The Establishment of A Catalog of Compartment Fire Model Algorithms and Associated Computer Subroutines

Reference

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The Establishment of a Catalog of Compartment Fire Model Algorithms and Associated Computer Subroutines

David W. Stroup

ABSTRACT

The Compartment Fire Model Research group of the Center for Fire Research, National Bureau of Standards has been charged with the development of a "benchmark" compartment fire model. As part of this activity, a catalog of available fire model algorithms is being compiled. This paper presents a proposal for the organization, format, and use of the catalog. Appendix A of this report is a copy of the proposed introductory text for the catalog. Appendix B presents the Table of Contents for the first edition of the catalog, and Appendix C contains several examples of catalog algorithm write-ups. Finally, Appendix D lists the references used in Appendix A.

Keywords: algorithms; building fires; cataloging; combustion physics; compartment fires; computer programs; fire chemistry; fire models; mathematical models; zone models.
The Compartment Fire Model Research group of the Center for Fire Research, National Bureau of Standards has been charged with the development of a "benchmark" compartment fire model. As part of this activity, a catalog of available fire model algorithms is being compiled. The catalog will contain algorithms which calculate various physical/chemical fire phenomena.

The description of each algorithm will include the input(s), output(s), and calculations performed. In addition, each algorithm will have a computer subroutine written for it in FORTRAN 77. The variables used as input and output throughout the catalog will be cross-referenced. This will enable a catalog user to easily determine which routines would be required to calculate a particular fire phenomena.

Appendix A is a draft of the introductory text of the catalog. It begins with a brief discussion of the purpose of the catalog. Following these remarks, there is a description of fire dynamics and fire models. Appendix A details how the catalog will be published and updated. It outlines the format used to present each algorithm as well as describing the method used to cross-reference variables. Through the use of an example, the utility of the catalog for upgrading and enhancing existing fire models is illustrated.

Appendix B is a tentative List of Algorithms for the first release of the catalog. It shows the major catalog divisions and the many algorithms to be included under each heading. The majority of these algorithms in the first

Appendix C presents several algorithm write-ups including those referenced in the example discussed in Appendix A. These write-ups are shown as they would appear in the actual catalog. Appendix D lists the references that are used in Appendix A (the catalog introduction).

In summary, the Appendices to this paper illustrate the proposed format for the Compartment Fire Model Algorithm Catalog. Comments on the text and ideas presented are heartily solicited.
APPENDIX A.

Compartment Fire Model Algorithm Catalog
1. INTRODUCTION

Many mathematical models and associated computer programs have been developed to predict enclosure fire dynamics [1-15]. These models differ in many respects. They differ in the number and complexity of fire compartments which may be analyzed; the amounts of computer time and memory required; the number and detail of individual physical phenomena accounted for; the amount of documentation available; and the degree of "user-friendliness". Regardless of the many differences, all of these models attempt to describe the same basic fire phenomena. It is possible to break existing fire models up into "elemental" pieces. These "elemental" pieces describe the physical/chemical effects associated with the fire phenomena.

It is the purpose of this catalog to present the available physical/chemical algorithms and corresponding subroutines in a form which may be used by fire researchers who wish to develop or improve fire modeling computer programs. Researchers may use routines from the catalog according to their needs and take advantage of the progress made by others. The catalog contains descriptions of the methodologies used to calculate each of the fire related physical/chemical phenomena. In addition, a FORTRAN 77 computer subroutine which implements the method is included with each algorithm write-up.

1 Numbers in brackets refer to references listed in Appendix D.
This catalog provides fire researchers with convenient access to each others' work. It eliminates the need for researchers to continually redevelop the same algorithms. For the most part, only the most accurate and efficient algorithms and subroutines are included in the catalog. The catalog is published in loose-leaf form so that old algorithms may be improved and new ones added as necessary. Finally, to be successful, this catalog will require user support and feedback which is heartily encouraged.

2. FIRE DYNAMICS

The physical and chemical processes simulated by the algorithms and subroutines in this catalog are relevant to compartment fire-generated phenomena. The generic fire scenario of interest can be briefly described as follows. An unwanted ignition is assumed to occur within an enclosed space. The fire may start in a couch, for example, or stacked commodities in a warehouse. Regardless of the method and location of ignition, the applicable physical/chemical phenomena discussed below will be the same.

Heat from the initial flame pyrolyzes the material of fire origin. The resulting vapors rise into the flame zone, ignite, and maintain the flame. The elevated temperature products of combustion are driven out of the combustion zone by buoyancy. In this way, a plume of upward moving elevated temperature gases is formed above the fire. The gas entrains some of the surrounding air and the mixture rises to the ceiling. When the plume impinges on the ceiling, it spreads out and forms a relatively thin, hot, sooty layer. As the
fire grows, this layer will thicken and the relatively sharp interface between it and the cool ambient air layer below will continuously drop. Eventually, the layer falls below the top of the highest vent, whereupon buoyancy-generated cross-vent pressure differentials will drive some of the layer gases out of the room. In addition to energy losses from the flow of hot gases out of the vent(s), the layer also loses energy by radiation and convection to the floor, ceiling, walls, and other objects within the room.

Due to heating from the elevated room temperature environment, combustible objects in the room remote from the fire, may eventually reach their ignition temperature, and ignite. If such ignitions begin to occur, they may follow one another very rapidly, until all combustible objects within the room are burning. This transition period between ignition of the first "target item" and full room involvement is called "flashover." It generally only lasts a few seconds. Following flashover, the fire may spread from the room of origin to other parts of the building, thus presenting a severe danger to life and property.

