (1-\Omega)\sigma T_a^4 \tag{D3}$$

where ϵ_d is the emissivity of the device surface. For the particular case that was carried out, the standoff distance is 5.4 mm, while the diameter of the glowing filament is 13 mm. According to Siegel and Howell (1981), Appendix C, the view factor for a disk of radius R, at a point a distance H along the axis normal to the disk, is

$$\Omega = \left(\frac{H^2}{R^2} + 1\right)^{-1} \tag{D4}$$

Hence $\Omega = 0.592$. We also assume that $T_a = 25$ °C ≈ 298 K, and that $\epsilon_d \approx 0.85$. It follows from equations (D1) and (D3) that

$$T_d^4 = \frac{10F}{\Omega \epsilon_d \sigma} - \frac{(1-\Omega)T_a^4}{\Omega \epsilon_d} \tag{D5}$$

If F = 1, this yields $T_d \approx 493$ °C, while F = 0.9 yields $T_d = 472.5$ °C. The device surface cannot be much colder than 500 °C, since it is observed to glow red. If $T_d = 472.5$ °C, then $\phi_{rad} \cong 9$ kW/m^2.

We will assume that the factor F remains constant for all irradiations. Thus for the case $\phi_{tot} = 25$ kW/m^2, $\phi_{rad}^* \approx 16$ kW/m^2, and equation (D5) implies that $T_d = 840.3$ K = 567.1 °C.

We proceed the same way for all four cases, and obtain the values in the first six columns of Table D-1 (with fluxes given in kW/m^2). Column 6, marked ϕ_c, is the convective flux, found as the difference between ϕ_{tot} and ϕ_{rad}. These values of ϕ_c are plotted vs ϕ_{tot} and a smooth curve passed through these points, including the point at the origin. That yields the smoothed convective fluxes ϕ_c, given in column 7.

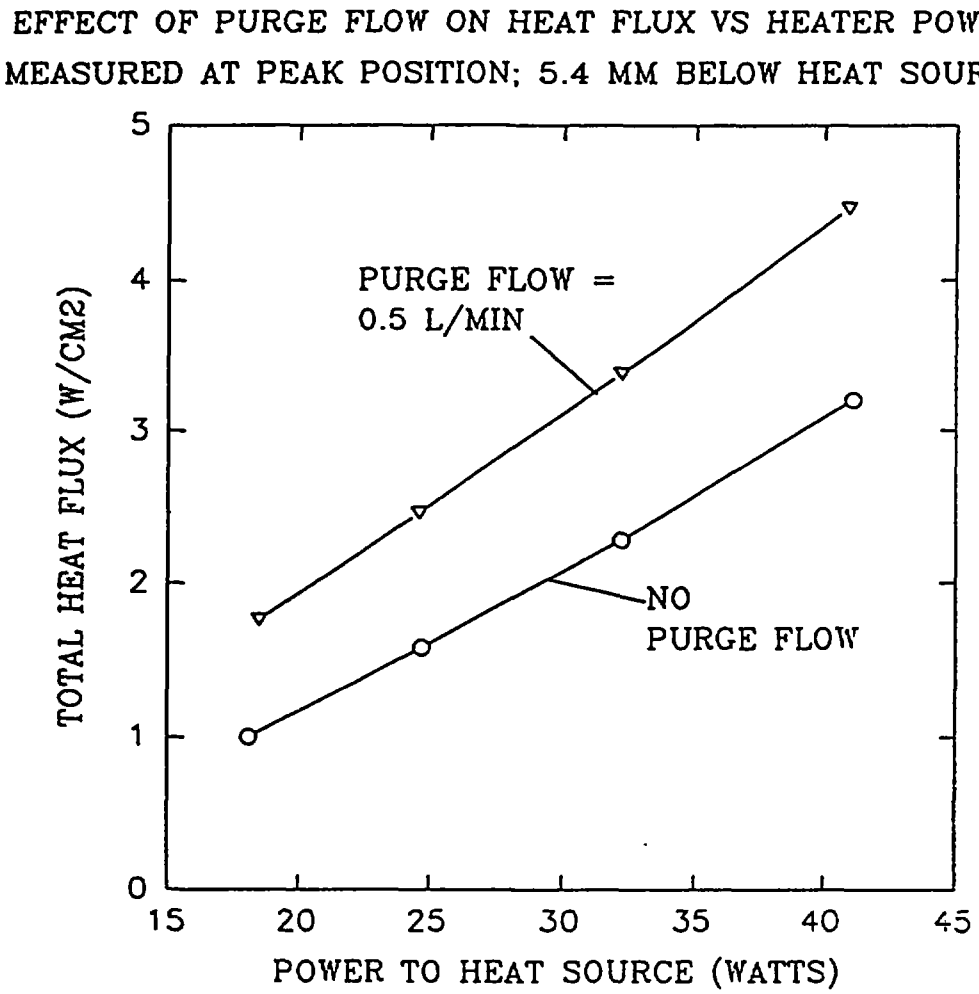


Figure D-1. Total heat flux impinging on gauge, with and without purge flow

Table D-1. Measured and Inferred Quantities From the Ignition Experiments

ϕ_{tot}	ϕ_{rad}/F	T_d(K)	T_d(°C)	ϕ_{rad}	ϕ_c	$\bar{\phi}_c$	hf	T_g(K)	h	f
18	10	745.7	472.5	9.0	9.0	8.9	19.67	698	22.0	0.893
25	16	840.3	567.1	14.4	10.6	10.7	19.56	760	22.9	0.854
34.5	23	921.0	647.8	20.7	13.2	13.0	20.71	837	23.9	0.865
44	32	1000.9	727.7	28.8	15.2	15.2	21.48	907	24.8	0.866

The convective flux can be written in the form

$$\phi_c = h(T_g - T_c) \tag{D6}$$

where T_g is the purge gas temperature, and T_c is the (cold) gauge temperature. In order to make progress we make one further plausible assumption: the purging gas takes up a (constant) fraction of the total energy delivered to the device. We can express this as

$$\theta_g = f\theta_g \tag{D7}$$

where Θ is the temperature referred to the gauge temperature:

$$\theta_i \equiv T_i - T_c \ . \tag{D8}$$

Thus, equations (D6) and (D7) yield

$$\phi_c = h\theta_g = fh\theta_d \tag{D9}$$

Since we have T_d (column 4) and ϕ_c (column 7), we readily infer the factor fh from equation (D9). This is given as column 8.