3. FIRE MODEL TYPES

Many attempts have been made to model the above fire phenomena mathematically. Fire models may be divided into two main groups. The first group is composed of probabalistic models. Models in this group "calculate" fire development based on the probability of one event following another. Routines from these models will not be discussed in this catalog.
The other group consists of deterministic models. In general, these models solve differential and/or algebraic equations to determine the time-varying fire characteristics. The deterministic models may be further sub-divided into categories which describe the assumptions used to solve the problem. The first of these groups is "field" models. Field fire models describe events within an enclosure volume by a set of coupled partial differential equations, which are applicable throughout the volume, and which stipulate boundary conditions at the surfaces of the volume. Field models are generally very complex and require large amounts of computer time and memory.

The other group consists of the "zone" models. The zone type fire models divide the room into zones, usually three. The three zones are an upper zone which includes the smoke layer, a lower zone which contains relatively cool and uncontaminated air, and a combustion/plume zone which transports the smoke from the fire below to the upper smoke layer. Models developed using the zone concept range from very simple to very complex.

The focus of attention of this catalog is on the physical/chemical algorithms which would be used in zone-type models and, possibly, in hybrid models which combine both zone-type and field-type descriptions of the fire-generated compartment environment.
This catalog of compartment fire model algorithms is intended to be used as a reference by persons desiring to develop their own fire models or enhance existing ones. Each algorithm write-up, contained in the catalog explains the methodology for calculating a fire related parameter. The format, used to present each algorithm, has been chosen to be as "user-friendly" as possible. The catalog is being issued in loose-leaf form. This will make it easy to update, and updates, including new and improved algorithms, will be issued periodically. The catalog is divided into eight sections. They are: Burning Object, Conductive Heat Transfer, Convective Heat Transfer, Hot Layer, Plume, Radiative Heat Transfer, Room Conservation, and Vents. Each section contains one or more algorithms which calculate result(s) related to that section heading. An individual algorithm is only described once. However, if the algorithm could logically be expected to be found under two or more headings, reference to the complete algorithm description may be found under each appropriate heading.

Each algorithm is described individually. The algorithm's name and brief title appears at the top of each page. The first section, Description, describes the methodology used in the algorithm. In addition, the major limitations of the algorithm are listed as are any other details which may be important to someone wishing to incorporate the algorithm into a fire model. The second section, Output, lists the output variable(s), with a brief description of the meaning of each variable. The number of output variables from a given subroutine are generally limited to one. This enables a catalog
user to build a complete fire model using relatively small pieces of the phenomena. It also makes it possible to include alternate algorithms for modeling the same phenomena. The third section, Input, includes a list of the required input variables along with a brief description of each variable. Each input variable is identified as to whether it is a physical constant, input data, or calculated physical variable. Input variables are cross-referenced so the user can easily find required input which is calculated by routines elsewhere in the catalog.

A fourth section, Calculations, presents the step-by-step procedure or algorithm used to calculate the result. The meaning of each calculation is briefly described next to the calculation. The fifth section, References, is a listing of reference sources where the user may obtain more information about the theory used to develop the algorithm, its limitations, and/or its implementation in other fire models. Section six, Subroutine Variables, relates the variables used in the output, input, and calculations sections to the associated FORTRAN variables. Finally, section seven, Computer Subroutine, presents the FORTRAN 77 computer subroutine which implements the algorithm.

5. AN EXAMPLE OF USING THE CATALOG

Suppose a fire researcher wishes to improve the modeling capabilities of the ASET (Available Safe Egress Time) computer code[7,8]. A likely improvement would involve use of a more fundamental means of estimating heat transfer to the compartment ceiling. This improvement would require an algorithm for calculating the transient heat conduction through the depth of the ceiling
material. Such an algorithm and its associated subroutine can be found in the section on Conduction Heat Transfer in the Catalog. In that section, there is an algorithm named TMPW01 (see Appendix C of this report). It may be used to calculate the transient heat conduction through a surface exposed to radiative and convective heating.

In the write-up of this algorithm, there is a listing of the required inputs. Many of these deal with characteristics of the wall or ceiling material and may be obtained from published data on thermophysical properties of materials. Another input, the layer height, is already calculated in the ASET model. Inputs describing the convective and radiative fluxes being received by the material are also required. For these, the modeler might use the simple assumptions already used in the ASET model. (In the ASET model the total rate of heat transfer to bounding surfaces of the compartment is represented as a constant fraction of the instantaneous fire heat release rate.) The alternative would be to compute these inputs using algorithms and subroutines referenced elsewhere in the catalog and to incorporate these subroutines into the ASET model.

The final input required by this routine is the infra-red absorptivity of the hot layer. The Catalog contains several algorithms useful for calculating this value. The simplest is ABSRB2 (see Appendix C of this report). It assumes the absorptivity is a constant fraction of the mass concentration of the soot in the hot layer. If this routine is selected, another input is required. This input represents the mass concentration of soot in the layer as a function of time. In this case, a simple way to represent this value would
be to use the product of combustion calculation capability of the ASET model. The soot concentration could be modeled as either a constant fraction of the heat release rate or as input data from fire tests.

Using these two subroutines, TMPW01 and ABSRB2, it would be possible to incorporate heating of a slab (ceiling, floor, or wall) into the ASET model. This would be the first step in developing an improved method of calculating the fraction of heat lost to the bounding surfaces of the room from elementary principles. The modeler would have to find a way to control the calling of these subroutines, but the subroutines themselves would not have to be developed again.
APPENDIX B.

List of Algorithms in the Catalog
1. Burning Object

ANGLE Calculates the angle of the flame cone based on radius of fire and height of flame.

BURN Calculates the rate of burning, on a mass basis, of the vapors released by a combustible object.

CHEM Calculates the rate at which chemical energy is released from a burning object.

FLUX Calculates the heat fluxes from the hot layer, plume(s), and walls, incident on the surface of a burning object.

HEIGHT Calculates the height of the flame of a burning object.

PFLUX Calculates the net heat flux from user determined sources to a potentially pyrolyzing surface.

PULRAD Calculates the radius of a pool fire.

PYRO Calculates the mass pyrolysis rate of a burning horizontal fuel slab.

SPREAD Calculates the rate of spread of a fire on a horizontal fuel slab.

TANPSI Calculates the tangent of the angle of the flame cone based on constant volumetric heating (open air burning).

TMGAS Calculates the gas flow rate, at a given time, from a burner with a variable gas flow rate.

2. Conduction Heat Transfer

CONDUC Calculates the heat conduction from the surface into the interior of a pyrolyzing fuel item.

TMPO01 Calculates the temperature of an object by a "shortcut" method when the object is heating or pyrolyzing.

TMPO02 Calculates the temperature profile within an object using a discrete grid.

TMPW01 Calculates the temperature profile within a wall (slab) using a discrete grid.
3. Convection Heat Transfer

CBLOCK Calculates the convective heat flux from the flame above to the surface of a burning pool.

CNVF Calculates the convective heat flux from the lower layer to the floor assuming that radiation (from the flames and from the hot layer) heats the floor, and that in turn will heat the (cool) lower layer of gas above it by convection.

CNVL Calculates the convective heat loss rate from the hot layer to the extended ceiling.

CNVL1 Calculates the rate of loss of energy from the hot layer in a room due to convective heating of the walls and ceiling.

CNW01 Calculates the convective heat flux to one side of a wall from the adjacent hot layer.

THERM Calculates the thermal conductivity of air as a function of temperature (required by CNVF).

VISC Calculates the kinematic viscosity of air as a function of temperature (required by CNVF).

4. Hot Layer

ABSRB2 Calculates the infra-red absorptivity of the hot layer.

ABSRB3 Calculates the infra-red absorptivity of the hot layer (requires EMSVTY and associated routines).

ASYMP Calculates the asymptotic expansion for the penta-gamma function (required by PENTA).

CHEBY Calculates the value of the Chebyshev polynomial of order N and argument x (required by SCRTH).

DLECK Calculates the 2.7 and 15 micrometer overlap correction for mixtures of CO₂ and H₂O (required by EGAS).

DXDCNC Calculates the mass concentration of carbon dioxide in the hot layer.

DXDPRD Calculates the rate at which the fire of an object produces carbon dioxide.

EGAS Calculates the emissivity of a given path of a mixture of carbon dioxide and water vapor at temperature t (required by EMSVTY).
<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
</tr>
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<tr>
<td>EMSVTY</td>
<td>Calculates the emissivities of the isothermal and homogeneous mixtures of soot, carbon dioxide, and water vapor at a total pressure of one atmosphere (required by ABSRB3).</td>
</tr>
<tr>
<td>LAYDPT</td>
<td>Calculates the depth of the hot layer.</td>
</tr>
<tr>
<td>MNXCNC</td>
<td>Calculates the mass concentration of carbon monoxide in the hot layer.</td>
</tr>
<tr>
<td>MNXPRD</td>
<td>Calculates the rate at which the fire of an object produces carbon monoxide.</td>
</tr>
<tr>
<td>OXYCNC</td>
<td>Calculates the mass concentration of oxygen in the hot layer.</td>
</tr>
<tr>
<td>PENTA</td>
<td>Calculates the value of the penta-gamma function of argument x.</td>
</tr>
<tr>
<td>POWL</td>
<td>Calculates the rate of change of the energy of the hot layer.</td>
</tr>
<tr>
<td>RBLOCK</td>
<td>Calculates the absorption of radiant flux directed toward the fuel surface as a result of a layer of cool, absorbing fuel gas close to the pyrolyzing surface.</td>
</tr>
<tr>
<td>SCRTH</td>
<td>Calculates the chebyshev polynomials for carbon dioxide and water vapor (required by EGAS).</td>
</tr>
<tr>
<td>SOOT</td>
<td>Calculates the transmissivity of the path of soot to a blackbody radiation source at a given temperature (required by EMSVTY).</td>
</tr>
<tr>
<td>SUTCNC</td>
<td>Calculates the mass concentration of soot in the hot layer.</td>
</tr>
<tr>
<td>SUTPRD</td>
<td>Calculates the rate at which the fire of an object produces soot.</td>
</tr>
<tr>
<td>TGO2M</td>
<td>Calculates the rate of change of mass of carbon dioxide in the hot layer.</td>
</tr>
<tr>
<td>TH2OM</td>
<td>Calculates the rate of increase of mass of water vapor in the hot layer.</td>
</tr>
<tr>
<td>TMNXM</td>
<td>Calculates the rate of increase of mass of carbon monoxide in the hot layer.</td>
</tr>
<tr>
<td>TMPL</td>
<td>Calculates the temperature of the hot layer.</td>
</tr>
<tr>
<td>TMSL</td>
<td>Calculates the rate of change of the mass of the hot layer.</td>
</tr>
<tr>
<td>TOXYM</td>
<td>Calculates the rate of change of mass of oxygen in the hot layer.</td>
</tr>
<tr>
<td>TSUTM</td>
<td>Calculates the rate of change of mass of soot in the hot layer.</td>
</tr>
<tr>
<td>WTRCNC</td>
<td>Calculates the mass concentration of water vapor in the hot layer.</td>
</tr>
</tbody>
</table>
WTRPRD Calculates the rate at which the fire from an object produces water vapor.