Next, we must find the heat transfer coefficient h for stagnant flow. The purge air comes down, strikes the fabric, and must move away radially. This configuration is approximated by the standard problem of stagnant flow. The heat transfer coefficient for this case is given in Kakaç *et al.* (1987). Their equation (2.176) on page 2-59 gives the Nusselt number:

$$\left(\frac{Nu}{Pr^{0.4}\sqrt{Re}}\right)_w = 0.767\left(\frac{\mu_e \rho_e}{\mu_w \rho_w}\right)^{0.43} \tag{D10}$$

which was found by Cohen (1961). The subscripts w and e, above, stand for "wall" and "edge" (of the boundary layer), respectively. The second factor on the right-hand side is approximately one, in this case. The Reynolds number is

$$Re = \frac{u_\infty \ell_c}{\nu} \tag{D11}$$

where ℓ_c is the characteristic length. One might think that the characteristic length here is the diameter of the opening. In fact, however, Cohen (1961) gives **Re** in the form

$$Re = \frac{du_\infty}{dx}\frac{\ell_c^2}{\nu} \tag{D12}$$

Since the (vertical) velocity goes from u_∞ to zero in the distance δ, we may write

$$\frac{du_\infty}{dx} \approx \frac{u_\infty}{\delta}; \tag{D13}$$

then equation (D12) indicates that the proper ℓ_c to use here is δ. u_∞ is readily inferred from the volumetric flow, dV/dt = 0.5 l/min. Thus

$$\dot{V} = \frac{\pi r^2 u_\infty \rho_g}{\rho_a} = \frac{\pi d^2 u_\infty T_a}{4T_g} \tag{D14}$$

which yields

$$u_\infty = 6.28(T_g/T_a) \qquad \text{cm/sec} \tag{D15}$$

The Nusselt number is given by

$$Nu = \frac{h\delta}{\kappa} \tag{D16}$$

where δ is the stand-off distance between the heater and the substrate, 5.4 mm. Combining these, and knowing $\kappa(T)$ and $\nu(T)$ for air, we obtain $h(T_g)$, as shown in Figure D-2. Note that this is independent of any estimates of F, the radiative and convective fluxes, etc.

We now proceed as follows: we guess a value for T_g; corresponding to this we have $h(T_g)$, and we then find $h(T_g)(T_g - T_a) \equiv \phi^*$. We must do this until $\phi^* = \bar{\phi}_c$, as given in Table D-1. This procedure converges quite rapidly, and we find the values of T_g and $h(T_g)$ shown in columns 9 and 10. Finally, dividing hf by the now-known values of h, we obtain the values of f shown in column 11. There are two things to be noted about f: it is almost as large as it can get (*i.e.*, close to unity), and it is approximately independent of ϕ_{tot}.

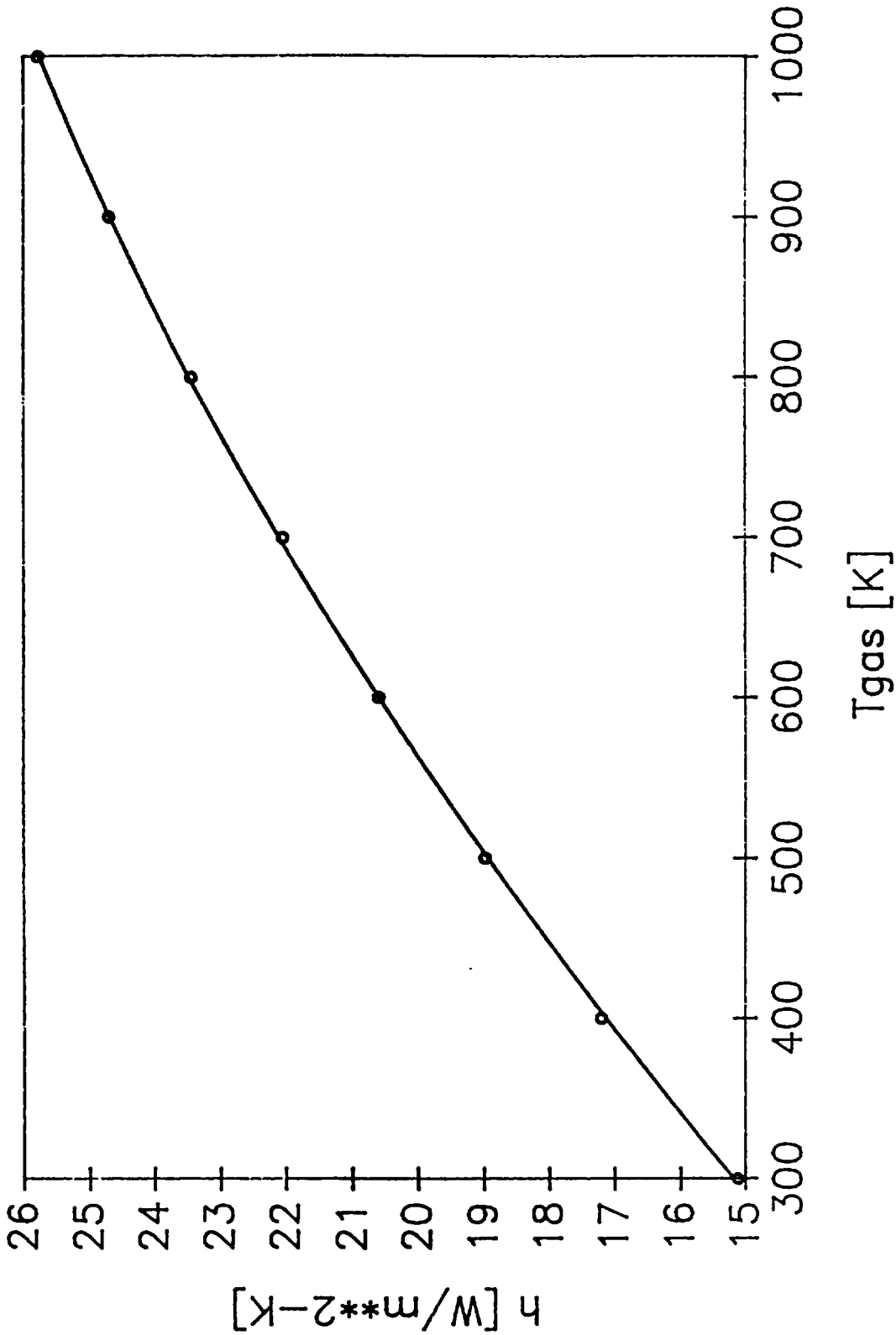


Figure D-2. Calculated heat transfer coefficient, as a function of the temperature T_g of the impinging purge gas jet

APPENDIX E

THERMOPHYSICAL DATA FOR COTTON

The fabric is a weave of cotton fibers. Cotton itself is a flexible, hollow tube of cellulose; the central channel is called the lumen, and occupies a fraction η of the total volume. Thus we would expect that the density of cotton is about

$$\rho(\text{cotton}) = (1-\eta)\rho_s,$$

where ρ_s is the density of the solid (largely α-cellulose). Measurements yield $\eta = 0.2 - 0.4$. However, Brandrup and Immergut (1989) gives the following data on page V-122. (The references given there to the original authors are omitted here for brevity):

Material	Density (g/mℓ)
Cellulose I	1.582-1.630
Cellulose II	1.583-1.62
Cellulose III	1.61
Cotton	1.545-1.585

Thus, the density of cotton appears to be very nearly the same as that of the solid (cellulose) implying that $\eta \approx 0$. We will hereafter ignore the apparently small difference between α-cellulose and cotton, and take the (mean) density to be $\rho_s = 1.565 \pm 0.02$ g/mℓ.