5. Plume

DPLUM Calculates the rate of change of the mass of a fire plume (Delichatsios model).

ENTPL Calculates the rate of entrainment of the layer gases into the upper part of the plume over an object (inside hot layer).

HPLUM Calculates the rate of change of the mass of a fire plume (modified Hasemi model).

MPLUM Calculates the rate of change of the mass of a fire plume (McCaffrey model).

OXYBRN Calculates the mass rate of oxygen burning in the plume of an object.

PLMHT Calculates the height of the plume over an object.

PLUM Calculates the dimensions and rate of change of mass and energy of a fire plume (virtual point source).

PTPLUM Calculates the dimensions of and throughput of mass and energy in a plume above an object (point-source).

TENPLM Calculates the rate at which the plume over an object adds energy to the hot layer.

TMSPLM Calculates the rate at which the plume over an object adds mass to the hot layer.

ZPLUM Calculates the rate of entrainment of mass in a fire plume (Cetegen, Zukoski, Kubota model).

6. Radiation Heat Transfer

PWRPLR Calculates the power (energy) absorbed by the layer due to radiation from the fire plume of a burning object.

RADFW Calculates the radiative flux from the fire plume of a burning object to the walls of the room.

RADLW Calculates the radiative flux from the hot layer to the portion of the walls and ceiling covered by the hot layer.

RDNL Calculates the energy losses and gains of the hot layer via radiation (using an empirical value of optical depth).
Calculates the total radiative heat loss from the flame of a burning object. [The flame is assumed to be a cone or conical shell.]

Calculates the radiative heat transfer to the portion of the walls and ceiling contiguous to the hot layer, from the flame(s) and the hot layer. [The layer is approximated by a cylinder, with the fire centrally located and itself further approximated by a point source at the centroid.]

Calculates the energy absorbed by a flame due to radiation from another flame which may be shaded by a fuel slab.

Calculates the radiative flux to the horizontal surface of an object from the layer via a cylinder approximation (even if the object is burning).

Calculates the radiative flux from the layer to the surface of a vertical object via a cylinder approximation (even if the object is burning).

Calculates the sum of the radiative fluxes from flames to objects.

Calculates the radiative flux from the walls and ceiling in a room to the top surface of an object (even if the object is burning).

7. Room Conservation of Mass

Check for conservation of mass in a room.

8. Vents

Calculates the width of the segment of a given vent which intersects the interface between the hot and cold layers.

Calculates the energy and mass flow through a vent.

Linear for large values of x and rounds out the \( \sqrt{x} \) singularity at small values of x (used by FLOW).

Calculates the mass flow rate of each of the gaseous species through a vent.

Calculates the area of a vent covered by the hot layer.
APPENDIX C.

Catalog Entries
Description

This routine calculates the rate at which chemical energy is released from a burning object. The energy release rate of an object is a function of the object's rate of burning and its heat of combustion. In this routine, an effective heat of combustion is used. This accounts for the energy required to raise the object's temperature from ambient to its pyrolysis temperature. The power output by combustion is then calculated using this effective heat of combustion and returned as a negative value.

Output

\( \dot{E}_f \)

Rate of chemical energy release from a burning object. [W]

Input

\( C_p \)

Specific heat of ambient air (Input Data). [J/kg-K]

\( H_c \)

Heat of combustion of the object as fuel (Input Data). [J/kg]
\( T_a \)  
Ambient temperature of the room containing the object (Input Data). [K]

\( T_p \)  
Temperature of object at onset of pyrolysis (Input Data). [K]

\( \dot{m}_b \)  
Burning rate of object (Calculated Value, see Burning Object section). [kg/sec]

Calculations

\[
H'_c = H_c - C_p(T_p - T_a)
\]
Effective heat of combustion.

\[
\dot{E}_f = -\dot{m}_b \times H'_c
\]
Negative of power output by combustion.

References


Subroutine Variables

\[
\text{TEOZZ} = \dot{E}_f
\]
\[
\begin{align*}
CP &= C_p \\
QF &= H_c \\
ZKAZ &= T_a \\
ZCOPY &= T_p \\
TMOZB &= \dot{m}_b
\end{align*}
\]
Computer Subroutine

SUBROUTINE CHEM (CP,QF,ZKAZZ,ZCOPY,TMOZB,TEOZZ)
C ******************************************************************************
C
C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C SUBROUTINE TO CALCULATE THE RATE AT WHICH CHEMICAL ENERGY IS
C RELEASED FROM A BURNING OBJECT.
C
C INPUT PARAMETERS:
C CP -- SPECIFIC HEAT OF AMBIENT AIR
C QF -- HEAT OF COMBUSTION OF THE OBJECT AS FUEL
C ZKAZZ -- AMBIENT TEMPERATURE OF THE ROOM CONTAINING THE
C OBJECT
C ZCOPY -- TEMPERATURE OF THE ONSET OF PYROLYSIS OF THE
C OBJECT
C
C INPUT VARIABLES:
C TMOZB -- MASS BURNING RATE OF OBJECT
C
C OUTPUT VARIABLE:
C TEOZZ -- CHEMICAL ENERGY RELEASE RATE OF THE OBJECT
C
C TQF = QF - CP * (ZCOPY - ZKAZZ)
C PATCH TO PREVENT TEOZZ FROM STAYING AT 0. AFTER AN OBJECT MOVES
C OUT OF THE HOT LAYER.
C TMB = TMOZB
C IF (TMOZB .LE. 0.D0) TMB = 1.D-6
C TEOZZ = -TMB * TQF
C
C RETURN
END
PYRO - Mass Pyrolysis Rate of Burning Object

Description

This subroutine calculates the mass pyrolysis rate of a burning horizontal fuel slab. The pyrolysis rate is taken to be proportional to the net heat flux to the surface and to the (instantaneous) burning area. The net heat flux is the radiation incident from all sources (principally the flame) plus the convective heating from the flame, minus the reradiation. For small flames convective heating is substantial, but rapidly falls in importance as the flame grows. Theoretical expressions for it exist, but they are very complex. In this algorithm, the reradiation is simply cut down for small flames in such a way that the observed growth rate of pyrolysis is followed. This ad hoc procedure turns out to be very simple. The energy loss by diffusion into the slab is ignored. The pyrolysis rate is also modified (in an arbitrary way) to take into account the smooth cessation of pyrolysis as the fuel nears burnout.

Output

\[ m_f \]

Mass pyrolysis rate of burning slab. [kg/sec]
**Input**

\( H_v \)  
Heat of vaporization of the object (Input Data). [J/kg]

\( \phi \)  
Flux impinging on the surface of the object (Calculated Value, see Burning Object section). [W/m²]

\( m_f \)  
Remaining mass of object (Calculated Value, see Burning Object section). [kg]

\( R \)  
Radius of fire on object (Calculated Value). [m]

\( \pi \)  
\( \pi \) (Physical Constant). [3.141592...]

**Calculations**

\[ \dot{m}_\beta = \begin{cases} -\pi R^2 \phi / H_v, & \phi > 0 \\ 0, & \phi \leq 0 \end{cases} \]  
Unadjusted rate of change of fuel mass (negative of pyrolysis rate).

\( G = m_f / (2\dot{m}_\beta) \)  
Convenient definition (for \( \dot{m}_\beta < 0 \))

\[ \dot{m}_f = \begin{cases} \dot{m}_\beta (1-e^G), & \phi > 0 \\ 0, & \phi \leq 0 \end{cases} \]  
Negative of pyrolysis rate, adjusted for smooth burnout.
References


Subroutine Variables

TMOZZ = \dot{m}_f
QVAP = H_v
PHI = \phi
ZMOZZ = m_f
ZRFZZ = R
PI = \pi
SUBROUTINE PYRO (QVAP, PHI, ZMOZZ, ZRFZZ, TMOZZ)

C *******************************************************

C IMPLICIT DOUBLE PRECISION (A-H, O-Z)

C SUBROUTINE TO CALCULATE THE MASS PYROLYSIS RATE OF A BURNING
C OBJECT.

C INPUT PARAMETERS:
C QVAP -- HEAT OF VAPORIZATION OF THE OBJECT

C INPUT VARIABLES:
C PHI -- FLUX IMPINGING ON THE SURFACE OF THE OBJECT
C ZMOZZ -- REMAINING MASS OF THE OBJECT
C ZRFZZ -- RADIUS OF THE FIRE ON THE OBJECT

C OUTPUT VARIABLE:
C TMOZZ -- NEGATIVE OF MASS PYROLYSIS RATE OF THE OBJECT

PARAMETER (PI = 3.1415927D0)

TMOZZA = TMOZZ

IF (PHI .GT. 0.D0) THEN
    TMO = -PI * ZRFZZ**2 * PHI / QVAP
ENDIF

IF (TMO .NE. 0.D0) THEN
    G = ZMOZZ / (2.D0 * TMO)
    IF (ABS(G) .LT. 30.D0) THEN
        TMOZZ = TMO * (1.D0 - DEXP(G))
    ELSE
        TMOZZ = TMO
    ENDIF
ELSE
    TMOZZ = 0.D0
ENDIF

RETURN
END
SPREAD - Fire Spread Rate on Horizontal Fuel Slab

Description

This routine calculates the spread rate of a fire on a horizontal fuel slab, ignited at the center of its top surface. The fire grows slowly until the entire surface (including the sides) is burning. The fire radius grows until it reaches a maximum such that the resulting area is the area of the top plus sides of the slab. This equivalent maximum radius, \( R_m \), is of course larger than the radius corresponding to the top surface. The spread rate until \( R = 0.95R_m \) is given by an expression which yields approximately exponential growth (as observed). Beyond that point, the spread rate is taken to slow down, as shown under the section "Calculations" below.

Output

\[ \dot{R} \]

Spread rate of a fire on a horizontal fuel slab. [m/sec]
**Input**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Spread rate parameter (Input Data)</td>
<td>[m/sec]</td>
</tr>
<tr>
<td>T_f</td>
<td>Flame temperature (Input Data)</td>
<td>[K]</td>
</tr>
<tr>
<td>R_m</td>
<td>Maximum burning radius of the object (Input Data)</td>
<td>[m]</td>
</tr>
<tr>
<td>R</td>
<td>Current radius of the fire on the object (Calculated Value, see Burning Object section)</td>
<td>[m]</td>
</tr>
<tr>
<td>φ</td>
<td>Flux incident on the surface of the object (Calculated Value, see Burning Object section)</td>
<td>[W/m^2]</td>
</tr>
<tr>
<td>σ</td>
<td>Stefan - Boltzmann constant (Physical Constant)</td>
<td>5.67 x 10^-8 W/m^2-K^-</td>
</tr>
</tbody>
</table>

**Calculations**

\[ C = \frac{\phi}{\sigma T_f^4} \]

Convenient non-dimensional grouping of terms.
\[
\begin{align*}
\dot{R} &= \begin{cases} 
AC(1+\frac{C}{2}+\frac{C^2}{3}), & R \leq 0.95R_m \\
(R_m-R)/10, & R > 0.95R_m
\end{cases} \\
\text{Rate of change of fire radius.}
\end{align*}
\]