For many polymers, there is only a weak dependence of the thermal conductivity on T, between 100 and 300 K (see Siegel and Howell (1981) Figure 68). One can get an idea of the variability of the thermal conductivity of cotton and of cotton fabrics from Figures AA-AC, in Kakaç *et al.*

Measurements at NIST by J.R. Lawson (private communication) have shown that the density of #10 duck is $\rho \approx 0.6$ g/cm^3, that of #6 duck is 0.72 g/cm^3, and that of all the other cotton duck fabrics measured is

$$\rho_f \equiv \rho(\text{fabric}) = 0.62 \text{ g/cm}^3 = 620 \text{ kg/m}^3.$$

The "void fraction" of the fabric is Φ. With $\rho_s = 1.565$, $\rho_f = 0.62$, and with ρ_a = density of air at STP = 1.774×10^{-3} g/cm^3, the relationship

$$\rho_f = (1 - \Phi)\rho_s + \Phi\rho_a$$

yields $\Phi = 0.6045$.

Next, consider the specific heat. Again, the values given in Brandrup and Immergut (1989) are:

Material	Specific Heat (J/g K)
Cellulose	1.34
Cotton	1.22
	1.15-1.18 (0-34 °C)
	1.32 (0-100 °C)
	1.327-1.251
	1.273-1.35

Where the temperature range is not listed, it is assumed to be the ambient (20 or 25 °C). We will thus not be far wrong it we take $c_s = 1.3$ J/g-K,

where the subscript "s" stands for "solid" (cotton or α-cellulose). We expect that, just as was the case for density,

$$c_f \equiv c(\text{fabric}) = \Phi c_{air} + (1 - \Phi)c_s.$$

Hence

$$c_f \approx 1.122 \text{ J/g-K}, \qquad \text{at } T \approx 300 \text{ K}.$$

This author has not been able to find the **temperature dependence** $c_s(T)$; we will defer that question for the moment.

Finally, we come to the thermal conductivity, κ. This is a quantity which is notoriously difficult to obtain accurately. Figure E-1, from Childs *et al.* (1973), shows the large variations in thermal conductivity depending on measuring conditions. Many of the low values (nos. 5, 6, and 8, for example) were measured in a vacuum. Numbers 4 and 9, on the other hand, were similar specimens, measured in air at 25 °C. However, #9 had over three times the density of #4 and would therefore have been expected to have a substantially higher thermal conductivity.

We list here four sources for the thermal conductivity:

a. The apparently most consistent data from Childs *et al.* (1973): curves 1, 2, and 3, and point 7, give

$$\kappa \approx 0.0365 \text{ W/m K} \qquad \text{at } T = 306 \text{ K} = 33 \text{ °C}$$

b. We have the following data for cotton paper, from Brandrup and Immergut (1989):

T (°C)	κ (W/m K)
30	0.049
40	0.071
50	0.084
60	0.090

A curve-fit to these points, if extrapolated, would predict that κ vanishes at (and below) $T \approx 10$ °C, which is nonsense.

c. Touloukian *et al.* (1970) give:

T (°C)	κ (W/m K)
0	0.056
20	0.058
100	0.067

The density of the material for these measurements is listed as 81 kg/m^3; hence $\Phi = 0.9493$. Then equation (14) gives

$$\kappa = 0.03408\kappa_s + 0.9828\kappa_g \qquad \text{(E1)}$$

while the tabular data are reasonably well fitted by

$$\kappa(T) = 0.056 + 1.1\text{x}10^{-4}T, \quad \text{with T in °C} \qquad \text{(E2)}$$

We have $\kappa_{air}(25\ °C) = 0.02624$ W/m K; now if the data in the table are the conductivities for the light cotton/air mixture, then at 20 °C, with $\kappa_g = \kappa_{air}$, equation (E1) yields $\kappa_s = 0.945$, which is an unreasonably large value. According to Kunii (1961), the value for the gas-phase thermal conductivity to be used in equation (14) is 1.7 times what it is in the ambient. If we use $\kappa_{gas} = 1.7\text{x}0.02624 = 0.04461$, the resulting value of κ_s is $\kappa_s = 0.415$ W/m K, still very large. If, on the other hand, the listed values are for κ_a, then $\kappa_s = 0.058$ and $\kappa_g = \kappa_a$ imply that $\kappa = 0.0278$, while for $\kappa_g = 1.7\kappa_a$, $\kappa = 0.0458$. Thus none of the combinations is plausible.

d. Ohlemiller has made measurements of the thermal conductivity of the (#12) cotton duck; the apparatus only works properly when the sample is thermally thick, however. Therefore he carried out a series of measurements, with an increasing number of layers of the fabric. It was then possible to infer the asymptotic value which would be reached if the number of layers had been increased to a very large number: It was assumed that

$$\kappa(n) = \kappa_\infty[1 - \exp(-n\Theta)],$$

where Θ = dimensionless thickness of one layer, and n = number of layers. The data were:

n	κ
0	0
6	0.050
12	0.077
18	0.099

The Asymptotic value of the series at the left is 0.9. That is $\kappa_\infty = 0.13$ J/m K.

$\kappa = 0.13$ is about twice the value (0.056) found in the Handbook, as quoted in c., just above. Recall that for this fabric, the void fraction is 0.6045. With $\Phi = 0.6045$, equation (14) gives

$$\kappa = 0.28505\kappa_s + 0.84554\kappa_{gas}$$

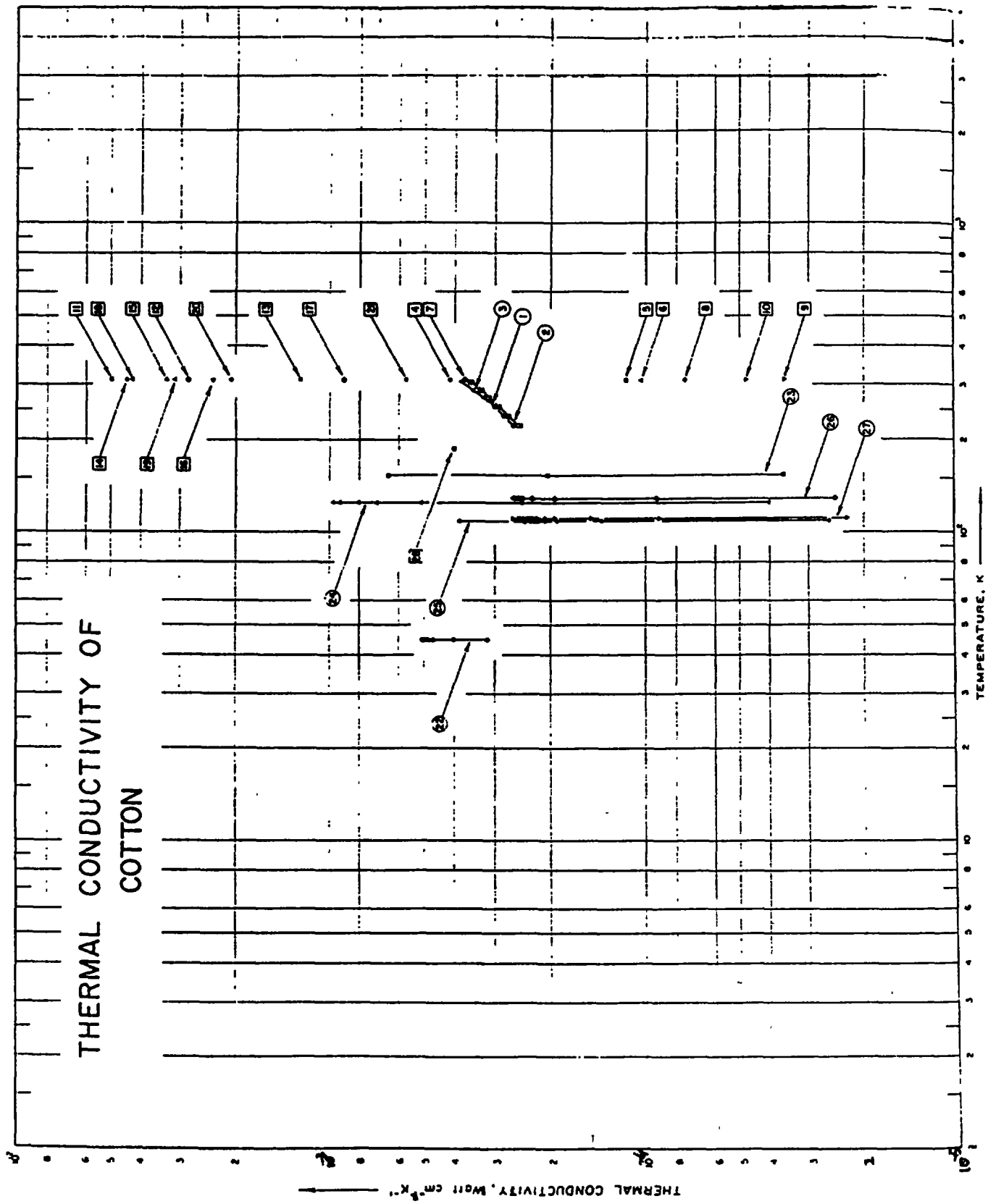


Figure E-1. Thermal conductivity of cotton as a function of temperature, as measured by different workers

If we use $\kappa_{gas} = \kappa_{air}$, we would then infer that $\kappa_s = 0.378$, which is an order of magnitude greater than the earlier estimates. If we use $\kappa_{gas} = 1.7\kappa_{air}$, then $\kappa = 0.13$ implies $\kappa_s = 0.324$, only a little smaller. The latter value is not too different from the 0.415 found in source c., above.

We thus take $\kappa_s \equiv \kappa_s(T_a = 25\ °C) \approx 0.324$ W/m K

and $\kappa(T_a) \approx 0.13$ W/m K

Assuming that the temperature dependence is like that given by eqaution (E2), we find that

$$\kappa(T) = 0.125 + 2.457\text{x}10^{-4}\,T, \tag{E3}$$

with T in °C. Alternatively, we might use equation (14) in its more general form, that is, including the temperature dependence

$$\kappa(T) = 0.28505\kappa_s(T) + 0.84554(1.7)\kappa_{air}(T) \tag{E4}$$

For air, $\kappa(T)$ is given by equation (52) in Childs *et al.* For the solid, a reasonable assumption is that the conductivity is proportional to the absolute temperature, and that it is also proportional to the density. Thus $\kappa_s(T)$ is given by

$$\kappa_s(T) = \kappa_s(T_a)\,\rho T/\rho_a T_a \cong 0.3237\,\rho T/\rho_a T_a \tag{E5}$$

We now turn to the question of the **temperature dependence** of c_f. For a number of materials, the thermal diffusivity is relatively insensitive to T. This is, in particular, the case for **wood** (see Parker 1985, 1987) which consists, to a significant extent, of cellulose and related compounds. If we assume that to be the case for cotton, then we could write

$$\kappa(T) = \alpha\rho c(T); \tag{E6}$$

c(T) is generally much easier to measure than $\kappa(T)$, and this would be a relatively good way to obtain $\kappa(T)$; the irony is that we do not have c(T) for cotton or cellulose.

If we take $\kappa_f = 0.13$ for the fabric at ambient temperature, we now find that

$$\alpha \equiv \kappa/\rho c \approx 0.13/(620)(1122) = 1.87\text{x}10^{-7}\ \text{m}^2/\text{s}$$

We therefore have, finally,

$$c(T) = \kappa/\rho\alpha \approx \kappa(T)/620(1.87\text{x}10^{-7}) = 8630\kappa(T)\ \text{J/kg K}$$

where $\kappa(T)$ is given by equation (E3), or by (E4), if preferred.

APPENDIX F

HEAT TRANSFER COEFFICIENT IN THE PRESENCE OF A SUBSTRATE

It is first assumed that there is no x-dependence of cigarette or substrate temperature. Now refer to Figure F-1; we need to know how the losses from point P on the cigarette to the substrate surface depend on θ. For the convective losses, it is clear that for small θ, they will depend on the substrate temperature in the neighborhood of P. In fact, for each angle θ, we may identify a mean value y associated with it. For $\theta = \pi/2$, buoyant convection carries gases directly away from the surface, so that the associated value of y is $y = \infty$, and the convective losses are precisely as they would be for the free cigarette. In general, we may write

$$\phi_c(\theta) = h_s(y)\,[T_c(\theta) - T_s(y)] \tag{F1}$$

where we have explicitly assumed that T_c may vary around the circumference.