References


Subroutine Variables

- \( \text{TRFZZ} = \dot{R} \)
- \( A = A \)
- \( T = T_f \)
- \( ZRFZM = R_m \)
- \( ZRFZZ = R \)
- \( \text{PHI} = \phi \)
- \( \text{SIGMA} = \sigma \)
Computer Subroutine

SUBROUTINE SPREAD (A,T,ZRFZM,PHI,ZRFZZ,TRFZZ)
C ************************************************************
C
C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C SUBROUTINE TO CALCULATE THE SPREAD RATE OF THE FIRE ON AN
C OBJECT.
C
C INPUT PARAMETERS:
C A -- FIRE SPREAD PARAMETER
C T -- FLAME TEMPERATURE
C ZRFZM -- MAXIMUM BURNING RADIUS OF THE OBJECT
C
C INPUT VARIABLES:
C PHI -- FLUX INCIDENT ON THE SURFACE OF THE OBJECT
C ZRFZZ -- RADIUS OF THE FIRE ON THE OBJECT
C
C OUTPUT VARIABLE:
C TRFZZ -- SPREAD RATE OF THE FIRE ON THE OBJECT
C
C PARAMETER (SIGMA = 5.67D-8)
C
C ZRFZZA = ZRFZZ
C
C C = PHI / (SIGMA * T**4)
IF (ZRFZZ .LE. 0.95D0*ZRFZM) THEN
   TRFZZ = A * C * (1.D0 + C/2.D0 + C*C/3.D0)
ELSE
   TRFZZ = (ZRFZM - ZRFZZ) / 10.D0
ENDIF
C
RETURN
END
Description

This algorithm calculates the time dependent temperature profile inside a slab. A slab of thickness, \( \theta \), is exposed to radiative and convective heat fluxes on its front and back surfaces. The temperature profile through the slab is calculated numerically by cutting the slab into pieces (parallel to its front surface), and solving the one-dimensional heat diffusion equation by finite differences (see for example Holman, *Heat Transfer*, pp. 72-98).

To calculate the slab temperature profile, the slab thermal properties (conductivity, diffusivity, specific heat, and density) and its thickness must be known. It is also necessary to know the convective and radiative fluxes to which the slab is exposed. These may be calculated elsewhere in the user's program or appropriate routines may be inserted directly into this subroutine. Of course, the user will have to make sure the necessary input data is available to the routine when needed. This routine may be used to calculate temperature profiles in walls, ceilings, or floors with the appropriately specified boundary conditions.

This algorithm requires that the present layer height be specified. This is usually available from most fire models. The absorption coefficient of the hot layer must also be specified or calculated in some way. Various methods for calculating this value may be found in the Hot Layer section of this catalog. The user must specify the time step to be used in the calculation as
well as the maximum number of layers into which the slab may be divided. The method outlined below will automatically calculate the number of layers required for stable calculations. If this exceeds the maximum allowable, the maximum number of layers will be used. The Stefan-Boltzmann constant must be specified for use in the radiation calculations.

Finally, the slab temperature profile at the end of the previous time step must be known. Initially, the entire slab is assumed to be at ambient temperature. After a calculation is completed, the new temperature profile must be stored and later returned as input for use in the calculation at the next time step.

This routine assumes that the interior part of the slab radiates to an environment at some temperature, $T_D$, while the exterior part of the slab radiates to an environment at ambient temperature, $T_a$.

**Output**

$T_i^{\text{new}}; i = 1,2,\ldots,N$ Slab temperature profile. [K]

**Input**

$q_{LWD}$ Convective heat flux from layer to interior side of slab (Calculated Value, see Convective Heat Transfer section). [W/m$^2$]
\( \dot{q}_{LWR} \) Radiative heat flux from layer to interior side of slab (Calculated Value, see Radiation Heat Transfer section). [W/m\(^2\)]

\( \dot{q}_{PWR} \) Radiative heat flux from plume(s) to interior side of slab (Calculated Value, see Radiation Heat Transfer section). [W/m\(^2\)]

\( \dot{q}_{AWD} \) Convective heat flux from layer to exterior side of slab (Calculated Value, see Convective Heat Transfer section). [W/m\(^2\)]

\( \dot{q}_{AWR} \) Radiative heat flux from layer to exterior side of slab (Calculated Value, see Radiation Heat Transfer section). [W/m\(^2\)]

\( \dot{q}_{PR} \) Radiative heat flux from plume(s) to exterior side of slab (Calculated Value, see Radiative Heat Transfer section). [W/m\(^2\)]

\( \Delta t \) Size of current time step (calculated within routine). [sec]

\( T_a \) Ambient temperature of air. [K]

\( T_D \) Temperature of lower layer. [K]
\( \theta \)  
Slab thickness (Input Data). [m]

\( k \)  
Slab thermal conductivity (Input Data). [W/m-K]

\( \alpha \)  
Slab thermal diffusivity (Input Data). [m^2/sec]

or \( C_p \)  
Slab specific heat (Input Data). [J/kg-k]

and \( \rho \)  
Slab material density (Input Data). [kg/m^3]

\( \kappa \)  
Infra-red absorptivity of the hot layer in the room (Calculated Value, see ABSRB routines in Hot Layer section). [m^-1]

\( \sigma \)  
Stefan-Boltzmann constant (Physical Constant). \([5.67 \times 10^{-8} \ W/m^2-K^4]\)

\( N_{\text{max}} \)  
Maximum allowable number of layers into which slab may be divided (Input Data).