It is now necessary to integrate this around the circumference, to obtain the total (convective) energy loss rate (per unit length). An expression was found relating θ and y; in order to enable explicit calculations to be carried out, it was assumed that $T_s(y)$ can be approximated by the expression

$$T_s(y) \sim T_o + \Delta T\, e^{-y^2/s^2} \tag{F2}$$

with

$$\Delta T \equiv T_s(y=0) - T_o\,. \tag{F3}$$

The integration is carried out in two steps. First, suppose that T_c does not vary around the circumference; the flux can then be integrated, with the result

$$\begin{aligned}\int_0^{\pi} \phi_c(\theta)\,d\theta \approx\ & \pi\left[h_o + \frac{\Delta h}{2}\, e^{\eta}\, erfc\sqrt{\eta}\,\right](T_c - T_o) \\ & - \frac{\pi}{2}\Delta T\left[h_o e^{\zeta}\, erfc\sqrt{\zeta} + \Delta h\, e^{\eta+\zeta}\, erfc\sqrt{\eta+\zeta}\right]\end{aligned} \tag{F4}$$

where

$$\sqrt{\eta} \equiv R/\sigma_y \qquad \text{and} \qquad \sqrt{\zeta} \equiv R/s \tag{F5}$$

Assuming s = R, $\sigma_y = 0.8R$, $h_o = 10$, and $\Delta h = 61$, equation (F4) yields

$$\int_o^{\pi} \phi_c\, d\theta \approx \frac{\pi}{2}\,[42.437(T_c - T_a) - 20.923\,\Delta T] \tag{F6}$$

Next, the variation in surface temperature around the circumference was taken into account. It was assumed that

$$T_c(\theta) \approx \begin{cases} T_c(\pi/2) - \tau(1 - 2\theta/\pi) & -\pi/2 \le \theta \le \pi/2 \\ T_c(\pi/2) & \pi/2 < \theta \le 3\pi/2 \end{cases} \tag{F7}$$

where

$$\tau = T_c(\pi/2) - T_c(0) \tag{F8}$$

Note that $T_c(\theta=0)$ is the minimum temperature around the circumference. Hence we may write $T_c(\theta=0) = T_{c,min}$. We will shortly see that τ is in fact a function of x and t. The time dependence of $T_c(\theta)$ has been suppressed for brevity. Assuming that the T_c used earlier is the maximum temperature, a simple integration around θ shows that $\pi(18.0366)\tau/2$ must be subtracted from the above result. Hereafter, T_c will always mean the peak temperature around the circumference.

We want to run the cigarette program with model input values of h, T_c, and/or T_a such that the "isolated" cigarette will have the indicated energy loss *via* convection. This can be achieved, for example, by using an effective heat transfer coefficient h*, such that

$$\int_0^{\pi} \phi_c(\theta) d\theta = \int_0^{\pi} h^*(T_c - T_a) d\theta = \pi h^*(T_c - T_a) \tag{F9}$$

Thus, from equation (F6),

$$h^* = 21.22 - 10.47\left(\frac{T_s - T_a}{T_c - T_a}\right) - 9.02\left(\frac{T_c - T_{c,min}}{T_c - T_a}\right) \qquad \text{W/m}^2\text{K} \tag{F10}$$

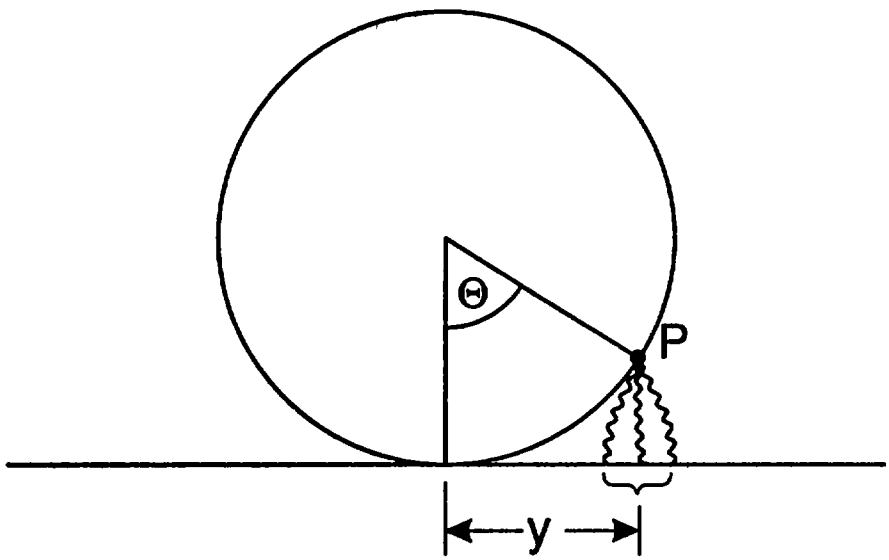


Figure F-1. Schematic of the exchange of energy between point P on the cigarette surface and the substrate surface.

APPENDIX G

CALCULATION OF THE CONVECTIVE VIEW FACTOR

The conductive flux distribution in the transverse direction, $\phi_c(x,y,t)$, is calculated in Appendix 5-D of Gann *et al.* (1988). The approximate expression

$$\phi(0,y,0) \approx \phi(0,0,0)\frac{a^2}{a^2 + y^2} \tag{G1}$$

is derived there, where $\phi_c(0,0,0)$ is the (peak) initial conduction/convection flux along the line of contact; this flux falls rapidly with time. The parameter a is of the order R/2. Equation (G1) gives $\Omega_c(y)$ implicitly.

Experimental measurements (Gann *et al.* (1988), Section 4) have shown that the (total) flux from a cigarette can be fitted approximately with a distribution of the form

$$\phi_{in}(x,y,t) = \phi_{max}\exp\left[\left(\frac{x - x_o - vt}{\sigma_x}\right)^2 - \frac{y^2}{\sigma_y^2}\right] \tag{G2}$$

If expanded as a power series, this agrees with equation (G1), to lowest order in y^2. The total energy output from the distribution (B2) is

$$\dot{E} = \iint \phi(x,y)dxdy = \pi\sigma_x\sigma_y\phi_{max} \tag{G3}$$

Reasonable agreement with experiment is obtained with $\sigma_x = 0.6$ cm and $\sigma_y \approx 0.32$ cm. This suggests that the above implicit expression for $\Omega_c(y)$, equation (G1), be modified to be a Gaussian. That is, the coefficient in equation (139) is

$$h_s(y) = h_o + \Delta h\, e^{-y^2/\sigma_y^2} \tag{G4}$$

where

h_o = background $\approx$ 10 W/m^{2}K and $\Delta h = h_c - h_o \approx 61$ W/m^{2}K.

APPENDIX H

LONGITUDINAL DEPENDENCE OF RADIATION FLUX TO THE SUBSTRATE

If the cigarette surface were at the uniform temperature T_c, and the view factor for the cigarette for some point P on the substrate were Ω (the fraction of energy emitted by the given substrate area which would be intercepted by the cylinder), one might think that the radiation flux reaching P is

$$\phi_p = \Omega \phi_c + (1 - \Omega)\phi_a \tag{H1}$$

where

$$\phi_c \equiv \epsilon_c \sigma T_c^4 \tag{H2}$$

is the flux from the cigarette and

$$\phi_a \equiv \sigma T_a^4$$

is the ambient flux. If one properly considers the reflections between cigarette and substrate, however, then with the further assumption that the surface temperature of the substrate, T_s, is also uniform, one finds that the correct expression would be

$$\phi_p = \frac{\Omega \phi_c + (1 - \Omega)\phi_a}{1 - a\Omega} + \frac{(1 - \epsilon_c)\Omega^2 \phi_s}{1 - a\Omega^2}, \tag{H3}$$

where

$$\phi_s \equiv \epsilon_s \sigma T_s^4 \tag{H4}$$

and

$$a \equiv (1-\varepsilon_s)(1-\varepsilon_c). \tag{H5}$$

Equation (H3) reduces to (H1) in the case $\varepsilon_c = 1$. The more general case, where neither T_s nor T_c are uniform over the surfaces, involves some very complex integrations which can generally not be carried out analytically.

Indeed, T_c is in fact **not** uniform, but highly peaked. The longitudinal (*i.e.*, parallel to the axis) net radiation flux distribution from the surface of the freely smoldering cigarette,

$$\phi_r(x) = \epsilon_c \sigma \left[T_c^4(x) - T_a^4\right] \tag{H6}$$

can be again be approximated by a Gaussian:

$$\phi_r(x) \approx \epsilon_c \sigma (\Delta T)^4 \exp\left[-\frac{(x - x_o)^2}{s^2}\right] \tag{H7}$$

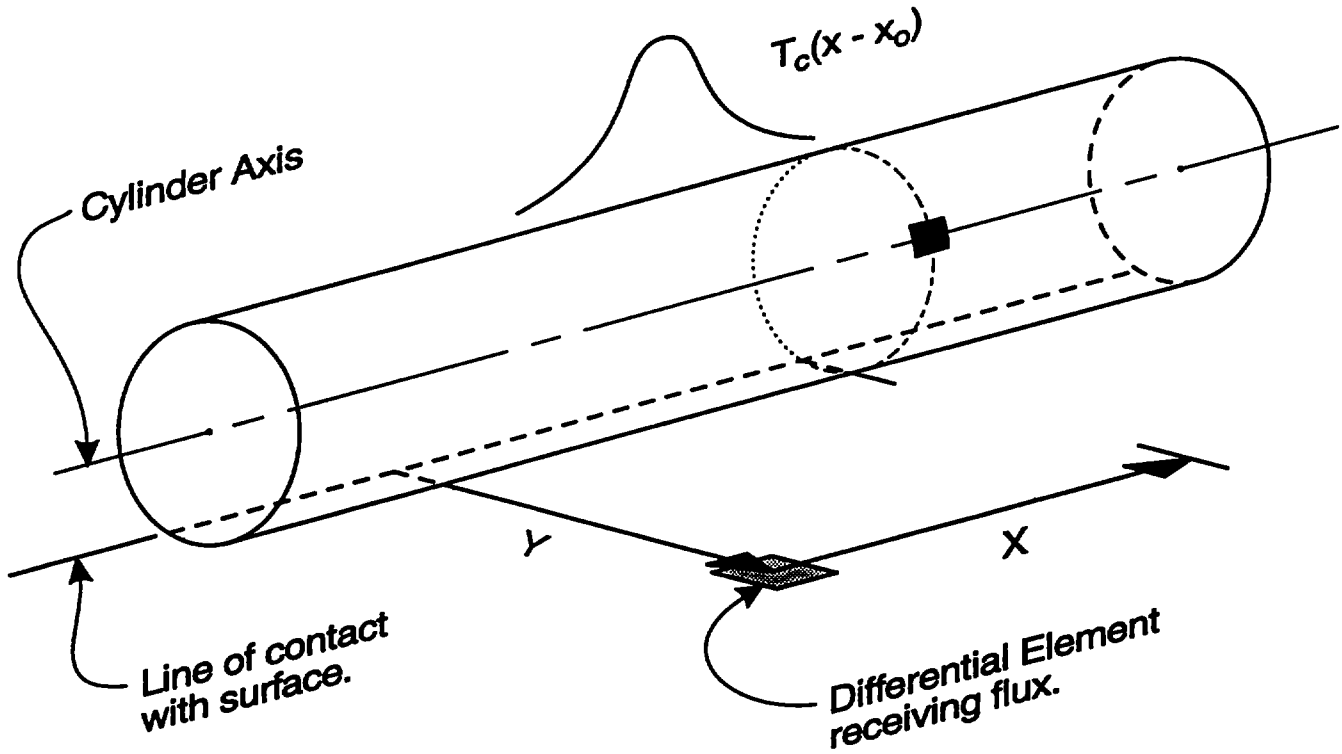


Figure H-1. The geometric relationship between a general point on the cigarette and another on the substrate. The profile above the cigarette is its surface temperature, with its peak at x_o.

Thus the peak flux from, and peak temperature on, the cigarette surface both occur at $x = x_0$; equation (H7) gives the peak flux, and equation (H8) defines ΔT:

$$T_{max}^4 = T_c^4(x_o) = T_a^4 + (\Delta T)^4 \tag{H8}$$

Thus, even if we had had the simple approximation (H1) rather than (H3), it must be generalized to

$$\phi_p = \epsilon_c \int \sigma T_c^4(x) d\Omega + (1 - \Omega)\phi_a \tag{H9}$$

where

$$\int d\Omega = \Omega$$

and where $d\Omega$ is the view factor from a differential element on the plane to the differential cylindrical shell of width dx, a distance x in the axial direction and a distance y in the orthogonal direction, as shown in Figure H-1. (See reference [20] in Siegel and Howell (1981).) However, we do not have an analytic expression for $d\Omega$.

Two alternative approximations were investigated: in one, the cylindrical shell is approximated (for $y > R$) as a wall of height $a \sim 2R$. In another, the Gaussian distribution (38a) was approximated by a band of constant (peak) temperature, of equivalent width. That is,

$$\int_{-\infty}^{\infty} \phi_{max} e^{-x^2/s^2} dx = \sigma \phi_{max} \tag{H10}$$

This equation yields

$$\sigma = \sqrt{\pi}\, s \tag{H11}$$

Thus, if $s = \sigma_x$, then with $\sigma_x \approx 6.1$ mm, $\sigma \approx 1$ cm. Neither of these approximations was satisfactory.

Although obtaining the general expression for Ω is a task of daunting complexity, we may obtain a crude approximation as follows: It is clear that the flux at (x,y) is most strongly determined by the cigarette temperature at the nearest points. These are just the points at x -- that is, on the normal to the cigarette at x. Carrying this through to its logical conclusion, we may assume that the flux at any point (x,y) depends only on the local temperature, $T_c(x)$. This achieves an enormous simplification.

In fact, since each point on the substrate receives radiation from other points on the cigarette as well, the actual distribution will have a slightly larger half-width than that on the cigarette. The effect can be expected to be small, however.

Thus at any given distance y from the contact line, the flux distribution over the substrate surface (along the x coordinate) obtained this way will be similar to the distribution on the cigarette surface, only scaled down appropriately, as we shall now see. There then remains the task of determining how the flux falls off with distance y from the cigarette surface.