\( h_L \)  
Smoke layer height (Calculated Value, see Hot Layer section). [m]

\( T_{01}^d; \ i = 1,2,\ldots,N \)  
Temperature profile of slab at start of time step
Calculations

\[ \alpha = \frac{k}{(\rho C_p)} \]

Calculate thermal diffusivity, if necessary.

\[ \delta x_i = \sqrt{2\alpha \Delta t} \]

Smallest permissible time space increment (calculated for the largest time increment to be used).

\[ N = 1 + \left[ \frac{\theta}{\delta x_i} \right] \]

N is the number of points where the temperature is calculated. \( i = 1 \) on inside surface, \( i = N \) on outside surface. (take integer part only of term in brackets)

\[ \delta x = \begin{cases} \frac{\theta}{(N-1)}, & 1 < N \leq N_{\text{max}} \\ \frac{\theta}{(N_{\text{max}}-1)}, & N > N_{\text{max}} \\ \theta, & N = 1 \end{cases} \]

Space increment actually used.

\[ a = \frac{2\alpha}{(\delta x)^2} \]

Computation parameter.

\[ b = \frac{\delta x}{k} \]

Computation parameter.
The calculation of the temperature distribution at time $t + \Delta t$ given the distribution at time $t$:

$$q_1'' = q_{LWD}'' + q_{LWR}'' + q_{PWR}''$$  \hspace{1cm} \text{Heat flux to side 1 (inside).}

$$q_N'' = q_{AWD}'' + q_{AWR}'' + q_{PR}''$$  \hspace{1cm} \text{Heat flux to side N (outside).}

$$\phi_1 = q_1'' - \sigma T_1^2 + e^{-\kappa h_0}T_N''$$  \hspace{1cm} \text{Net flux to inside of wall after re-radiation.}

$$\phi_N = q_N'' + \sigma T_a^2 - \sigma T_N^2$$  \hspace{1cm} \text{Net flux to outside of slab.}

$$T_1(t+\Delta t) = T_1(t) (1-a\Delta t) + a\Delta t (T_2(t)+b\phi_1)$$  \hspace{1cm} \text{Inside surface temperature calculation.}

$$T_i(t+\Delta t) = T_i(t) (1-a\Delta t) + \frac{\Delta t}{2} [T_{i-1}(t)+T_{i+1}(t)]$$  \hspace{1cm} \text{Interior node temperature calculation.}  

(i = 2, 3, ..., N-1)

$$T_N(t+\Delta t) = T_N(t) (1-a\Delta t) + a\Delta t (T_{N-1}(t)-b\phi_N)$$  \hspace{1cm} \text{Outside surface temperature calculation.}
References


Subroutine Variables

\[
\begin{align*}
ZKW & = T_{new}^i; \ i = 1,2, \ldots, N \\
FQLWD(1) & = q_{LWD} \\
FQLWR(1) & = q_{LWR} \\
FQPWR(1) & = q_{PWR} \\
FQLWD(2) & = q_{AWD} \\
FQLWR(2) & = q_{AWR} \\
FQPWR(2) & = q_{PR} \\
DT & = \Delta t \\
ZKAZZ & = T_a \\
ZKDZZ & = T_D \\
ZNWZZ & = \theta \\
ZJWZZ & = k \\
ZGWZZ & = \alpha \\
ZCWZZ & = C_p
\end{align*}
\]
VMWZZ = ρ
ZULZZ = κ
SIGMA = σ
MXLYRS = N_{max}
ZHLZZ = h_L
ZKWO = T^{old}_i; i = 1, 2, ..., N
SUBROUTINE TMPW01 (ZNWZZ,ZJWZZ,ZGWZZ,ZCWZZ,VMWZZ,ZKAZZ, & ZKDZZ,ZKWO,ZHLZZ,MXLYRS,FQLWD,FQLWR,FQPWR,DT,ZKW)
C ************************************************************
C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C SUBROUTINE TO CALCULATE THE TEMPERATURE PROFILE WITHIN A SLAB
C USING A DISCRETE GRID. THE SLAB IS HEATED OR COOLED ON EACH
C SIDE BY CONVECTION AND RADIATION AND THE HEAT DIFFUSES
C THROUGH IT BY CONDUCTION.
C
C INPUT PARAMETERS:
C ZNWZZ -- SLAB THICKNESS
C ZJWZZ -- SLAB THERMAL CONDUCTIVITY
C ZGWZZ -- SLAB THERMAL DIFFUSIVITY
C ZCWZZ -- SLAB MATERIAL SPECIFIC HEAT
C VMWZZ -- SLAB MATERIAL DENSITY
C ZKAZZ -- AMBIENT AIR TEMPERATURE (EXPOSING EXTERIOR
C SIDE OF SLAB)
C
C INPUT VARIABLES:
C ZKDZZ -- LOWER LAYER TEMPERATURE (EXPOSING INTERIOR
C SIDE OF SLAB)
C ZKWO -- PREVIOUS TIME STEP SLAB TEMPERATURE PROFILE
C ZHLZZ -- SMOKE LAYER HEIGHT
C MXLYRS -- MAXIMUM NUMBER OF LAYERS INTO WHICH THE SLAB
C MAY BE DIVIDED
C FQLWD(1) -- CONVECTIVE HEAT FLUX FROM LAYER TO
C INTERIOR SIDE OF SLAB
C FQLWR(1) -- RADIATIVE HEAT FLUX FROM LAYER TO INTERIOR
C SIDE OF SLAB
C FQPWR(1) -- RADIATIVE HEAT FLUX FROM PLUME(S) TO
C INTERIOR SIDE OF SLAB
C FQLWD(2) -- CONVECTIVE HEAT FLUX FROM LAYER TO EXTERIOR
C SIDE OF SLAB
C FQLWR(2) -- RADIATIVE HEAT FLUX FROM LAYER TO EXTERIOR
C SIDE OF SLAB
C FQPWR(2) -- RADIATIVE HEAT FLUX FROM PLUME(S) TO
C EXTERIOR SIDE OF SLAB
C DT -- SIZE OF TIME STEP
C
C OUTPUT VARIABLE:
C ZKW -- TEMPERATURE PROFILE WITHIN SLAB AT NEW TIME
C
C PARAMETER (SIGMA = 5.67D-8)
C
C INITIAL CALCULATIONS
C IF (ZGWZZ .LE. 0.0) ZGWZZ = ZJWZZ / (VMWZZ * ZCWZZ)
DXM = DSQRT (2.DO * ZGWZZ * DT)
M = IFIX( ZNWZZ / DXM ) + 1
N = MIN0 (M, MXLYRS)
IF (N .LE. 1) N = 2
DX = ZNWZZ / (FLOAT( N - 1 ))
AW = 2.DO * ZGWZZ / (DX * DX)
BW = DX / ZJWZZ

C WALL TEMPERATURE CALCULATIONS
C
TEMP = 1.DO - AW * DT
NM1 = N - 1

C CALCULATE INTERIOR NODE TEMPERATURES
DO 10 I = 2, NM1
   ZKW(I) = ZKW0(I) * TEMP + AW * (DT / 2.DO) * (ZKW0(I-1)
      & + ZKW0(I+1))
10 CONTINUE

C CALCULATE SLAB HEAT FLUXES
   FQWA = FQLWD(1) + FQLWR(1) + FQPWR(1)
   FQW1 = FQWA - SIGMA * (ZKW0(1)**4 - DEXP (-ZHLZZ * ZKDZZ**4)
      & ZULZZ)
   FQWB = FQLWD(2) + FQLWR(2) + FQPWR(2)
   FQW2 = FQWB + SIGMA * (ZKAZZ**4 - ZKW0(N)**4)

C CALCULATE INTERIOR NODE TEMPERATURE
   ZKW(1) = ZKW0(1) * TEMP + AW * DT * (ZKW0(2) + BW * FQW1)
C CALCULATE EXTERIOR NODE TEMPERATURE
   ZKW(N) = ZKW0(N) * TEMP + AW * DT * (ZKW0(N-1) + BW * FQW2)
C
RETURN
END
ABS RB2 - Infra-red Absorptivity of the Hot Layer

Description

This routine calculates the infra-red absorptivity of the hot layer. In this routine, the absorption coefficient is assumed to be gray and due mostly to the smoke concentration in the layer. Therefore, it is modeled as being a constant multiple, 265, of the concentration (by mass) of smoke (particulates, mainly C, and condensed hydrocarbons) in the hot layer in a room. The proportionality constant used in the equation below was obtained by comparing the infra-red absorptivity as measured in the July 6, 1977 full-scale fire test (channel 126), with the smoke concentration calculated in a standard run of NBS/Harvard 5.

Output

\[ \kappa \]

Infra-red absorptivity of the hot layer. [m⁻¹]

Input

\[ Y_s \]

Mass concentration of smoke in the hot layer (Calculated Value, see Hot Layer section). [gms of smoke/gms of hot layer gas]
Calculation

\[ \kappa = 265 \times Y_s \]

References


Subroutine Variables

\[ \text{ZYKZZ} = \kappa \]
\[ \text{ZYLSZ} = Y_s \]
SUBROUTINE ABSRB2 (ZYLSZ, ZULZZ)
C**************************************************************
C
C IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
C THIS SUBROUTINE CALCULATES THE INFRA-RED ABSORPTIVITY OF THE
C HOT LAYER. WE ASSUME THE ABSORPTION COEFFICIENT IS IN FACT
C AND DUE MOSTLY TO THE SMOKE CONCENTRATION IN THE LAYER. THE
C PROPORTIONALITY CONSTANT USED IN THE EQUATION BELOW WAS
C OBTAINED BY COMPARING THE I.R. ABSORPTIVITY AS MEASURED IN
C THE JULY 6, 1977 FULL-SCALE FIRE TEST (SEE CHANNEL 126), WITH
C SMOKE CONCENTRATION CALCULATION CALCULATED BY LAYR03 IN A
C STANDARD RUN OF HARVARD 5.0.
C
C INPUT VARIABLES:
C ZYLSZ -- MASS CONCENTRATION OF SMOKE IN THE HOT LAYER
C
C OUTPUT VARIABLE:
C ZULZZ -- INFRA-RED ABSORPTIVITY OF THE HOT LAYER
C
C ZULZZ = 265.0 * ZYLSZ
C
C RETURN
C END
APPENDIX D.

References


The Establishment of a Catalog of Compartment Fire Model Algorithms and Associated Computer Subroutines

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The Compartment Fire Model Research group of the Center for Fire Research, National Bureau of Standards, has been charged with the development of a "benchmark" compartment fire model. As part of this activity, a catalog of available fire model algorithms is being compiled. This paper presents a proposal for the organization, format, and use of the catalog. Appendix A of this report is a copy of the proposed introductory text for the catalog. Appendix B presents the Table of Contents for the first edition of the catalog, and Appendix C contains several examples of catalog algorithm write-ups. Finally, Appendix D lists the references used in Appendix A.

algorithms; building fires; cataloging; combustion physics; compartment fires; computer programs; fire chemistry; fire models; mathematical models; zone models

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