From Sparrow and Cess (1978), we find that for a thin but infinitely long strip on the substrate, parallel to the cylinder axis and a distance y from it, the configuration (view) factor $F_{sc} = \Omega$ is

$$\Omega(y) = \frac{R^2}{R^2 + y^2} \tag{H12}$$

where R is the cylinder radius. This is precisely of the same form as the factor for conduction. (See equation (B1).) This is a one-dimensional calculation; clearly, for the two-dimensional case, the flux will fall off faster. A simple expression which falls off faster but has the same y-dependence for small y is the Gaussian dependence $\exp(-y^2/R^2)$. More generally, the variance of the distribution may be somewhat different from R (though it may be expected to be *proportional* to R); call it σ_y. Thus we will use

$$\Omega(y) = e^{-y^2/\sigma_y^2} \tag{H14}$$

Since we found above that $\sigma_y \approx 3.2$ mm for R = 4mm, we may take, in general,

$$\sigma_y = 0.8R \tag{H14}$$

The improvement (over simply assuming that the heat flux profile is Gaussian in the y direction) which would be obtained by carrying out the formidable integrations indicated above, hardly justifies the effort. This holds even more strongly for the more complete expression, equation (H3). We thus use

$$\Omega_c(y) \approx \Omega(y) \approx \exp\left(-y^2/\sigma_y^2\right) \tag{H15}$$

for the sake of simplicity.

Now consider the net flux from the cigarette to the substrate: along the line of contact, $\Omega = 1$; therefore equation (H3) yields

$$\phi_{net,rad} = \frac{\epsilon_s \epsilon_c}{1-a}\sigma\left(T_c^4 - T_s^4\right) \tag{H16}$$

where a is given by equation (H5).

The radiation flux is treated in the same way as the convective flux, that is,

$$\phi_{net,r} = \epsilon_r \Omega \sigma (T_c^4 - T_s^4) - (1-\Omega)\epsilon_s \sigma (T_s^4 - T_a^4), \tag{H17}$$

where ϵ_r is given by equation (142), and this is split into an effective radiation from cigarette to substrate,

$$\phi_{cig,r} = \epsilon_r \Omega \sigma\left(T_c^4 - T_a^4\right) \tag{H18}$$

while the substrate radiates away at the rate

$$\phi_{sub,r} = \left[\epsilon_r \Omega + \epsilon_s (1-\Omega)\right]\sigma\left(T_s^4 - T_a^4\right) \tag{H19}$$

Note that we have taken the reflections from the cigarette partially into account, by using ϵ_r rather than ϵ_c; however, we have not made the fuller analysis, as in getting equation (H3).

All of the above holds for $0 \le x \le L$.

APPENDIX I

TRANSIENT DEPRESSION OF CIGARETTE TEMPERATURE UPON DEPOSITION ON A SUBSTRATE

As noted above, finding $T_{c,min}(t)$ is a very complex problem; a simple approximation is possible, however: this problem has been solved for the special case of two semi-infinite solid slabs (homogeneous, isotropic, uniform) of different temperatures, coming into contact (Carslaw and Jaeger (1959), Section 2.15). In the vicinity of the contact line, and for a short period, this solution will be approximately (and locally) valid.

It is assumed there that there is perfect thermal contact between the two surfaces, so that the temperatures at the interface immediately reach the mean value

$$\bar{T} = \frac{T_a + T_c}{1 + r} \tag{I1}$$

where r is the ratio of the thermal inertias of the materials:

$$r = \sqrt{\frac{(k\rho c)_s}{(k\rho c)_c}} \tag{I2}$$

The temperature of the substrate varies with z and t according to

$$T_s(z,t) = T_a + \bar{T}\, erfc\left[\frac{z}{2\sqrt{\alpha_s t}}\right] \tag{I3}$$

where z is to be taken as positive into the substrate, and α_s is the thermal diffusivity of the substrate. The temperature of the other "slab" (the bottom of the cigarette) is

$$T_c(z,t) = \bar{T}\left[1 + r\, erf\left(\frac{z}{2\sqrt{\alpha_c t}}\right)\right] - T_a \tag{I4}$$

Since the thermal contact between cigarette and substrate is **not** perfect, their actual surface temperatures correspond to small finite depths z, in equations (I3) and (I4).

For a common fabric/foam substrate, the thermal properties are (Section II.D.2): k_s = 0.1435 W/mK, ρ_s = 620 kg/m^3, and c_s = 1122 J/kg K. Hence $\alpha_s = 2.063 \times 10^{-7}$ m^2/s and the thermal inertia = 316 Ws$^{1/2}$/m^{2}K. For a cigarette, we find (Mitler, 1988) k_c = 0.316 W/mK, ρ_c = 620 kg/m^3, and c_c = 1043 J/kg K. Hence $\alpha_c = 1.165 \times 10^{-6}$ m^2/s and the thermal inertia = 293, not very different from that of the substrate. With these two values, we find r = 1.0795. With T_c = 600 °C and T_a = 20 °C, equation (I1) yields $\langle T \rangle \approx 298$ °C.

For this cotton fabric/foam, the temperature fall in a couple of seconds is estimated to be 50-70 °C at the flux peak, at the side of the cigarette; that is, at $\theta = \pi/2$. Hence the assumption made above that the cigarette temperature is unaffected at the side is not quite correct. At $\theta = 0$, in fact, the temperature fall

was greater than 200 °C; the precise temperature could not be measured. Thus, $\delta T_{max} \approx 200$ °C. Then from equation (I4) we find that $erf(x/2\sqrt{\alpha_c t}) \approx 0.38$, for t ≈ 2 s. Assuming that the thermal diffusivities do not vary a great deal among cigarettes, we may take this term to be a constant. In general, then, assuming that $x/2\sqrt{\alpha_c t} \approx const.$, we may write, from equation (I4),

$$\delta T_{max} \approx T_c + T_a - [1 + 0.38\, r]\, \bar{T}$$

or

$$\delta T_{max} \approx 0.62\, r\, \bar{T} \qquad \text{(I5)}$$

Glass, as a substrate, is a more effective heat sink than a cotton fabric. Indeed, we find that the thermal inertia for ordinary glass is about 1690; hence in this case, r = 1690/316 = 5.35, and with T_c = 600 °C and T_a = 20 °C,

$$\bar{T} = \frac{620}{1 + r} = 97.7\ ^\circ C$$

and

$$\delta T_{max} \approx 324\ ^\circ C$$

APPENDIX J

MASS TRANSFER COEFFICIENTS

Baker and Crellin (1977) measured the diffusion of CO through cigarette paper. For CO in nitrogen, D_o = 0.21 cm^2/s, while for oxygen in nitrogen, D_o = 0.199 cm^2/s. These are close enough that we may take the results for CO to be valid for oxygen. They found the relationship:

$$D_p = A\sqrt{Z} \tag{J1}$$

between the diffusion coefficient of CO through the inherently porous cigarette wrapping paper, and the permeability Z of the paper, to hold. Here:

D_p is in 10^{-3} cm^2/s

and Z is in units of cm^3/min (10 cm^2 10 cm water)$^{-1}$

The value of A is 0.57, in the appropriate units. Permeabilities range between 16 and 2000, in these units, so D_p ranges between 1 and 22, with many of the papers in the region about:

$$D_p = 7 \times 10^{-3} \text{ cm}^2/\text{s}.$$

Cigarette paper thickness is $\delta = 43 \pm 5$ μm. Taking the mean, this yields:

$$\gamma_p = D_p/\delta \approx 1.6 \text{ cm/s}$$

For $\gamma_g = \gamma_b$, the boundary-layer value, we use equation (118). Then at the peak surface temperature ($T_s \approx 600$ °C), the mean value of temperature to be used in equation (118) is 310 °C = 583 K. We then get:

$$\gamma_b \approx 3.3 \text{ cm/s}.$$

According to these results, the resistance to diffusion through the paper is only about twice that through the boundary layer. The combined value, according to equation (122), is

$$\gamma \approx 1.1 \text{ cm/s}.$$

APPENDIX K

NOMENCLATURE

B = Biot number
C_g = specific heat of the gases
C_s = specific heat of the solid
D_e = diffusion coefficient for oxygen
D_{io} = diffusion coefficient for species i in the background "o" [equation (26)]
D_p = mean pore diameter
E_p = activation energy for the pyrolytic reaction
g = acceleration of gravity
h = heat transfer coefficient
h_{in} = mean convective heat transfer coefficient between cigarette and surface
h_q = heat transfer coefficient between cigarette and quiescent air
h_c = convective heat transfer coefficient; heat of combustion per unit mass
h_e = convective heat transfer coefficient (at the end)
h_r = heat transfer coefficient for radiation; see equations (15) and (106)
H_c = molar heat of combustion
k = thermal conductivity of the cigarette (see Section III.D.1, assumption #8)
k_g = thermal conductivity of the gas
k_{op} = normalized reaction rate (in min^{-1})
k_s = thermal conductivity of the solid shreds
l_c = a characteristic dimension [see equation (34)]
L = length of tobacco column
m = mass of tobacco column
n_A = no. of grams of ash yielded by the burning of one gram of char
n_c = no. of grams of char produced by the pyrolysis of one gram of tobacco
n_{O2} = no. of grams of oxygen which react with one gram of char
Nu = Nusselt number
Pr = Prandtl number
Q_{co} = energy released from char oxidation (lower heat of combustion)
Q_p = energy absorbed in (endothermic) pyrolysis
$\dot{Q}_i$ = energy loss rates: see Section III.B.7
$\dot{Q}$ = mean power produced during combustion
r = radial coordinate; ratio of thermal inertias [see equation (I2)]; stoichiometric fuel/oxygen ratio
R = universal gas constant; cigarette radius
Ra = Rayleigh number
Re = $u_o l_c/\nu$ = Reynolds number
R_p, R_{op} = pyrolysis rate (in gm/cm^3s)
R_{co} = char oxidation rate
Sc = Schmidt number (Sc = ν/D)
S_i = source/sink term [equation (26)]
T = absolute temperature
$T_{c,min}$ = cigarette surface temperature at contact line
T_{cig} = cigarette surface temperature
T_s = surface temperature of the substrate
u_r = radial (convective) gas velocity

V = total volume of the cigarette
V_s = total volume occupied by the solids in the cigarette
x = coordinate; axis of cylinder representing cigarette
X_{ox} = volume fraction of oxygen
y = oxygen mass fraction
Y_s = surface value of y
y_a = ambient value of y
y_o = "local" ambient (inside cigarette); used in heterogeneous models
y_s = value of y at cigarette (or shred) surface
y_T = tobacco mass fraction
Z_p = pre-exponential factor in reaction rate equation (108)
Z_{CO} = pre-exponential factor in reaction rate equation (110)

Greek Symbols

α = thermal diffusivity of gas
β = volumetric coefficient of (gas) expansion; parameter in equation (56)
γ = mass transfer coefficient for air + paper
γ_b = mass transfer coefficient for air (the boundary layer) alone
δ = characteristic penetration depth
ϵ = emissivity of the fabric (assuming that α, the absorptivity, = ϵ)
ϵ_A = emissivity of the (paper) ash
ϵ_{cig} = emissivity of cigarette
ϵ_T = emissivity of the shreds
ϵ_s = emissivity/absorptivity of the substrate (assumed constant)
θ = e-folding distance in equations (40)-(43)
κ = thermal conductivity of the substrate
κ_s, κ_g = solid and gas-phase thermal conductivities, respectively
ν = kinematic viscosity of air
ρ_g = mass density of the gases
ρ_T = tobacco density
ρ_s = mass density of the solid
σ = Stefan-Boltzmann constant
τ = total duration of the smolder
ϕ = void fraction in the cigarette (*i.e.*, the volume fraction of gas, rather than of tobacco shreds)
Φ = total void fraction (including the void space in the shreds, and is therefore larger than ϕ)
ϕ_a = ambient radiation flux = σT_a^4
ϕ_c = radiation flux from cigarette; convective flux (substrate)
ϕ_c^* = model convective heating flux from cigarette (see equation (9))
ϕ_{in} = heating flux reaching the substrate surface
ϕ_{net} given by equation (6)
ϕ_{out} = surface heat loss of the surface to the ambient, for the areas away from the cigarette
ϕ_r = radiation flux (substrate)
Ω = $\Omega(r)$ = radiation view factor of the cigarette as seen by the substrate at the point r
Ω_c = fraction giving influence of convection at a given point

Subscripts

a = ambient; ash
c = convection; cigarette; char
g = gas
m = maximum
o = original; ambient
p = pyrolysis; peak
r = radial; radiation; effective
s = surface; substrate; solid
t = tobacco; total
x = in x-direction (axial)

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This paper describes the user-friendly computer models CIGARET and SUBSTRAT. CIGARET calculates the time-dependent behavior of a cigarette smoldering quietly in the air, away from surfaces. The model incorporates diffusion and convection of gases, as well as the kinetics of char oxidation. It calculates the internal heat fluxes, as well as the internal distributions of temperature, gas velocity, and oxygen concentration. SUBSTRAT determines whether a two-layer solid (with an air gap in between), exposed to a moving heating flux such as is produced by a cigarette, will ignite. Among the processes taken into consideration are three-dimensional heat conduction in the substrate and its pyrolysis. This model has successfully simulated the thermal runaway signifying smoldering ignition of the substrate when it is exposed to a set of external heating fluxes. SUBSTRAT and CIGARET have been designed to work in tandem to simulate the most frequent cause of fatal fires: cigarette ignition of upholstered furniture and bedding. Users' guides are included.

KEY WORDS (MAXIMUM 9 KEY WORDS; 28 CHARACTERS AND SPACES EACH; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES)

cigarettes; cigarette model; computer model; free smolder; furniture fires; ignition; mathematical modeling; modeling; pyrolysis; simulation; smoldering; substrates

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